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Report No. CG-D-08-92

**Development of a Model to Predict  
Chemical Permeation of the  
U.S. Coast Guard  
Chemical Response Suit**

R. Goydan and J.R. Powell

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15 Acorn Park  
Cambridge, MA 02140-2390



FINAL REPORT  
OCTOBER 1991

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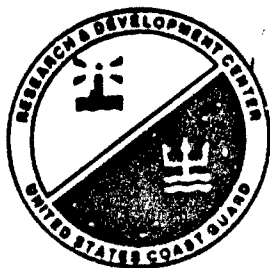
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# Technical Report Documentation Page

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| 16. Abstract<br><br><p>A predictive model was developed and computerized to enable Coast Guard field personnel to determine with 95% certainty whether totally encapsulated suits would be adequate barriers to untested chemicals. The model was based on permeation test results at 25 degrees centigrade of 163 chemicals against Challenge 5100 and 125 chemicals against Challenge 5200 fluoropolymer suit materials. Additional tests contained in the data base included tests at other temperatures and 36 mixtures.</p> <p>The model enables prediction as to whether permeation will be detected within three hours at 25 degrees centigrade, based on structure and size of the chemical of interest. Mixtures were found to exhibit no synergistic effects, i.e., each component behaves as it would alone (permeates or does not permeate). Compounds that tend to permeate have six carbons or less, carbon-carbon multiple bonds, halogen atoms, and are small non-polar organic compounds or small non-acidic, non-ionic inorganic compounds.</p> |                                                             |                                                                                                                                                                   |           |
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# METRIC CONVERSION FACTORS

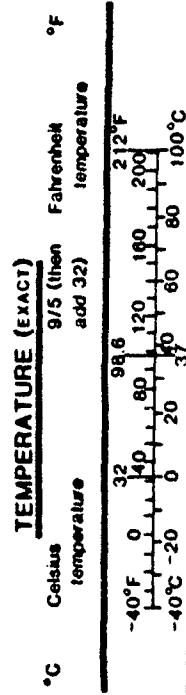
## Approximate Conversions to Metric Measures

| Symbol                     | When You Know          | Multiply By                | To Find             | Symbol          |
|----------------------------|------------------------|----------------------------|---------------------|-----------------|
| <b>LENGTH</b>              |                        |                            |                     |                 |
| in                         | inches                 | 2.5                        | centimeters         | cm              |
| ft                         | feet                   | 30                         | centimeters         | cm              |
| yd                         | yards                  | 0.9                        | meters              | m               |
| mi                         | miles                  | 1.6                        | kilometers          | km              |
| <b>AREA</b>                |                        |                            |                     |                 |
| in <sup>2</sup>            | square inches          | 6.5                        | square centimeters  | cm <sup>2</sup> |
| ft <sup>2</sup>            | square feet            | 0.09                       | square meters       | m <sup>2</sup>  |
| yd <sup>2</sup>            | square yards           | 0.8                        | square meters       | m <sup>2</sup>  |
| mi <sup>2</sup>            | square miles           | 2.6                        | square kilometers   | km <sup>2</sup> |
|                            | acres                  | 0.4                        | hectares            | ha              |
| <b>MASS (WEIGHT)</b>       |                        |                            |                     |                 |
| oz                         | ounces                 | 28                         | grams               | g               |
| lb                         | pounds                 | 0.45                       | kilograms           | kg              |
|                            | short tons (2000 lb)   | 0.9                        | tonnes              | t               |
| <b>VOLUME</b>              |                        |                            |                     |                 |
| tsp                        | teaspoons              | 5                          | milliliters         | ml              |
| tbsp                       | tablespoons            | 15                         | milliliters         | ml              |
| fl oz                      | fluid ounces           | 30                         | milliliters         | ml              |
| c                          | cups                   | 0.24                       | liters              | l               |
| pt                         | pints                  | 0.47                       | liters              | l               |
| qt                         | quarts                 | 0.95                       | liters              | l               |
| gal                        | gallons                | 3.8                        | liters              | l               |
| ft <sup>3</sup>            | cubic feet             | 0.03                       | cubic meters        | m <sup>3</sup>  |
| yd <sup>3</sup>            | cubic yards            | 0.76                       | cubic meters        | m <sup>3</sup>  |
| <b>TEMPERATURE (EXACT)</b> |                        |                            |                     |                 |
| °F                         | Fahrenheit temperature | 5/9 (after subtracting 32) | Celsius temperature | °C              |

\*1 in = 2.54 (exactly) For other exact conversions and more detailed tables, see NBS Misc. Publ. 286, Units of Weights and Measures. Price \$2.25. SD Catalog No. C13 10 286

## Approximate Conversions from Metric Measures

| Symbol                     | When You Know                     | Multiply By       | To Find                | Symbol          |
|----------------------------|-----------------------------------|-------------------|------------------------|-----------------|
| <b>LENGTH</b>              |                                   |                   |                        |                 |
| mm                         | millimeters                       | 0.04              | inches                 | in              |
| cm                         | centimeters                       | 0.4               | inches                 | in              |
| m                          | meters                            | 3.3               | feet                   | ft              |
| m                          | meters                            | 1.1               | yards                  | yd              |
| km                         | kilometers                        | 0.6               | miles                  | mi              |
| <b>AREA</b>                |                                   |                   |                        |                 |
| cm <sup>2</sup>            | square centimeters                | 0.16              | square inches          | in <sup>2</sup> |
| m <sup>2</sup>             | square meters                     | 1.2               | square yards           | yd <sup>2</sup> |
| km <sup>2</sup>            | square kilometers                 | 0.4               | square miles           | mi <sup>2</sup> |
| ha                         | hectares (10,000 m <sup>2</sup> ) | 2.5               | acres                  |                 |
| <b>MASS (WEIGHT)</b>       |                                   |                   |                        |                 |
| g                          | grams                             | 0.035             | ounces                 | oz              |
| kg                         | kilograms                         | 2.2               | pounds                 | lb              |
| t                          | tonnes (1000 kg)                  | 1.1               | short tons             |                 |
| <b>VOLUME</b>              |                                   |                   |                        |                 |
| ml                         | milliliters                       | 0.03              | fluid ounces           | fl oz           |
| l                          | liters                            | 0.125             | cups                   | c               |
| l                          | liters                            | 2.1               | pints                  | pt              |
| l                          | liters                            | 1.06              | quarts                 | qt              |
| l                          | liters                            | 0.26              | gallons                | gal             |
| m <sup>3</sup>             | cubic meters                      | 35                | cubic feet             | ft <sup>3</sup> |
| m <sup>3</sup>             | cubic meters                      | 1.3               | cubic yards            | yd <sup>3</sup> |
| <b>TEMPERATURE (EXACT)</b> |                                   |                   |                        |                 |
| °C                         | Celsius temperature               | 9/5 (then add 32) | Fahrenheit temperature | °F              |



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## SECTION 1

### EXECUTIVE SUMMARY

#### 1.1 INTRODUCTION

Emergency spill response personnel wear protective clothing to minimize exposures to potentially hazardous chemicals. Consequently, the materials used to construct the clothing must provide superior chemical resistance, preferably to the broad range of chemicals that are used in commerce. One high performance encapsulating suit is the U.S. Coast Guard's Chemical Response Suit (CRS) in which the principal material of construction is a fabric with fluoropolymer films on its surfaces (Challenge® 5100 and Challenge® 5200, Chemical Fabrics Corporation). Permeation testing has demonstrated that these fabrics provide good resistance to a wide range of chemicals, however, some chemicals do permeate the fabrics. Since there is virtually an unlimited number of chemicals and chemical mixtures and because testing of all such potential challenges is impractical, there was the desire to develop a predictive model to provide reasonable estimates of the permeation resistance. The development of such a model could lead to targeted decisions as to which chemicals and mixtures should be tested, better clothing selection decisions, and improved worker safety.

#### 1.2 PERMEATION DATA BASE

The results of over 300 tests were provided by the Coast Guard on the permeation of a broad range of pure chemicals and chemical mixtures through Challenge 5100 and 5200. Although the Challenge materials contain different substrates (aramid vs. glass fiber), the outer, fluoropolymer film layers appear to be the same total thickness, approximately 0.008 cm, as measured by cross-section.

The permeation tests had been performed in accordance with ASTM Method F739-85. Early tests were continued until steady-state permeation rates were achieved, however, the majority of the tests was terminated at 3 hours. The 3-hour limit was specified because it is the maximum duration for Coast Guard CRS use. Breakthrough times and permeation rates as a function of time were measured. However, permeation versus time curves or raw data were not made available to us for all material/chemical combinations tested. In general, the method detection sensitivity was less than  $0.05 \mu\text{g}/\text{cm}^2\text{-min}$  but did vary for each chemical and sometimes varied in subsequent tests with the same chemical. The lack of a constant detection sensitivity and single test duration made it difficult to develop a model to quantitatively predict the permeation behavior, particularly regarding breakthrough times. Definition of a standard breakthrough detection sensitivity for permeation testing is now under consideration by the ASTM and, if adopted, would facilitate the comparison of permeation test results.

At 25°C, permeation test results were reported for 163 chemicals for Challenge 5100 and 125 chemicals for Challenge 5200. Permeation test results were also reported for a small number of tests at 30°, 35°, and 40°C. The Coast Guard data set also included results for

permeation tests conducted with 29 chemical mixtures, however, only breakthrough times were measured. To further expand the mixture permeation data base, supplementary mixture tests were conducted by Arthur D. Little. Permeation tests were conducted for five, two-component and two, three-component mixtures. In these tests, the permeation rate of each mixture component was measured as a function of time.

### 1.3 PURE CHEMICAL PERMEATION

For Challenge 5100, permeation was detected within 3 hours for 20 of the 163 chemicals. For Challenge 5200, permeation was detected for 47 of the 128 chemicals. In general, permeation results for chemicals tested against both materials were similar although Challenge 5100 may provide a slightly better barrier. Thus, in our analysis and model development efforts, we treated the materials as equivalent and combined the data sets. Permeation rate versus time curves were available to us for most of the tests in which permeation was detected. We first analyzed the curves to assess the permeation mechanism.

#### 1.3.1 Permeation Mechanism

The permeation-time curves were analyzed to determine whether the permeation was controlled by a solution-diffusion process or was occurring by some other mechanism. Mathematical relationships based on Fick's law were used to calculate values for the solubility (S) and the diffusion coefficient (D) from the permeation-time data. For the 35 cases studied, an excellent fit to the permeation data was possible using Fick's law with a constant D. For these chemicals, the D values ranged from  $10^{-10}$  to  $10^{-9}$  cm<sup>2</sup>/s and the S values generally ranged from 0.0001 to 1.0 g/cm<sup>3</sup>. On this basis, we concluded that the permeation process was occurring by a solution-diffusion mechanism. The small set of permeation curves for analysis, and the lack of well-developed methods for predicting D and S for chemicals in fluoropolymers at present, limited the development of a quantitative model for predicting permeation behavior. Consequently, our focus was to develop an empirical model to predict the permeation behavior. We also analyzed the permeation-time curves for the chemicals tested at multiple temperatures to investigate the effect of temperature. The data set, however, was inconsistent and no quantitative conclusions could be reached regarding the effect of elevated temperature on the permeation resistance.

#### 1.3.2 Predictive Model

Using the full permeation database measured at 25°C, we developed an empirical model to predict permeation of Challenge 5100 or Challenge 5200 within 3 hours at 25°C at a representative detection sensitivity of 0.05 µg/cm<sup>2</sup>-min. We explored correlations with the chemical's structure, size, and shape. We found that the simplest and most accurate model was one based on chemical structure that addresses both molecular size and electronic structure. In general, chemicals with 6 or greater non-hydrogen atoms do not permeate the Challenge materials. Compounds of small size and with the following structure types tend to permeate:

- carbon-carbon multiple bonds (non-aromatic),
- halogen atoms (F and Cl),
- small non-acidic, non-ionic inorganic compounds, or
- small non-polar organics.

Thus, a set of rules was developed, in the form of questions with yes or no answers regarding chemical structure that leads to a Yes/No prediction of permeation. The set of rules was applied to the present data base and was found to accurately predict the behavior for 88% to 93% of the chemicals tested. The rules were organized into a decision tree and programmed for use on a personal computer.

#### 1.4 CHEMICAL MIXTURE PERMEATION

The permeation data for 29 chemical mixtures provided by the Coast Guard included both two- and three-component mixtures. The behavior can be summarized as follows. If a mixture component was found to permeate when tested as a pure chemical, it was found to permeate from the mixture and at approximately the same or slightly longer breakthrough time. If the mixture component did not permeate when tested as a pure chemical, it also was not found to permeate from a mixture. No synergistic effects were observed.

To better understand mixture permeation, we conducted supplementary tests that involved two- and three-component mixtures of three chemicals to explore the effect of concentration on the mixture permeation behavior. The permeation rates as a function of time of the mixture components were generally proportional to their concentration in the mixture (i.e., as the concentration was decreased, the breakthrough time increased and the steady-state permeation rate decreased).

##### 1.4.1 Predictive Model

Although based on a limited data set, a general rule was developed to predict chemical mixture permeation through the Challenge materials, again at 25°C and within 3 hours, as follows. If the chemical permeates in pure form, it will permeate from a mixture at a permeation rate proportional to its concentration in the mixture. If the chemical does not permeate in pure form, it will not permeate from a mixture.

#### 1.5 COMPUTERIZED PREDICTION MODEL AND DATABASE

A computerized version of the permeation data set and prediction model was developed using SuperCard 1.5 (Silicon Beach Software) to run on Macintosh computers. For every chemical entered into the database, there is one card that stores information on the chemical identity, permeation data (if available), and permeation model prediction (if generated.) System operational features include capabilities to search the database, run the permeation prediction model, enter data or model predictions into the database (access to this feature is restricted), and print entries from the database. A user manual was also developed.

## 1.6 CONCLUSIONS AND RECOMMENDATIONS

The permeation resistance of Challenge 5100 and Challenge 5200 has been widely tested and the results indicate that these materials are effective barriers to a broad range of chemicals and chemical mixtures. When permeation was detected, it was found to follow a simple Fickian diffusion mechanism with a constant diffusion coefficient. No quantitative predictive model based on the Fick's law approach was developed however. Also, no definitive conclusions could be reached regarding the effect of temperature on the permeation resistance of the Challenge materials based on the available data set.

An empirical model or rule system was developed that enables the prediction as to whether permeation will be detected within three hours at 25°C based on the structure and size of the chemical of interest. Based on a smaller set of data, the permeation of mixtures or the components thereof was found to behave similarly to the results for the chemicals tested individually. If a chemical permeates the Challenge material as a pure chemical then it will permeate from a mixture. Conversely, if a chemical does not permeate in pure form then it will not permeate from a mixture.

A computerized version of the permeation database and prediction model was developed for use by personnel with minimal permeation or chemistry training. The computer system should facilitate thorough and efficient reviews of existing data and assessments of probable permeation behavior by field (or other) users who must make clothing selection decisions. Although use of the model was targeted as an aid for making clothing selection decisions, it is also useful to focus decisions regarding priority chemicals and mixtures for future testing.

Further research should be undertaken to address some of the uncertainties in the data set, the predictive model described herein, and other approaches being evaluated to predict the permeation behavior. Specific recommendations include:

- A field evaluation of the computerized permeation database and predictive model should be undertaken to assess the product's usefulness and identify ways to optimize the product to better meet Coast Guard's needs.
- Future permeation tests, if performed, should be conducted so that chemical breakthrough is determined at a constant, normalized permeation detection rate, if feasible.
- Selected permeation tests at elevated temperatures should be repeated to confirm the results reported to date and to better understand the effect of temperature on the permeation resistance of the Challenge materials.
- Permeation tests with additional chemical mixtures should be undertaken to further validate the mixture permeation rule.

- The computerized permeation database should be updated as more data are generated and the predictive model should be continually tested as new data become available to expand and improve its accuracy.
- In the long term, similar computer databases and predictive models could be developed for other important components of the Coast Guard CRS (e.g., glove materials, face shield material) or alternative materials for the encapsulating suit fabric that may adopted at a later date. Development of such databases and models provide a better understanding of the barrier properties of critical materials and help to focus priorities for testing.

## SECTION 2

### INTRODUCTION

#### 2.0 BACKGROUND

Since 1978, the U.S. Coast Guard has been responsible for inspecting marine chemical-transporting vessels and responding to chemical spills into waters in the United States. At that time, a research and development project was initiated to develop chemical protective clothing and equipment for use during spill response activities. Because of the variety of chemicals that are handled in commerce, the Coast Guard required a protective clothing ensemble that was an effective barrier to a broad range of chemicals. For example, the Coast Guard's Chemical Hazard Response Information System (CHRIS) includes spill response information for over 1100 chemicals [1]. Early, commercially-available protective ensembles and materials that were evaluated included butyl rubber, Viton/chlorobutyl laminate, and chlorinated polyethylene [2,3]. In general, these materials were found to provide only fair resistance to the CHRIS chemicals.

In the mid-1980s, the Coast Guard renewed its search for improved protective materials and identified a proprietary fluoropolymer-film based composite fabric, Challenge 5100. To support the development of an ensemble using this material, an extensive testing program was undertaken to assess the fabric's performance as a primary suit material [4]. In addition to chemical resistance evaluations, the program involved evaluation of physical properties, critical suit seams, other suit components, etc., that will not be considered here.

To evaluate the chemical resistance of the Challenge 5100 material, a permeation test program was undertaken by the Coast Guard Research and Development Center beginning in 1985 and continuing through 1990 [5,6]. During that time, a second fabric, the Challenge 5200 material, was introduced and incorporated into the testing program. In general, good resistance to permeation was demonstrated in over 300 permeation tests with these fabrics for a wide range of chemicals. Since there is virtually an unlimited number of chemicals and chemical mixtures and because testing of all potential challenges is impractical, there was the desire to develop a predictive model to provide reasonable estimates of the permeation resistance.

#### 2.1 OBJECTIVE

The objective of this project was to develop a model to predict permeation of the Challenge materials based on the permeation data set available from the Coast Guard. At the minimum, the model was to predict whether measurable permeation will or will not occur after a specified duration. If sufficient data were available and the permeation process occurred by a solution-diffusion process, a further objective was to develop a model that accurately predicts permeation behavior as a function of time.

## 2.2 SCOPE AND APPROACH

The permeation model developed in this study is based on permeation data provided by the Coast Guard as well as a small set of chemical mixture permeation data generated in our laboratories. Our approach was to compile and analyze the permeation data set, assess the permeation mechanism, and then develop, test, and refine a predictive model. Much of our initial effort was directed toward compiling and analyzing the data set, which was reported in a series of reports and using a series of formats. Also, additional data were being reported to us throughout the model development program.

Both theoretical and empirical approaches to a predictive model were investigated. Initially the emphasis was on theoretical approaches based on Fick's laws of diffusion since, if successful, such models can be extrapolated with greater confidence to conditions other than those considered in the model development. In addition, we investigated empirical approaches including correlations with chemical structure, size, and shape. The ultimate goal was a generalized model that could be applied rapidly and reliably by field personnel who must make clothing selection decisions. In addition to developing a model to predict pure chemical permeation, we also analyzed two smaller data sets, one for mixtures and one for tests at elevated temperature, to investigate the effects of temperature and mixture composition on the permeation behavior.

The program began with a model development phase based on a review of the existing data set. At the conclusion of this phase, a prototype model was proposed and a series of chemical permeation tests were recommended to test the prototype model. The results of these tests were then used to refine the prototype model and establish the accuracy and limitations of the final model. At the conclusion of the effort, a computerized version of the data set and the predictive model were developed to facilitate its use in the field.

## SECTION 3

### PERMEATION DATA SET

#### 3.1 CRS MATERIALS TESTED

Since 1985, the Coast Guard has been evaluating the suitability of two proprietary fabrics to meet their requirements for a totally encapsulating suit material. The two materials are manufactured by the Chemical Fabrics Corporation (Merrimack, NH) and involve composite structures in which outer, fluoropolymer (Teflon®) films provide the chemical resistance. Challenge 5100, the first of these materials, is a composite structure of fluoropolymer films applied to both sides of a woven aramid reinforcing substrate. The second material, Challenge 5200, is a similar composite structure with the outer, fluoropolymer films applied to a glass fiber reinforcing substrate.

Preliminary evaluation of the Challenge 5100 material indicated very good resistance to chemical permeation and good physical properties relative to those of other materials that the Coast Guard had previously evaluated [4]. Consequently, the Challenge 5100 material was selected for an extensive testing program, one aspect of which was to evaluate the permeation resistance of the material to a large set of priority chemicals [5,6]. In the midst of this testing program the manufacturer introduced the Challenge 5200 material, as a next generation version of the Challenge 5100 material, and this new material was incorporated into the Coast Guard testing program [7].

Although requested, the manufacturer would not provide information regarding the fluoropolymer composition, barrier layer thicknesses, or whether differences exist between the fluoropolymer films of the fabrics. Rough measurements were made in our laboratory to compare the barrier layer thicknesses, however, no analyses were undertaken to compare the fluoropolymer layer compositions. Fluoropolymer layer thicknesses were estimated by examination of the materials' cross-section using a microscope:

- Challenge 5100
  - total composite thickness: 0.048 cm
  - outer fluoropolymer layer: 0.0045 cm
  - inner fluoropolymer layer: 0.0035 cm
  - total fluoropolymer thickness: 0.0080 cm
- Challenge 5200
  - total composite thickness: 0.026 cm
  - outer fluoropolymer layer: 0.0040 cm
  - inner fluoropolymer layer: 0.0040 cm
  - total fluoropolymer thickness: 0.0080 cm

The presence of fluoropolymer layers on both the inner and outer surfaces of the materials was confirmed by attenuated total reflectance (ATR) infrared analysis of the sample surfaces.

Based on these measurements, the two fabrics appear to contain the same total fluoropolymer film thickness even though Challenge 5200 is approximately one half the thickness of Challenge 5100. As discussed later, comparison of the permeation test results for the two materials appear to support this conclusion.

### 3.2 PERMEATION TEST METHOD AND DATA REPORTING FORMAT

The majority of the permeation test data analyzed in this effort was generated by Texas Research International (TRI) under contract to the Coast Guard [6,7]. Essentially all tests with pure chemicals, several tests at elevated temperatures and most of the chemical mixture tests were performed by TRI. Some early tests were conducted by the Coast Guard Research and Development Center. A small number of mixture permeation tests were performed by Arthur D. Little and are described in Section 3.2.2. In general, the permeation tests were conducted in accordance with ASTM F739-85 but with minor modifications in some cases.

#### 3.2.1 Tests Performed by Texas Research International

Most tests conducted by TRI were performed using an automated permeation test system in which three test replicates were performed simultaneously. The system uses an open-loop testing mode with photoionization detection. In general, the collection medium flow rate was set at 100 cc/min. In most tests, a 2.54 cm diameter test cell was used, however, in many of the early tests the ASTM F739 standard cell of 5.08 cm diameter was used. The small diameter cell has a 5.07 cm<sup>2</sup> exposed surface area whereas the 5.08 cm diameter cell has a 20.3 cm<sup>2</sup> area. Alternative detection methods were used for chemicals that could not be detected by photoionization.

After charging the challenge side of the permeation cell with the test chemical, the collection side of the test cell was monitored periodically. In early tests (i.e., most of the Challenge 5100 tests), the detector responses were monitored for 3 hours or until a steady-state permeation rate was achieved in tests in which permeation was detected within 3 hours. In later tests (i.e., most of the Challenge 5200 tests), the detector responses were monitored for 3 hours (although sometimes this was extended to 4 to 7 hours). For tests in which permeation was detected but steady-state was not reached within 3 hours, the maximum permeation rate measured during the test was reported. As discussed later, there were very few cases in which the permeation rate reached steady-state within 3 hours.

The results of the permeation tests were reported to us by the Coast Guard in various summary reports, summary tables, and individual data sheets with attached instrument response curves over the course of this program. A significant portion of our efforts involved compiling the reported results into a consistent format and analyzing the data set to understand the permeation behavior.

Breakthrough was determined to occur by TRI when the detector response exceeded a minimum detectable limit (MDL). The detector response was calibrated separately for each chemical using a syringe pump and single point calibration technique [8]. The detector

response (mV) was used to calculate the response factor (mV/ppm) and the MDL in concentration units of parts per million (ppm). The response factor, determined at a single low concentration, was assumed to be a linear response with a zero intercept and used as a constant to convert the detector responses measured in the permeation test to concentration values. The concentration values were converted to permeation rates using the collection medium flowrate and the clothing material surface area. In most cases, only the final permeation rate was reported in permeation rate units. The results as a function of time were reported in graphs showing detector response (mV) plotted versus time. From these curves, we converted the response data to permeation rates as a function of time for our analyses. Because response factors (mV/ppm) were not reported to us for all chemicals, we converted the instrument response graphs using the reported permeation rate value and the mV response reading at that time. Thus, there may be some uncertainty in our values as a function of time.

Several tests with chemical mixtures were also performed. These tests involved binary and ternary mixtures of liquid chemicals and were conducted using the automated system described above. In these tests, only breakthrough times were reported. In several tests, however, only a generic MDL and breakthrough time were reported without identifying which component had actually broken through. No permeation rate or instrument response data as a function of time were provided to us for these tests.

In summarizing the data set, it is important to note that an individual MDL value was determined for each chemical/test and used to judge whether permeation occurred. MDL values ranged from 0.001 ppm to 40 ppm depending upon the instrument sensitivity for the chemical of interest. In several cases in which tests were repeated for the same chemical (or performed with both Challenge 5100 and 5200), the reported MDLs for that chemical varied by several orders of magnitude. This range makes it difficult to compare the results of tests in which permeation was not detected. To better normalize the data set, we converted the MDL values from concentrations (ppm) to minimum detectable permeation rate (MDR) values in units of  $\mu\text{g}/\text{cm}^2\text{-min}$  using the reported flowrates and exposed surface areas. Use of MDRs eliminates some apparent discrepancies in the data set and allows for more direct comparison of the results [9]. In particular, this was important when comparing results in which permeation was or was not detected at apparently the same MDL but at different test conditions. As discussed later, this data set illustrates the difficulty in interpreting permeation test results when a constant detection limit (i.e., MDR) is not used and many tests are terminated before permeation is detected. Consequently, throughout this report, the data tables reporting breakthrough times and permeation rates, also report the detection limit for the chemical and the duration of the permeation test.

### 3.2.2 Tests Performed by Arthur D. Little

To further expand the chemical mixture database, supplementary permeation tests were conducted by Arthur D. Little under this contract. Permeation tests were conducted for seven different mixtures involving carbon disulfide, vinyl acetate, and ethanol. The standard ASTM F739 permeation test cell was used providing a clothing material surface area of  $20.3\text{ cm}^2$ . The tests were conducted in a closed-loop mode with air as the collection medium. The total

collection medium volume was 6 liters and was continuously recirculated at a rate of 10 liters/min for the test duration. A Miran 80A Infrared Spectrophotometer (Foxboro Company, Foxborough, MA) was employed to detect the concentration of the chemical in the collection medium. Calibration curves of concentration ( $\mu\text{g/L}$ ) versus absorbance were generated over the range of expected concentration values. Individual MDLs and MDRs were determined for the three test chemicals. The spectrophotometer was calibrated prior to testing each day that tests were conducted.

All tests were performed until either each component of the mixture being tested reached a steady-state permeation rate or eight hours had elapsed. Only ethanol failed to reach steady-state in this time period. In all cases, the permeation rates as a function of time were recorded so that the effect of mixture composition and concentration on the permeation behavior could be observed.

### 3.3 PURE CHEMICAL DATA SET

#### 3.3.1 Summary

The results of permeation tests conducted with over 300 chemical/material combinations were available for analysis in this study. As noted earlier, the results of the permeation tests were reported to us by the Coast Guard in various summary reports, summary tables, and individual data sheets during this program. Thus, the compilation and analysis of the test results continued throughout the model development effort.

Table 1 summarizes the permeation tests that were conducted at (or near) 25°C. In total, 163 chemicals were tested against Challenge 5100 while only 128 chemicals were tested against Challenge 5200. Of these, only 39 chemicals were tested against both materials. Complete tables of the permeation test results, as compiled by us, are provided in Appendix A with Table A-1 reporting the Challenge 5100 results and Table A-2 reporting the Challenge 5200 results. Table A-2 also includes results for 21 chemicals that were reported by the manufacturer, Chemical Fabrics Corporation [10]. Most of these chemicals were also tested by TRI. The source of the data is indicated in the Appendix A tables. Permeation tests were also conducted at elevated temperatures with Challenge 5200 as summarized in Table 2. These tests were conducted at 30°, 35°, and 40°C using chemicals that, in general, had also been tested at 25°C. Complete tables of the permeation test results, again as compiled by us, are provided in Appendix B.

The Appendix A and Appendix B tables report the chemical name, the MDL (ppm), the MDR ( $\mu\text{g}/\text{cm}^2\text{-min}$ ), and the permeation test results in terms of the average breakthrough time (min) average reported permeation rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ), an indicator as to whether the rate was at steady-state or at the test conclusion, and the breakthrough times and permeation rates reported for each of the three replicate tests, when applicable. In approximately 20% of the cases, permeation-time curves were not provided so we could not conclude whether permeation had reached steady-state. These cases are noted in the tables. In general, the permeation-time curves that were received showed instrument responses that increased smoothly from the baseline over time. Several curves, however, showed a lot of noise,

TABLE 1. SUMMARY OF PERMEATION TESTS AT 25°C

| Condition                                                                       | No. of chemicals |                |
|---------------------------------------------------------------------------------|------------------|----------------|
|                                                                                 | Challenge 5100   | Challenge 5200 |
| Total chemicals tested                                                          | 163              | 128            |
| - Chemicals tested multiple times                                               | 11               | 22             |
| Chemicals for which permeation was detected within 3 hours                      | 20               | 47             |
| - Chemicals for which curves for permeation as a function of time were provided | 18               | 37             |
| - Chemicals for which permeation rate reached steady-state                      | 10               | 6              |
| - Chemicals for which the test was terminated before steady-state*              | 8                | 31             |

\* Typically 3-hour test duration.

TABLE 2. SUMMARY OF PERMEATION TESTS FOR CHALLENGE 5200 AT ELEVATED TEMPERATURES

| Condition                                                                       | No. of chemicals |      |      |
|---------------------------------------------------------------------------------|------------------|------|------|
|                                                                                 | 30°C             | 35°C | 40°C |
| Total chemicals tested                                                          | 18               | 20   | 9    |
| - Chemicals tested multiple times                                               | 1                | 0    | 0    |
| Chemicals for which permeation was detected within 3 hours                      | 8                | 10   | 7    |
| - Chemicals for which curves for permeation as a function of time were provided | 0                | 9    | 7    |
| - Chemicals for which permeation rate reached steady-state                      | **               | 0    | 1    |
| - Chemicals for which the test was terminated before steady-state*              | **               | 9    | 6    |

\* Typically 3-hour test.

\*\* Unknown because permeation-time curves were not provided.

spikes, or drifting behavior and were considered unusable results. These tests were discussed with the Coast Guard and, in several cases, repeated.

The numbers of chemicals that were tested multiple times are noted in Tables 1 and 2. The results of these repeat tests are compared in Table 3 for Challenge 5100 and in Table 4 for Challenge 5200. In general, the reproducibility was only fair and was better for Challenge 5100. For the 11 chemicals tested multiple times with Challenge 5100, seven were either in good agreement or the lack of agreement could be related to differences in the detection limit (or possibly the test temperature, 25° vs. 27°C). For example, in the first test with acetone, no permeation was detected at 25°C within 210 minutes at an MDR of 0.047  $\mu\text{g}/\text{cm}^2\text{-min}$ . In the repeat test, permeation was detected at 27°C at an average of 71 minutes at an MDR of 0.00004  $\mu\text{g}/\text{cm}^2\text{-min}$ , an MDR that is three orders of magnitude lower. In other cases, discrepancies exist within replicates or reported permeation rates varied by several orders of magnitude. For the 22 chemicals tested multiple times against Challenge 5200, the results for about ten were in good agreement or their differences could be related to MDR differences. But, as Table 4 illustrates, there are also over ten cases in which either the repeat results do not agree regarding breakthrough time or the reported permeation rate values differ by over an order of magnitude. The testing laboratory suggests that the variations are due to differences in the lots of the Challenge materials tested.

This lack of reproducibility in some of the data set confounded our analyses and limited attempts to develop a model to predict quantitative breakthrough times or permeation rates. Thus, as detailed in Section 4, our model development efforts ultimately focussed on developing an empirical model that predicts whether permeation will be detected at a representative MDR within 3 hours at 25°C. Only a small effort was undertaken to predict the permeation behavior as a function of time for the chemicals found to permeate.

### 3.3.2 Chemicals for Which Permeation Was Detected at 25°C

For Challenge 5100, 20 chemicals were found to permeate within 3 hours, at their reported MDRs. The test results for these chemicals are summarized in Table 5. For ten of these chemicals, the permeation-time curves show that permeation had reached steady-state, often at much longer than 3 hours. In comparison, 47 of the 128 chemicals tested against Challenge 5200 were detected to permeate within 3 hours. The test results for these chemicals are reported in Table 6. For this fabric, only 6 tests were continued until steady-state. The remaining permeation tests were terminated at 3 hours (or longer in some cases.)

The larger percentage of chemicals that permeate Challenge 5200 material is not necessarily because Challenge 5200 is a less resistant barrier but could be because the chemicals tested against Challenge 5200 were more carefully selected, from a permeation standpoint, based on earlier Challenge 5100 test results. Most of the Challenge 5100 results had been obtained before the start of this program whereas the Challenge 5200 testing continued throughout the model development effort. Thus, as the Coast Guard began to understand better the permeation behavior of Challenge 5100, it began to specify testing with chemicals that had a higher probability of permeating Challenge 5200 [20]. In Tables 5 and 6, the chemicals tested after our preliminary model was developed are indicated with a (+).

TABLE 3. SUMMARY OF REPEAT PERMEATION TESTS WITH  
CHALLENGE 5100 AT 25°C

| Chemical name                           | Test # | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average<br>BT<br>(min) | Average<br>reported rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |       |
|-----------------------------------------|--------|---------------|--------------------------------------------------|------------------------|------------------------------------------------------------------------|-------|
| Acetone<br>(27°C)                       | 1      | 1.2           | 0.047                                            | >210                   | --                                                                     |       |
|                                         | 2      | 0.001         | 0.00004                                          | 71                     | 1.6                                                                    | (3hr) |
| Acetonitrile                            | 1      | nd            | nd                                               | >270                   | --                                                                     |       |
|                                         | 2      | 1.0           | 0.033                                            | >180                   | --                                                                     |       |
| Allyl Chloride                          | 1      | 0.16          | 0.0025                                           | 134                    | 0.011                                                                  | (ss)  |
|                                         | 2      | 0.060         | 0.0037                                           | 143                    | 0.013                                                                  | (6hr) |
| Ammonium Hydroxide                      | 1      | 2.0           | 0.057                                            | 30, >180†              | 26.7                                                                   | (3hr) |
|                                         | 2      | 7.2           | 0.020                                            | >180                   | --                                                                     |       |
| 1,2-Dichloroethylene                    | 1      | 0.010         | 0.0008                                           | 15                     | 1.1                                                                    | (ss)  |
|                                         | 2      | 0.010         | 0.0008                                           | 23                     | 0.13                                                                   | (ss)  |
| Dichloromethane<br>(USCG)               | 1      | 0.27          | 0.0042                                           | 51                     | 0.020                                                                  | (ss)  |
|                                         | -      | 0.030         | *                                                | 61                     | nd                                                                     |       |
| Ethyl Ether<br>(27°C)                   | 1      | 0.13          | 0.0078                                           | >180                   | --                                                                     |       |
|                                         | 2      | 0.010         | 0.0006                                           | 92                     | 0.005                                                                  | (3hr) |
|                                         | 3      | 0.006         | 0.0004                                           | 117                    | 1.07                                                                   | (3hr) |
| Sodium Hydroxide, 50%<br>(USCG)         | 1      | 0.50          | 0.016                                            | >180                   | --                                                                     |       |
|                                         | -      | nd            | nd                                               | >4260                  | --                                                                     |       |
| Tetrachloroethylene<br>(USCG)<br>(27°C) | 1      | 0.11          | 0.015                                            | >624                   | --                                                                     |       |
|                                         | -      | nd            | nd                                               | 108                    | nd                                                                     |       |
|                                         | 2      | 0.001         | 0.0001                                           | 26, >180†              | 18.0                                                                   | (3hr) |
| Trichloroethylene                       | 1      | 0.070         | 0.0017                                           | 148                    | 0.031                                                                  | (ss)  |
|                                         | 2      | 0.010         | 0.0011                                           | 138                    | 0.031                                                                  | (6hr) |
| Vinylidene Chloride                     | 1      | 0.49          | 0.038                                            | >180                   |                                                                        |       |
|                                         | 2      | 0.010         | 0.0008                                           | 51                     | 0.022                                                                  | (3hr) |

\* MDL = minimum detectable concentration determined by syringe pump calibration; MDR = minimum detectable permeation rate calculated from MDL, carrier gas flowrate, and material surface area. Values entered as (\*) could not be converted, (nd) indicates not determined.

\*\* Reported rate is the rate at the conclusion of the permeation test or the maximum reached during the test. Test durations are noted in parenthesis, (ss) indicates steady-state permeation value.

† Conflicting results were measured within the three replicates for this test.

TABLE 4. SUMMARY OF REPEAT PERMEATION TESTS WITH  
CHALLENGE 5200 AT 25°C

| Chemical name      | Test #      | MDL* (ppm) | MDR* ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average RT (min) | Average reported rate** ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |        |
|--------------------|-------------|------------|-----------------------------------------------|------------------|------------------------------------------------------------------|--------|
| Acetone            | 1           | 1.0        | 0.040                                         | >180             | --                                                               |        |
|                    | (27°C) 2    | 0.010      | 0.0004                                        | 116              | 0.0004                                                           | (3hr)  |
|                    | (27°C) 3    | 0.001      | 0.00004                                       | >180             | --                                                               |        |
|                    | (ChemFab) - | 0.10       | *                                             | >300             | --                                                               |        |
| Ammonia Gas        | 1           | 0.30       | 0.0041                                        | 31               | 0.11                                                             | (ss)   |
|                    | 2           | 0.070      | $\mu\text{L}$ 0.0010                          | 25               | 0.24                                                             | (3hr)  |
|                    | (27°C) 3    | 0.030      | $\mu\text{L}$ 0.0004                          | 32               | 0.15                                                             | (3hr)  |
|                    | (ChemFab) - | 0.10       | *                                             | >300             | --                                                               |        |
| Ammonium Hydroxide | 1           | 0.25       | 0.0071                                        | >180             | --                                                               |        |
|                    | (27°C) 2    | 7.2        | 0.20                                          | 120              | 0.34                                                             | (3hr)  |
| Benzonitrile       | 1           | 0.010      | 0.0008                                        | >180             | --                                                               |        |
|                    | 2           | 0.020      | 0.0017                                        | >180             | --                                                               |        |
| 1,3-Butadiene Gas  | 1           | 0.068      | 0.0030                                        | 5                | 0.039                                                            | (5hr)  |
|                    | 2           | 0.010      | $\mu\text{L}$ 0.00044                         | 24               | 0.080                                                            | (3hr)  |
| Chlorine Gas       | 1           | 1.0        | 0.057                                         | 70               | 0.020                                                            | (nc)   |
|                    | 2           | 38.0       | 2.2                                           | 60               | 170.3                                                            | (nc)   |
|                    | (ChemFab) - | 0.30       | *                                             | >300             | --                                                               |        |
| Cyclopropane Gas   | 1           | 0.020      | $\mu\text{L}$ 0.0007                          | 92               | 0.0008                                                           | (3hr)  |
|                    | (27°C) 2    | 0.002      | 0.0001                                        | 78               | 0.0008                                                           | (3hr)  |
| Dichloromethane    | 1           | 0.005      | 0.0003                                        | 64               | 0.26                                                             | (3hr)  |
|                    | (27°C) 2    | 0.007      | 0.0005                                        | 83               | 3.7                                                              | (3hr)  |
|                    | (ChemFab) - | 0.10       | *                                             | 64               | 0.12                                                             |        |
| Dimethyl Sulfide   | 1           | 0.010      | 0.0008                                        | 95               | 0.0005                                                           | (3hr)  |
|                    | 2           | 0.010      | 0.0008                                        | 48               | 0.0002                                                           | (3hr)  |
| Ethanethiol        | 1           | 0.020      | 0.0010                                        | 65               | 0.0028                                                           | (3hr)  |
|                    | (27°C) 2    | 0.003      | 0.0002                                        | 83               | 15.3                                                             | (3hr)  |
| Ethyl Ether        | (27°C) 1    | 0.010      | 0.0006                                        | 127              | 0.38                                                             | (20hr) |
|                    | (27°C) 2    | 0.010      | 0.0006                                        | 92               | 0.0080                                                           | (3hr)  |
|                    | (27°C) 3    | 0.003      | 0.0002                                        | 149              | 2.1                                                              | (3hr)  |
|                    | (27°C) 4    | 0.010      | 0.0006                                        | 40               | 173.3                                                            | (3hr)  |
| Ethylene Oxide Gas | 1           | 3.0        | 0.11                                          | 57               | 0.73                                                             | (3hr)  |
|                    | 2           | 0.65       | 0.023                                         | 25               | 0.14                                                             | (3hr)  |
|                    | (ChemFab) - | 0.34       | *                                             | 64               | 0.76                                                             |        |

TABLE 4. SUMMARY OF REPEAT PERMEATION TESTS WITH  
CHALLENGE 5200 AT 25°C

| Chemical name                  | Test # | MDL* (ppm) | MDR* (µg/cm <sup>2</sup> -min) | Average BT (min) | Average reported rate** (µg/cm <sup>2</sup> -min) |
|--------------------------------|--------|------------|--------------------------------|------------------|---------------------------------------------------|
| Hydrogen Sulfide Gas<br>(27°)  | 1      | 0.030      | 0.0008                         | 4                | 0.0028 (3hr)                                      |
|                                | 2      | 0.010      | 0.0003                         | 8                | 0.0070 (3hr)                                      |
|                                | 3      | 0.030      | 0.0008                         | 15               | 0.0078 (nc)                                       |
| Methyl Bromide Gas             | 1      | 0.40       | 0.031                          | 21               | 0.035 (3hr)                                       |
|                                | 2      | 0.020      | µL 0.0015                      | 20               | 0.0065 (3hr)                                      |
| Methyl Chloroformate<br>(27°C) | 1      | 0.050      | 0.0038                         | 81               | 0.012 (3hr)                                       |
|                                | 2      | 0.10       | 0.0076                         | 95               | 0.95 (3hr)                                        |
| Nitromethane                   | 1      | 0.73       | 0.036                          | 168              | 0.054 (nc)                                        |
|                                | 2      | 0.70       | 0.035                          | >180             | --                                                |
| Sulfur Dioxide Gas             | 1      | 47.0       | mL 0.020                       | 60               | 0.090 (3hr)                                       |
|                                | 2      | 1.0        | mL 0.052                       | 40               | 2.3 (3hr)                                         |
| Trichloroethylene<br>(27°C)    | 1      | 0.010      | 0.0011                         | 49               | 0.19 (3hr)                                        |
|                                | 2      | 0.010      | 0.0011                         | 72               | 0.0028 (3hr)                                      |
| Trimethylamine                 | 1      | 0.15       | 0.0072                         | 20               | nd (nc)                                           |
|                                | 2      | 0.014      | 0.0007                         | >180             | --                                                |
|                                | 3      | 0.15       | 0.0072                         | 25               | nd (nc)                                           |
| Vinyl Acetate                  | 1      | 0.020      | 0.0014                         | 69               | 0.25 (nc)                                         |
|                                | 2      | 0.004      | 0.0003                         | 73               | 38.0 (3hr)                                        |
|                                | 3      | 0.004      | 0.0003                         | 109              | 11.3 (3hr)                                        |
| Vinyl Chloride Gas             | 1      | 0.010      | µL 0.0005                      | 12               | 0.084 (3hr)                                       |
|                                | 2      | 0.020      | µL 0.0010                      | 7                | 0.060 (3hr)                                       |
| Vinylidene Chloride<br>(27°C)  | 1      | 0.49       | 0.038                          | 124              | 1.1 (3hr)                                         |
|                                | 2      | 0.010      | 0.0008                         | 40               | 0.086 (3hr)                                       |
|                                | 3      | 0.030      | 0.0023                         | 61               | 0.082 (3hr)                                       |

\* MDL = minimum detectable concentration determined by syringe pump calibration; MDR = minimum detectable permeation rate calculated from MDL, carrier gas flowrate, and material surface area. Values entered as (\*) could not be converted, µL indicates values reported as µL instead of µg, (mL) indicates mL instead of µg.

\*\* Reported rate is the rate at the conclusion of the permeation test or the maximum reached during the test. Test durations are noted in parenthesis, (ss) indicates steady-state permeation value, and (nc) indicates that no permeation time curve was provided.

TABLE 5. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE S100 AT 25C

| Chemical +                           | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average     |                                                                | Replicate #1 |                                                              | Replicate #2 |                                                              | Replicate #3 |                                                              |        |
|--------------------------------------|---------------|--------------------------------------------------|-------------|----------------------------------------------------------------|--------------|--------------------------------------------------------------|--------------|--------------------------------------------------------------|--------------|--------------------------------------------------------------|--------|
|                                      |               |                                                  | BT<br>(min) | Reported<br>rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |        |
| Acetone                              | 1.160         | 0.0469                                           | >           | 210                                                            |              |                                                              |              |                                                              |              |                                                              |        |
| Acetone (27C) +                      | 0.001         | 0.00004                                          |             | 71                                                             | 1.630 (3hr)  | 44                                                           | 1.3000       | 104                                                          | 1.2000       | 64                                                           | 2.4000 |
| Acrolein                             | 0.120         | 0.0054                                           |             | 41                                                             | 0.033 (ss)   | 44                                                           | 0.0395       | 38                                                           | 0.0268       |                                                              |        |
| Acrylonitrile                        | 0.460         | 0.0049                                           |             | 65                                                             | 0.014 (ss)   | 54                                                           |              | 76                                                           | 0.0143       |                                                              |        |
| Allyl Chloride                       | 0.160         | 0.0025                                           |             | 134                                                            | 0.011 (ss)   | 102                                                          | 0.0107       | 166                                                          | 0.0103       |                                                              |        |
| Allyl Chloride                       | 0.060         | 0.0037                                           |             | 143                                                            | 0.013 (6hr)  | 136                                                          | 0.0098       | 116                                                          | 0.0210       | 176                                                          | 0.0068 |
| Ammonium Hydroxide +                 | 2.000         | 0.0565                                           |             | 7                                                              | (nc)         | 30                                                           | 26.6667      | > 180                                                        |              |                                                              |        |
| Ammonium Hydroxide +                 | 7.200         | 0.2033                                           | >           | 180                                                            |              |                                                              |              |                                                              |              |                                                              |        |
| Carbon Disulfide                     | 0.100         | 0.0061                                           |             | 20                                                             | 0.050 (ss)   | 22                                                           | 0.0460       | 21                                                           | 0.0608       | 18                                                           | 0.0432 |
| Chloroprene (2-Chloro-1,3-Butadiene) | 0.030         | 0.0021                                           |             | 179                                                            | 0.005 (ss)   | 192                                                          | 0.0025       | 184                                                          | 0.0032       | 160                                                          | 0.0087 |
| 1,2-Dichloroethylene                 | 0.010         | 0.0008                                           |             | 15                                                             | 1.079 (ss)   | 20                                                           | 0.1933       | 4                                                            | 2.9333       | 20                                                           | 0.1115 |
| 1,2-Dichloroethylene                 | 0.010         | 0.0008                                           |             | 23                                                             | 0.130 (ss)   | 21                                                           | 0.1417       | 24                                                           | 0.1177       |                                                              |        |
| Dichloromethane                      | 0.270         | 0.0042                                           |             | 51                                                             | 0.020 (ss)   | 47                                                           | 0.0228       | 50                                                           | 0.0161       | 55                                                           | 0.0212 |
| Dichloromethane (USCG R&DC)          | 0.030         | *                                                |             | 61                                                             | (nc)         | 54                                                           |              | 65                                                           |              | 63                                                           |        |
| Ethyl Ether                          | 0.130         | 0.0078                                           | >           | 180                                                            |              |                                                              |              |                                                              |              |                                                              |        |
| Ethyl Ether +                        | 0.010         | 0.0006                                           |             | 92                                                             | 0.005 (3hr)  | 88                                                           | 0.0060       | 84                                                           | 0.0078       | 104                                                          | 0.0012 |
| Ethyl Ether (27C) +                  | 0.006         | 0.0004                                           |             | 117                                                            | 1.070 (3hr)  | 124                                                          | 1.4000       | 112                                                          | 0.9000       | 116                                                          | 0.9000 |
| Ethyl Vinyl Ether                    | 0.030         | 0.0017                                           |             | 113                                                            | 0.008 (3hr)  | 148                                                          | 0.0040       | 92                                                           | 0.0117       | 100                                                          | 0.0075 |
| Freon 12 (Gas) +                     | 3.500         | 0.3414 $\mu\text{L}$                             |             | 7                                                              | (nc)         | 160                                                          | 0.0001       | > 180                                                        |              | > 180                                                        |        |
| Methyl Bromide (Gas) +               | 0.010         | 0.0008 $\mu\text{L}$                             |             | 27                                                             | 0.0004 (ss)  | 28                                                           | 0.0002       | 28                                                           | 0.0005       | 24                                                           | 0.0005 |
| Propylene (Gas) +                    | 0.010         | 0.0003                                           |             | 61                                                             | 0.0003 (ss)  | 60                                                           | 0.0002       | 48                                                           | 0.0005       | 76                                                           | 0.0002 |
| Propylene Oxide                      | 0.680         | 0.0080                                           |             | 154                                                            | 0.021 (ss)   | 137                                                          | 0.0238       | 170                                                          | 0.0182       |                                                              |        |
| Tetrachloroethylene                  | 0.110         | 0.0147                                           | >           | 624                                                            |              |                                                              |              |                                                              |              |                                                              |        |
| Tetrachloroethylene (USCG R&DC)      | ND            | ND                                               |             | 108                                                            | (nc)         | 108                                                          |              |                                                              |              |                                                              |        |
| Tetrachloroethylene (27C) +          | 0.001         | 0.0001                                           |             | 7                                                              | (3hr)        | 180                                                          |              | 8                                                            | 33.0000      | 44                                                           | 3.0000 |
| Trichloroethylene                    | 0.070         | 0.0017                                           |             | 148                                                            | 0.031 (ss)   | 143                                                          | 0.0340       | 156                                                          | 0.0272       | 146                                                          | 0.0318 |
| Trichloroethylene                    | 0.010         | 0.0011                                           |             | 138                                                            | 0.031 (6hr)  | 155                                                          | 0.0148       | 140                                                          | 0.0233       | 120                                                          | 0.0540 |

(Continued)

TABLE 5. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE S100 AT 25C

| Chemical +             | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average     |                                                                | Replicate #1 |                                                              | Replicate #2 |                                                              | Replicate #3 |                                                              |
|------------------------|---------------|--------------------------------------------------|-------------|----------------------------------------------------------------|--------------|--------------------------------------------------------------|--------------|--------------------------------------------------------------|--------------|--------------------------------------------------------------|
|                        |               |                                                  | BT<br>(min) | Reported<br>rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
| Vinyl Acetate          | 0.210         | 0.0036                                           | 106         | 0.059 (ac)                                                     | 74           | 0.0550                                                       | 137          | 0.0622                                                       |              |                                                              |
| Vinyl Methyl Ether +   | 0.540         | 0.0253                                           | 60          | 2.242 (3hr)                                                    | 60           | 3.5833                                                       | 60           | 2.3667                                                       | 60           | 0.7750                                                       |
| Vinyl-Jeneo Chloride   | 0.490         | 0.0383                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Vinyl-Jeneo Chloride + | 0.010         | 0.0008                                           | 51          | 0.022 (3hr)                                                    | 52           | 0.0117                                                       | 52           | 0.0110                                                       | 48           | 0.0433                                                       |

+ Received after initial model development effort.

\* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL, the open-loop carrier gas flow rate, and the clothing material surface area. Values entered as (\*) could not be converted. ND indicates not determined.

Note:  $\mu\text{L}$  indicates the MDR and reported rate are in units of  $\mu\text{L}/\text{cm}^2\text{-min}$ .

\*\* Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses. (ac) indicates a steady-state permeation rate value. (nc) indicates that no permeation time curve was available.

TABLE 6. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE 5200 AT 25C

| Chemical +                   | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average     |                                                                | Replicate #1 |                                                              | Replicate #2 |                                                              | Replicate #3 |                                                              |
|------------------------------|---------------|--------------------------------------------------|-------------|----------------------------------------------------------------|--------------|--------------------------------------------------------------|--------------|--------------------------------------------------------------|--------------|--------------------------------------------------------------|
|                              |               |                                                  | BT<br>(min) | Reported<br>rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
| Acetone                      | 1.000         | 0.0404                                           | > 180       |                                                                | 116          | 0.0002                                                       | 116          | 0.0005                                                       | 116          | 0.0005                                                       |
| Acetone (27C) +              | 0.010         | 0.0004                                           | 116         | 0.0004 (3hr)                                                   |              |                                                              |              |                                                              |              |                                                              |
| Acetone (27C) +              | 0.001         | 0.00004                                          | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Allyl Chloride +             | 0.030         | 0.0019                                           | 56          | 0.2833 (3hr)                                                   | 68           | 0.2867                                                       | 64           | 0.1498                                                       | 36           | 0.4133                                                       |
| Ammonia (Gas)                | 0.300         | 0.0041                                           | 31          | 0.1144 (hr)                                                    | 36           | 0.0783                                                       | 24           | 0.1583                                                       | 32           | 0.1067                                                       |
| Ammonia (Gas) +              | 0.070         | 0.0010 $\mu\text{L}$                             | 25          | 0.2378 (3hr)                                                   | 18           | 0.2683                                                       | 23           | 0.2867                                                       | 35           | 0.1583                                                       |
| Ammonia (Gas) (27C) +        | 0.030         | 0.0004 $\mu\text{L}$                             | 32          | 0.1490 (hr)                                                    | 32           | 0.1200                                                       | 32           | 0.2183                                                       | 32           | 0.1100                                                       |
| Ammonium Hydroxide +         | 0.250         | 0.0071                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Ammonium Hydroxide (27C) +   | 7.200         | 0.2033                                           | 120         | 0.3390 (3hr)                                                   | 120          | 0.2500                                                       | 120          | 0.4500                                                       | 120          | 0.3167                                                       |
| Bromochloromethane           | 0.030         | 0.0031                                           | 98          | 0.0188 (7hr)                                                   | 93           | 0.0188                                                       | 109          | 0.0147                                                       | 93           | 0.0230                                                       |
| Bromochloromethane           | 0.010         | 0.0009                                           | 120         | 0.0281 (3hr)                                                   | 144          | 0.0245                                                       | 84           | 0.0325                                                       | 132          | 0.0272                                                       |
| 1,3-Butadiene (Gas)          | 0.068         | 0.0030                                           | 5           | 0.0389 (5hr)                                                   | 8            | 0.0240                                                       | 4            | 0.0375                                                       | 4            | 0.0552                                                       |
| 1,3-Butadiene (Gas) +        | 0.010         | 0.0004 $\mu\text{L}$                             | 24          | 0.0795 (3hr)                                                   | 24           | 0.1300                                                       | 24           | 0.0700                                                       | 24           | 0.0383                                                       |
| 2-Butene (Gas) (27C) +       | 0.040         | 0.0018                                           | 55          | 0.1300 (3hr)                                                   | 72           | 0.1000                                                       | 36           | 0.2000                                                       | 56           | 0.1000                                                       |
| Carbon Disulfide             | 0.010         | 0.0006                                           | 20          | 0.0335 (3hr)                                                   | 20           | 0.0497                                                       | 20           | 0.0208                                                       | 20           | 0.0300                                                       |
| Chlorine (Gas) +             | 1.000         | 0.0572                                           | 70          | 0.0182 (hr)                                                    | 90           | 0.0138                                                       | 60           | 0.0267                                                       | 60           | 0.0143                                                       |
| Chlorine (Gas) +             | 38.000        | 2.1734                                           | 60          | 170.33 (hr)                                                    | 30           | 320.00                                                       | 90           | 140.00                                                       | 60           | 51.0000                                                      |
| Chloromethane +              | 0.070         | 0.0036                                           | 60          | 0.6330 (hr)                                                    | 68           | 0.3667                                                       | 52           | 1.2500                                                       | 60           | 0.2833                                                       |
| 1-Chloropropane (27C)        | 2.000         | 0.1267                                           | 260         | 0.2367 (7hr)                                                   | 285          | 0.1433                                                       | 269          | 0.2350                                                       | 225          | 0.3317                                                       |
| Cyanogen (Gas) +             | 0.500         | 0.0210                                           | 30          | 0.0600 (hr)                                                    |              |                                                              |              |                                                              |              |                                                              |
| Cyclopropane (Gas) +         | 0.020         | 0.0007 $\mu\text{L}$                             | 92          | 0.0008 (3hr)                                                   | 96           | 0.0003                                                       | 72           | 0.0013                                                       | 108          | 0.0005                                                       |
| Cyclopropane (Gas) (27C) +   | 0.002         | 0.0001                                           | 78          | 0.0008 (3hr)                                                   | 76           | 0.0008                                                       | 80           | 0.0013                                                       | 80           | 0.0002                                                       |
| 1,2-Dichloroethylene +       | 0.010         | 0.0008                                           | 24          | 0.3578 (hr)                                                    | 28           | 0.2350                                                       | 28           | 0.4050                                                       | 16           | 0.3833                                                       |
| cis-1,2-Dichloroethylene     | 0.010         | 0.0008                                           | 69          | 0.1550 (3hr)                                                   | 56           | 0.2200                                                       | 80           | 0.0967                                                       | 72           | 0.1483                                                       |
| trans-1,2-Dichloroethylene + | 0.010         | 0.0008                                           | 19          | 1.3967 (hr)                                                    | 19           | 1.4317                                                       | 19           | 1.4700                                                       | 19           | 1.2883                                                       |
| Dichloromethane (27C) +      | 0.007         | 0.0005                                           | 83          | 3.6700 (3hr)                                                   | 84           | 4.0000                                                       | 88           | 3.0000                                                       | 76           | 4.0000                                                       |
| Dichloromethane +            | 0.005         | 0.0003                                           | 64          | 0.2630 (3hr)                                                   | 68           | 0.2300                                                       | 52           | 0.3700                                                       | 72           | 0.1900                                                       |
| Dimethyl Sulfide +           | 0.010         | 0.0008                                           | 95          | 0.0005 (3hr)                                                   | 116          | 0.0005                                                       | 76           | 0.0005                                                       | 92           | 0.0005                                                       |
| Dimethyl Sulfide +           | 0.010         | 0.0008                                           | 48          | 0.0002 (3hr)                                                   | 60           | 0.0002                                                       | 40           | 0.0002                                                       | 44           | 0.0003                                                       |

(Continued)

TABLE 6. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE 5200 AT 25C

| Chemical +                     | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average |                                          | Replicate #1 |                                          | Replicate #2 |                                          | Replicate #3 |                                          |
|--------------------------------|---------------|--------------------------------------------------|---------|------------------------------------------|--------------|------------------------------------------|--------------|------------------------------------------|--------------|------------------------------------------|
|                                |               |                                                  | BT      | rate**                                   | BT           | rate                                     | BT           | rate                                     | BT           | rate                                     |
|                                |               |                                                  | (min)   | ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | (min)        | ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | (min)        | ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | (min)        | ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
| Ethanol +                      | 0.020         | 0.0010                                           | 65      | 0.0028 (3hr)                             | 60           | 0.0030                                   | 76           | 0.0025                                   | 60           | 0.0030                                   |
| Ethanol (27C) +                | 0.003         | 0.0002                                           | 83      | 15.3300 (3hr)                            | 88           | 4.0000                                   | 88           | 16.0000                                  | 72           | 26.0000                                  |
| Ethyl Ether (27C)              | 0.010         | 0.0006                                           | 127     | 0.3761 (20hr)                            | 104          | 0.4050                                   | 136          | 0.3033                                   | 140          | 0.4200                                   |
| Ethyl Ether (27C) +            | 0.010         | 0.0006                                           | 92      | 0.0080 (3hr)                             | 92           | 0.0143                                   | 96           | 0.0035                                   | 88           | 0.0072                                   |
| Ethyl Ether (27C) +            | 0.003         | 0.0002                                           | 149     | 2.1000 (3hr)                             | 144          | 4.9000                                   | 156          | 0.9000                                   | 148          | 0.5000                                   |
| Ethyl Ether (27C) +            | 0.010         | 0.0006                                           | 40      | 173.33 (3hr)                             | 44           | 130.00                                   | 36           | 220.00                                   | 40           | 170.00                                   |
| Ethyl Vinyl Ether              | 0.020         | 0.0012                                           | 23      | 0.6694 (3hr)                             | 40           | 0.3933                                   | 8            | 0.5517                                   | 20           | 1.0633                                   |
| Ethylene Oxide (Gas) +         | 3.600         | 0.1066                                           | 57      | 0.7250 (3hr)                             | 68           | 0.8250                                   | 60           | 0.8483                                   | 44           | 0.5017                                   |
| Ethylene Oxide (Gas) +         | 0.650         | 0.0231                                           | 25      | 0.1420 (3hr)                             | 20           | 0.1418                                   | 24           | 0.1683                                   | 32           | 0.1160                                   |
| Hydrogen Sulfide (Gas) +       | 0.030         | 0.0008 $\mu\text{L}$                             | 4       | 0.0028 (3hr)                             | 4            | 0.0017                                   | 4            | 0.0005                                   | 4            | 0.0017                                   |
| Hydrogen Sulfide (Gas) (27C) + | 0.010         | 0.0003 $\mu\text{L}$                             | 8       | 0.0070 (3hr)                             | 8            | 0.0055                                   | 8            | 0.0077                                   | 8            | 0.0068                                   |
| Hydrogen Sulfide (Gas) +       | 0.030         | 0.0008 $\mu\text{L}$                             | 15      | 0.0078 (ac)                              | 20           | 0.0017                                   | 12           | 0.0133                                   | 12           | 0.0083                                   |
| Isoprene                       | 0.010         | 0.0005                                           | 9       | 0.1820 (3hr)                             | 8            | 0.0615                                   | 8            | 0.1295                                   | 12           | 0.3550                                   |
| Methane (27C) +                | 1.000         | 0.0129                                           | 7       | 18.0000 (ac)                             | 7            | 16.0000                                  | 6            | 27.0000                                  | 8            | 11.0000                                  |
| Methyl Acetate +               | 0.020         | 0.0012                                           | 112     | 0.0053 (3hr)                             | 84           | 0.0072                                   | 144          | 0.0042                                   | 108          | 0.0048                                   |
| Methyl Acrylate +              | 7.000         | 0.4861                                           | 7       | 0.0053 (3hr)                             | 116          | 0.7683                                   | 112          | 0.7700                                   | 180          | >                                        |
| Methyl Bromide (Gas) +         | 0.400         | 0.0306                                           | 21      | 0.0347 (3hr)                             | 20           | 0.0367                                   | 20           | 0.0367                                   | 24           | 0.0308                                   |
| Methyl Bromide (Gas) +         | 0.020         | 0.0015 $\mu\text{L}$                             | 20      | 0.0065 (3hr)                             | 20           | 0.0053                                   | 20           | 0.0073                                   | 20           | 0.0067                                   |
| Methyl Chloride (Gas) (27C) +  | 0.060         | 0.0024 $\mu\text{L}$                             | 16      | 0.0020 (ac)                              | 16           | 0.0020                                   | 16           | 0.0020                                   | 16           | 0.0020                                   |
| Methyl Chloroformate +         | 0.050         | 0.0038                                           | 81      | 0.0120 (3hr)                             | 76           | 0.0092                                   | 76           | 0.0198                                   | 92           | 0.0068                                   |
| Methyl Chloroformate (27C) +   | 0.100         | 0.0076                                           | 95      | 0.9500 (3hr)                             | 116          | 0.7500                                   | 72           | 1.2000                                   | 96           | 0.8900                                   |
| Methyl Iodide +                | 0.370         | 0.0424                                           | 32      | 17.2333 (3hr)                            | 32           | 27.0000                                  | 32           | 10.8000                                  | 32           | 13.9000                                  |
| Methyl Isocyanate +            | 0.010         | 0.0005                                           | 92      | 0.0202 (3hr)                             | 96           | 0.0207                                   | 72           | 0.0188                                   | 108          | 0.0212                                   |
| Nitric Oxide (Gas) +           | 1.000         | 0.0508 $\mu\text{L}$                             | 30      | 2.0000 (ac)                              |              |                                          |              |                                          |              |                                          |
| Nitrogen Dioxide (Gas) (27C) + | 0.500         | 0.0186 $\mu\text{L}$                             | 4       | 4.9900 (ac)                              | 4            | 5.3333                                   | 4            | 6.3500                                   | 4            | 3.2833                                   |
| Nitrogen Tetraoxide (Gas) +    | 0.080         | 0.0059 $\mu\text{L}$                             | 15      | 13.7600 (ac)                             | 24           | 16.2000                                  | 4            | 18.7000                                  | 16           | 6.4000                                   |
| Nitromethane                   | 0.730         | 0.0359                                           | 168     | 0.0538 (ac)                              | 168          | 0.0447                                   | 168          | 0.0630                                   | 168          | 0.0537                                   |
| Pentane +                      | 0.010         | 0.0006                                           | 81      | 0.0440 (ac)                              | 88           | 0.0500                                   | 64           | 0.0500                                   | 92           | 0.0333                                   |
| Phonene (Gas) +                | 0.500         | *                                                | 60      | 3.3300 (ac)                              | 60           | 3.3300                                   | 60           | 3.3300                                   | 60           | 3.3300                                   |

(Continued)

TABLE 6. CHEMICALS FOR WHICH PERMEATION WAS DETECTED WITH CHALLENGE 5200 AT 25C

| Chemical +                  | MDL* (ppm) | MDR* ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average  |                                                          | Replicate #1 |                                                        | Replicate #2 |                                                        | Replicate #3 |                                                        |
|-----------------------------|------------|-----------------------------------------------|----------|----------------------------------------------------------|--------------|--------------------------------------------------------|--------------|--------------------------------------------------------|--------------|--------------------------------------------------------|
|                             |            |                                               | BT (min) | Reported rate** ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT (min)     | Reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT (min)     | Reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT (min)     | Reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
| Propylene Oxide (27C) +     | 0.010      | 0.0005                                        | 89       | 0.0001 (3hr)                                             | 96           | 0.0001                                                 | 96           | 0.0001                                                 | 76           | 0.0002                                                 |
| Sulfur Dioxide (Gas) +      | 47.000     | 2.4292 mL                                     | 60       | 0.0895 (3hr)                                             | 60           | 0.0717                                                 | 60           | 0.1250                                                 | 60           | 0.0717                                                 |
| Sulfur Dioxide (Gas) +      | 1.000      | 0.0517 mL                                     | 40       | 2.3000 (ac)                                              | 30           | 2.3000                                                 | 60           | 2.3000                                                 | 30           | 2.3000                                                 |
| Trichloroethylene +         | 0.010      | 0.0011                                        | 49       | 0.1949 (3hr)                                             | 52           | 0.2017                                                 | 56           | 0.1630                                                 | 40           | 0.2200                                                 |
| Trichloroethylene (27C) +   | 0.010      | 0.0011                                        | 72       | 0.0028 (3hr)                                             | 80           | 0.0022                                                 | 76           | 0.0042                                                 | 60           | 0.0022                                                 |
| Trimethylamine +            | 0.150      | 0.0072                                        | 20       | (ac)                                                     | 20           |                                                        |              |                                                        |              |                                                        |
| Trimethylamine +            | 0.014      | 0.0007                                        | > 180    |                                                          |              |                                                        |              |                                                        |              |                                                        |
| Trimethylamine +            | 0.150      | 0.0072                                        | 25       | (ac)                                                     | 20           |                                                        |              |                                                        |              |                                                        |
| Vinyl Acetate               | 0.020      | 0.0014                                        | 69       | 0.2522 (ac)                                              | 68           | 0.2433                                                 | 24           | 0.3350                                                 | 76           | 0.1783                                                 |
| Vinyl Acetate +             | 0.004      | 0.0003                                        | 73       | 38.0000 (3hr)                                            | 65           | 50.0000                                                | 85           | 35.0000                                                | 69           | 29.0000                                                |
| Vinyl Acetate +             | 0.004      | 0.0003                                        | 109      | 11.2800 (3hr)                                            | 72           | 25.2000                                                | 132          | 2.1900                                                 | 124          | 6.4400                                                 |
| Vinyl Chloride (Gas) +      | 0.010      | 0.0005 $\mu\text{L}$                          | 12       | 0.0840 (3hr)                                             | 12           | 0.0860                                                 | 12           | 0.0952                                                 | 12           | 0.0715                                                 |
| Vinyl Chloride (Gas) +      | 0.020      | 0.0010 $\mu\text{L}$                          | 7        | 0.0600 (3hr)                                             | 4            | 0.0600                                                 | 8            | 0.0400                                                 | 8            | 0.0400                                                 |
| Vinyl Methyl Ether +        | 33.000     | 1.5448                                        | 28       | 19.1000 (3hr)                                            | 36           | 7.6500                                                 | 24           | 35.0500                                                | 24           | 14.6000                                                |
| Vinylidene Chloride         | 0.490      | 0.0343                                        | 124      | 1.0028 (3hr)                                             | 120          | 1.4800                                                 | 120          | 0.8800                                                 | 132          | 0.8883                                                 |
| Vinylidene Chloride +       | 0.010      | 0.0008                                        | 40       | 0.0860 (3hr)                                             | 32           | 0.1570                                                 | 40           | 0.0655                                                 | 48           | 0.0352                                                 |
| Vinylidene Chloride (27C) + | 0.030      | 0.0023                                        | 61       | 0.0822 (3hr)                                             | 64           | 0.0567                                                 | 60           | 0.0900                                                 | 60           | 0.1000                                                 |
| Vinylidene Fluoride (Gas) + | 0.040      | 0.0021                                        | 32       | 0.0760 (3hr)                                             | 32           | 0.0700                                                 | 32           | 0.0900                                                 | 32           | 0.0700                                                 |

+ Received after initial model development effort.

\* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area. Values entered as (\*) could not be converted. ND indicates not determined.

Note:  $\mu\text{L}$  indicates the MDR and reported rate are in units of  $\mu\text{L}/\text{cm}^2\text{-min}$ , mL indicates MDR and reported rate are in units mL/cm<sup>2</sup>-min.

\*\* Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses. (ac) indicates a steady-state permeation rate value. (ac) indicates that no permeation time curve was available.

### 3.3.3 Comparison of Challenge 5100 with Challenge 5200 Results

As noted above, there were 39 chemicals tested against both Challenge 5100 and Challenge 5200. The results of these tests are compared in Table 7. In the broadest sense, there is good agreement between the results for the two fabrics: chemicals detected to permeate Challenge 5100 within 3 hours were also detected to permeate Challenge 5200 and vice versa. In all, there were 7 chemicals with some discrepancy. For 6 of these chemicals, the discrepancy was within one fabric (e.g., repeat test results for the same fabric conflicted, results within the 3 replicates of a test conflicted). For the remaining case (vinylidene fluoride), the results conflict, however, the MDR for the Challenge 5200 test was an order of magnitude lower than for the Challenge 5100 test.

For the remaining 32 chemicals, the results are in agreement. For 20 of these chemicals, no permeation was detected for either material. For the other 12 chemicals, permeation was detected through both materials. It is difficult, however, to make specific comparisons between the breakthrough times and reported permeation rates for these permeating chemicals because of differences in the MDRs and the test durations. In spite of these differences, the following generalizations are possible:

- the results were approximately equal for four chemicals,
- the permeation resistance was somewhat better for Challenge 5100 for seven chemicals, and
- the permeation resistance was somewhat better for Challenge 5200 for only one chemical.

Our conclusion based on this analysis is that the barrier properties of the two materials are similar. Therefore, for the purposes of predictive model development, the data set was combined and a single model developed to address both materials. Again, we also concluded that the variability in the permeation method and detection limits make the development of a quantitative predictive model difficult. Analysis of the overall data set and the development of an empirical model to predict pure chemical permeation of the Challenge materials are discussed in Section 4.

### 3.4 CHEMICAL MIXTURE DATA SET

Table 8 summarizes the permeation tests that were conducted with chemical mixtures at (or near) 25°C including both the TRI and Arthur D. Little tests. Compared to the data set for pure chemicals reported above, very few of the infinite number of chemical mixtures possible were tested. Consequently, only general guidelines regarding mixture permeation behavior are possible. The TRI mixture permeation test results, as compiled by us, are provided in Appendix C. The Arthur D. Little mixture permeation test results are documented in Appendix D using the ASTM F1194-89 format for reporting the results of chemical permeation testing. Both these data sets are discussed further in Section 5.

TABLE 7. COMPARISON OF PERMEATION TEST RESULTS WITH  
CHALLENGE 5100 AND 5200 AT 25°C

| Chemical                          | Material | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average<br>BT<br>(min) | Average<br>reported rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |       |
|-----------------------------------|----------|---------------|--------------------------------------------------|------------------------|------------------------------------------------------------------------|-------|
| Acetone<br>(27°C)                 | 5100     | 1.2           | 0.047                                            | >210                   | --                                                                     |       |
|                                   | 5200     | nd            | nd                                               | 70                     | 1.6                                                                    | (3hr) |
|                                   |          | 1.0           | 0.040                                            | >180                   | --                                                                     | (3hr) |
|                                   |          | (27°C)        | 0.010                                            | 116                    | 0.0004                                                                 |       |
|                                   |          | (27°C)        | 0.001                                            | >180                   | --                                                                     |       |
|                                   |          | (ChemFab)     | 0.10                                             | >300                   | --                                                                     |       |
| Acetonitrile                      | 5100     | nd            | nd                                               | >270                   | --                                                                     |       |
|                                   | 5200     | 1.0           | 0.033                                            | >180                   | --                                                                     |       |
|                                   |          | 2.0           | 0.066                                            | >180                   | --                                                                     |       |
| Acetyl chloride                   | 5100     | 35.5          | 2.25                                             | >186                   | --                                                                     |       |
|                                   | 5200     | 0.020         | 0.0013                                           | >180                   | --                                                                     |       |
| Allyl chloride                    | 5100     | 0.060         | 0.0037                                           | 143                    | 0.013                                                                  | (ss)  |
|                                   |          | 0.16          | 0.0099                                           | 134                    | 0.011                                                                  | (6hr) |
|                                   |          | 0.030         | 0.0019                                           | 56                     | 0.28                                                                   | (3hr) |
|                                   | 5200     |               |                                                  |                        |                                                                        |       |
| Ammonia gas<br><br>(ChemFab)      | 5100     | 0.040         | 0.0005                                           | >180                   | --                                                                     |       |
|                                   | 5200     | 0.30          | 0.0041                                           | 31                     | 0.11                                                                   | (ss)  |
|                                   |          | 0.070         | $\mu\text{L}$ 0.0010                             | 25                     | 0.24                                                                   | (3hr) |
|                                   |          | 0.030         | $\mu\text{L}$ 0.0004                             | 32                     | 0.15                                                                   | (3hr) |
|                                   |          | 0.10          | *                                                | >300                   | --                                                                     |       |
|                                   |          |               |                                                  |                        |                                                                        |       |
| Ammonium hydroxide                | 5100     | 2.0           | 0.057                                            | 30, >180†              | 26.7                                                                   | (3hr) |
|                                   |          | 7.2           | 0.20                                             | >180                   | --                                                                     |       |
|                                   |          |               |                                                  |                        |                                                                        |       |
|                                   | 5200     | 0.25          | 0.0071                                           | >180                   | --                                                                     |       |
|                                   |          | 7.2           | 0.20                                             | 120                    | 0.34                                                                   | (3hr) |
| Butylamine                        | 5100     | 0.32          | 0.019                                            | >180                   | --                                                                     |       |
|                                   | 5200     | 0.010         | 0.0006                                           | >180                   | --                                                                     |       |
| Carbon Disulfide<br><br>(ChemFab) | 5100     | 0.10          | 0.0061                                           | 20                     | 0.050                                                                  | (ss)  |
|                                   | 5200     | 0.010         | 0.0006                                           | 20                     | 0.034                                                                  | (3hr) |
|                                   |          | 0.30          | *                                                | 143                    | 0.050                                                                  | (nc)  |
|                                   |          |               |                                                  |                        |                                                                        |       |
| m-Cresol (Cresols)                | 5100     | 0.030         | 0.0026                                           | >240                   | --                                                                     |       |
|                                   | 5200     | 0.010         | 0.0009                                           | >180                   | --                                                                     |       |
| Dibromomethane                    | 5100     | 0.050         | 0.0070                                           | >180                   | --                                                                     |       |
|                                   | 5200     | 0.030         | 0.0042                                           | >180                   | --                                                                     |       |
| 1,2-Dichloroethylene              | 5100     | 0.010         | 0.0008                                           | 15                     | 1.1                                                                    | (ss)  |
|                                   |          | 0.010         | 0.0008                                           | 23                     | 0.13                                                                   | (ss)  |
|                                   |          | 0.010         | 0.0008                                           | 24                     | 0.36                                                                   | (nc)  |

TABLE 7. COMPARISON OF PERMEATION TEST RESULTS WITH  
CHALLENGE 5100 AND 5200 AT 25°C

| Chemical                                                          | Material | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average<br>BT<br>(min) | Average<br>reported rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |        |
|-------------------------------------------------------------------|----------|---------------|--------------------------------------------------|------------------------|------------------------------------------------------------------------|--------|
| Dichloromethane<br>(USCG)<br>(27°C)<br><br>(ChemFab)              | 5100     | 0.27          | 0.0042                                           | 51                     | 0.020                                                                  | (ss)   |
|                                                                   |          | 0.030         | *                                                | 61                     | nd                                                                     | (nc)   |
|                                                                   | 5200     | 0.007         | 0.0005                                           | 83                     | 3.7                                                                    | (3hr)  |
|                                                                   |          | 0.005         | 0.0003                                           | 64                     | 0.26                                                                   | (3hr)  |
|                                                                   |          | 0.10          | *                                                | 64                     | 0.12                                                                   | (nc)   |
| Diethylamine<br>(USCG)<br>(ChemFab)                               | 5100     | nd            | nd                                               | >270                   | --                                                                     |        |
|                                                                   | 5200     | 0.40          | *                                                | >300                   | --                                                                     |        |
| Dimethylformamide (USCG)<br>(ChemFab)                             | 5100     | nd            | nd                                               | >192                   | --                                                                     |        |
|                                                                   | 5200     | 0.70          | *                                                | >300                   | --                                                                     |        |
| Ethyl acetate<br><br>(ChemFab)                                    | 5100     | 0.49          | 0.035                                            | >258                   | --                                                                     |        |
|                                                                   | 5200     | 0.010         | 0.0007                                           | >180                   | --                                                                     |        |
|                                                                   |          | 0.10          | *                                                | >300                   | --                                                                     |        |
| Ethyl acrylate                                                    | 5100     | 1.7           | 0.14                                             | >1020                  | --                                                                     |        |
|                                                                   | 5200     | 0.050         | 0.0040                                           | >180                   | --                                                                     |        |
| Ethyl ether<br><br>(27°C)<br>(27°C)<br>(27°C)<br>(27°C)<br>(27°C) | 5100     | 0.13          | 0.0078                                           | >180                   | --                                                                     |        |
|                                                                   |          | 0.010         | 0.0006                                           | 92                     | 0.005                                                                  | (3hr)  |
|                                                                   |          | 0.006         | 0.0004                                           | 117                    | 1.1                                                                    | (3hr)  |
|                                                                   | 5200     | 0.010         | 0.0006                                           | 127                    | 0.38                                                                   | (20hr) |
|                                                                   |          | 0.010         | 0.0006                                           | 92                     | 0.0080                                                                 | (3hr)  |
|                                                                   |          | 0.003         | 0.0002                                           | 149                    | 2.1                                                                    | (3hr)  |
|                                                                   |          | 0.010         | 0.0006                                           | 40                     | 173.3                                                                  | (3hr)  |
| Ethyl vinyl ether                                                 | 5100     | 0.030         | 0.0017                                           | 113                    | 0.0080                                                                 | (3hr)  |
|                                                                   | 5200     | 0.020         | 0.0012                                           | 23                     | 0.67                                                                   | (3hr)  |
| Freon 12 gas                                                      | 5100     | 3.5           | $\mu\text{L}$ 0.34                               | 160, >180†             | 0.0001                                                                 | (3hr)  |
|                                                                   | 5200     | 0.10          | 0.0098                                           | >180                   | --                                                                     |        |
| Gasoline (Gasoline JP-4)                                          | 5100     | 1.7           | *                                                | >894                   | --                                                                     |        |
|                                                                   | 5200     | 0.1           | *                                                | >180                   | --                                                                     |        |
| Hexane                                                            | 5100     | 0.25          | 0.017                                            | >300                   | --                                                                     |        |
|                                                                   | 5200     | 0.10          | 0.0070                                           | >300                   | --                                                                     |        |
| Methanol<br>(ChemFab)                                             | 5100     | 4.1           | 0.11                                             | >852                   | --                                                                     |        |
|                                                                   | 5200     | 0.40          | *                                                | >300                   | --                                                                     |        |
| Methyl acrylate                                                   | 5100     | 0.12          | 0.0083                                           | >180                   | --                                                                     |        |
|                                                                   | 5200     | 7.0           | 0.49                                             | 114, >180†             | 0.77                                                                   | (3hr)  |
| Methyl bromide gas                                                | 5100     | 0.010         | $\mu\text{L}$ 0.0008                             | 27                     | 0.0004                                                                 | (ss)   |
|                                                                   | 5200     | 0.40          | 0.031                                            | 21                     | 0.035                                                                  | (3hr)  |
|                                                                   |          | 0.020         | $\mu\text{L}$ 0.0015                             | 20                     | 0.0065                                                                 | (3hr)  |
| Methyl ethyl ketone<br>(ChemFab)                                  | 5100     | 0.65          | 0.038                                            | >180                   | --                                                                     |        |
|                                                                   | 5200     | 1.0           | *                                                | >120                   | --                                                                     |        |

TABLE 7. COMPARISON OF PERMEATION TEST RESULTS WITH  
CHALLENGE 5100 AND 5200 AT 25°C

| Chemical                                             | Material | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average<br>BT<br>(min) | Average<br>reported rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |       |
|------------------------------------------------------|----------|---------------|--------------------------------------------------|------------------------|------------------------------------------------------------------------|-------|
| Methyl vinyl ketone                                  | 5100     | 0.050         | 0.0028                                           | >180                   | --                                                                     |       |
|                                                      | 5200     | 0.010         | 0.0006                                           | >180                   | --                                                                     |       |
| Nitrobenzene<br>(ChemFab)                            | 5100     | 0.080         | 0.0079                                           | >180                   | --                                                                     |       |
|                                                      | 5200     | 1.0           | *                                                | >300                   | --                                                                     |       |
| Nitromethane                                         | 5100     | 0.26          | 0.013                                            | >180                   | --                                                                     |       |
|                                                      | 5200     | 0.73          | 0.036                                            | 168                    | 0.054                                                                  | (nc)  |
|                                                      |          | 0.70          | 0.035                                            | >180                   | --                                                                     |       |
| Potassium hydroxide                                  | 5100     | 1.0           | 0.045                                            | >180                   | --                                                                     |       |
|                                                      | 5200     | 0.50          | 0.023                                            | >180                   | --                                                                     |       |
| Propylene oxide<br>(27°C)                            | 5100     | 0.68          | 0.0080                                           | 154                    | 0.021                                                                  | (ss)  |
|                                                      | 5200     | 0.010         | 0.0005                                           | 89                     | 0.0002                                                                 | (3hr) |
| Sodium hydroxide (50%)<br>(USCG)<br><br>(ChemFab)    | 5100     | 0.50          | 0.016                                            | >4260                  | --                                                                     |       |
|                                                      |          | nd            | nd                                               | >180                   | --                                                                     |       |
|                                                      | 5200     | 0.50          | 0.016                                            | >180                   | --                                                                     |       |
|                                                      |          | 0.20          | *                                                | >300                   | --                                                                     |       |
| Tetrachloroethylene<br>(USCG)<br>(27°C)<br>(ChemFab) | 5100     | 0.11          | 0.015                                            | >624                   | --                                                                     |       |
|                                                      |          | nd            | nd                                               | 103                    | nd                                                                     |       |
|                                                      |          | 0.001         | 0.0001                                           | 26, >180†              | 18.0                                                                   | (3hr) |
|                                                      | 5200     | 0.20          | *                                                | >300                   | --                                                                     |       |
| Tetrahydrofuran (USCG)<br>(ChemFab)                  | 5100     | nd            | nd                                               | >330                   | --                                                                     |       |
|                                                      | 5200     | 0.10          | *                                                | >300                   | --                                                                     |       |
| Toluene<br>(ChemFab)                                 | 5100     | 0.060         | 0.0045                                           | >180                   | --                                                                     |       |
|                                                      | 5200     | 0.10          | *                                                | >300                   | --                                                                     |       |
| Trichloroethylene                                    | 5100     | 0.070         | 0.0017                                           | 148                    | 0.031                                                                  | (ss)  |
|                                                      |          | 0.010         | 0.0011                                           | 138                    | 0.031                                                                  | (6hr) |
|                                                      | 5200     | 0.010         | 0.0011                                           | 49                     | 0.19                                                                   | (3hr) |
|                                                      |          | 0.010         | 0.0011                                           | 72                     | 0.0028                                                                 | (3hr) |
| Vinyl acetate                                        | 5100     | 0.21          | 0.0036                                           | 106                    | 0.059                                                                  | (ss)  |
|                                                      | 5200     | 0.020         | 0.0014                                           | 69                     | 0.25                                                                   | (nc)  |
|                                                      |          | 0.004         | 0.0003                                           | 73                     | 38.0                                                                   | (3hr) |
|                                                      |          | 0.004         | 0.0003                                           | 109                    | 11.3                                                                   | (3hr) |
| Vinyl methyl ether                                   | 5100     | 0.54          | 0.025                                            | 60                     | 2.2                                                                    | (3hr) |
|                                                      | 5200     | 33.0          | 1.5                                              | 28                     | 19.1                                                                   | (3hr) |

TABLE 7. COMPARISON OF PERMEATION TEST RESULTS WITH  
CHALLENGE 5100 AND 5200 AT 25°C

| Chemical            | Material | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average<br>BT<br>(min) | Average<br>reported rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |       |
|---------------------|----------|---------------|--------------------------------------------------|------------------------|------------------------------------------------------------------------|-------|
| Vinylidene chloride | 5100     | 0.49          | 0.038                                            | >180                   | --                                                                     |       |
|                     |          | 0.010         | 0.0008                                           | 51                     | 0.022                                                                  | (3hr) |
|                     | 5200     | 0.49          | 0.038                                            | 124                    | 1.1                                                                    | (3hr) |
|                     |          | 0.010         | 0.0008                                           | 40                     | 0.086                                                                  | (3hr) |
|                     |          | 0.030         | 0.0023                                           | 61                     | 0.082                                                                  | (3hr) |
| Vinylidene fluoride | 5100     | 0.70          | 0.036                                            | >180                   | --                                                                     |       |
|                     | 5200     | 0.040         | 0.0021                                           | 32                     | 0.076                                                                  | (3hr) |

\* MDL = minimum detectable concentration determined by syringe pump calibration; MDR = minimum detectable permeation rate calculated from MDL, carrier gas flowrate, and material surface area. Values entered as (\*) could not be converted, (nd) indicates not determined, and  $\mu\text{L}$  indicates values reported as  $\mu\text{L}$  instead of  $\mu\text{g}$ .

\*\* Reported rate is the rate at the conclusion of the permeation test or the maximum reached during the test. Test durations are noted in parenthesis, (ss) indicates steady-state permeation value, and (nc) indicates that no permeation time curve was provided.

† Conflicting results were measured within the three replicates for this test.

TABLE 8. SUMMARY OF MIXTURE PERMEATION TESTS AT 25°C

| Condition                                                              | No. of mixtures |                  |
|------------------------------------------------------------------------|-----------------|------------------|
|                                                                        | TRI             | Arthur D. Little |
| Total mixtures tested against Challenge 5100 material                  | 15              | --               |
| - Binary mixtures                                                      | 14              | --               |
| - Ternary mixtures                                                     | 1               |                  |
| - Tests for which permeation rates as a function of time were measured | 0               | --               |
| Total mixtures tested against Challenge 5200 material                  | 14              | 7                |
| - Binary mixtures                                                      | 10              | 5                |
| - Ternary mixtures                                                     | 4               | 2                |
| - Tests for which permeation rates as a function of time were measured | 0               | 7                |

## SECTION 4

### DEVELOPMENT OF A MODEL TO PREDICT PURE CHEMICAL PERMEATION

#### 4.1 FICK'S LAW ANALYSIS

Our first step in analyzing the data set was to assess the mechanism by which the chemicals permeate the Challenge materials as a function of time. Such an assessment is important because the direction and success of predictive model development often depend on the permeation mechanism. For example, if the permeation appears to be a solution-diffusion process, then a Fick's law model can be pursued and the permeation behavior as a function of time can be predicted using theoretical relationships. If the mechanism is not solution-diffusion (e.g., analogous to an inert gas penetrating a film or microporous substrate), then a more empirical model might be pursued to predict whether permeation will occur.

##### 4.1.1 Analysis of Permeation-Time Behavior

The available permeation-time curves were analyzed to assess whether the behavior could be accurately described by a solution-diffusion mechanism using Fick's laws of diffusion [11]. Mathematical relationships based on Fick's law describe the permeation rate,  $J$ , and the cumulative amount permeated,  $M$ , at any time following initiation of chemical contact for solution-diffusion processes. These relationships require two fundamental parameters: the diffusion coefficient,  $D$ , and the solubility,  $S$ , of the permeant in the material of interest. For a planar film of thickness,  $l$ , the appropriate solutions to Fick's second law of diffusion with standard initial conditions and simple boundary conditions are:

$$J = (DS/l) \left[ 1 + 2 \sum_{n=1}^{\infty} (-1)^n \exp(-\pi^2 n^2 \psi) \right] \quad \text{Eq. (1)}$$

and

$$M = (Sl) \left[ \psi - 1/6 - 2 \sum_{n=1}^{\infty} [(-1)^n / (\pi n)^2] \exp(-(n\pi)^2 \psi) \right] \quad \text{Eq. (2)}$$

|           |   |                                                        |
|-----------|---|--------------------------------------------------------|
| where $J$ | = | permeation rate, $\mu\text{g}/\text{cm}^2\text{-min}$  |
| $M$       | = | cumulative amount permeated, $\mu\text{g}/\text{cm}^2$ |
| $\psi$    | = | $Dt/l^2$ , dimensionless                               |
| $D$       | = | diffusion coefficient, $\text{cm}^2/\text{min}$        |

$S$  = equilibrium solubility,  $\mu\text{g}/\text{cm}^3$   
 $l$  = membrane thickness, cm  
 $t$  = time, min

The derivation of these equations assumes that there is continuous contact of the chemical with the clothing material surface for the test duration, there are no external resistances at the clothing material surfaces, and the diffusion coefficient and clothing material thickness are constants. The last assumption is not always valid and, particularly for rubbery polymer systems, the concentration dependence of  $D$  and swelling must be considered for accurate predictions of the permeation behavior.

Using these equations, one can calculate values for the breakthrough time on the basis of a minimum detectable permeation rate or a minimum cumulative amount permeated. These equations can also be used to solve for values of  $D$  and  $S$  given a set of  $J$  versus  $t$  or  $M$  versus  $t$  data [12]. For this data set, the permeation-time curves provide sets of  $J$  versus  $t$  data that can also be converted to  $M$  versus  $t$  data by analysis of the areas under the permeation-time curves as a function of time. Two approaches to extract values for  $D$  and  $S$  were pursued depending on the type of curve available. For permeation curves in which steady-state was reached, values for  $D$  and  $S$  were solved for directly by converting the later time data (i.e., steady-state data) to cumulative amounts permeated and applying Eq. (2). For permeation-time curves in which permeation rates were still increasing with time (i.e., in the transition region of a Fickian permeation curve), values for  $D$  and  $S$  were determined using Eq. (1) and an iterative curve-fitting technique. Both techniques are described in Appendix E.

Once values for  $D$  and  $S$  were determined, Eq. (1) was used to calculate permeation rates as a function of time for comparison with the reported permeation data. In general, the measured permeation-time curves could be accurately described using the Fick's law model. Figure 1 shows an example curve fit for a case in which the permeation rate data reached steady-state. A second example is shown in Figure 2 for a test that was terminated before reaching steady-state. Figure 2 also illustrates an important capability of this analysis technique that can simplify data comparisons. With the values of  $D$  and  $S$  and Eq. (1), the permeation behavior at any time can be calculated, including the steady-state permeation rate and the time required to reach steady-state. Thus, permeation results from different tests can be more readily compared by calculating a permeation rate at a set test duration or by calculating the steady-state permeation rate.

Values for  $D$ ,  $S$ , and the steady-state permeation rate calculated using Eq. (1) are reported in Table 9 for Challenge 5100 at 25°C, Table 10 for Challenge 5200 at 25°C, Table 11 for Challenge 5200 at 35°C, and Table 12 for Challenge 5200 at 40°C. Analyses were not possible for the 30°C data because permeation-time curves were not provided to us for that data set.

In general, an excellent fit to the permeation data was possible using Fick's law with the assumption of a constant  $D$ . As reported in Tables 9 through 12, the  $D$  values ranged from  $10^{-10}$  to  $10^{-9}$   $\text{cm}^2/\text{s}$ . These values are quite low compared to other protective clothing polymers, particularly elastomers, that have typical values in the range from

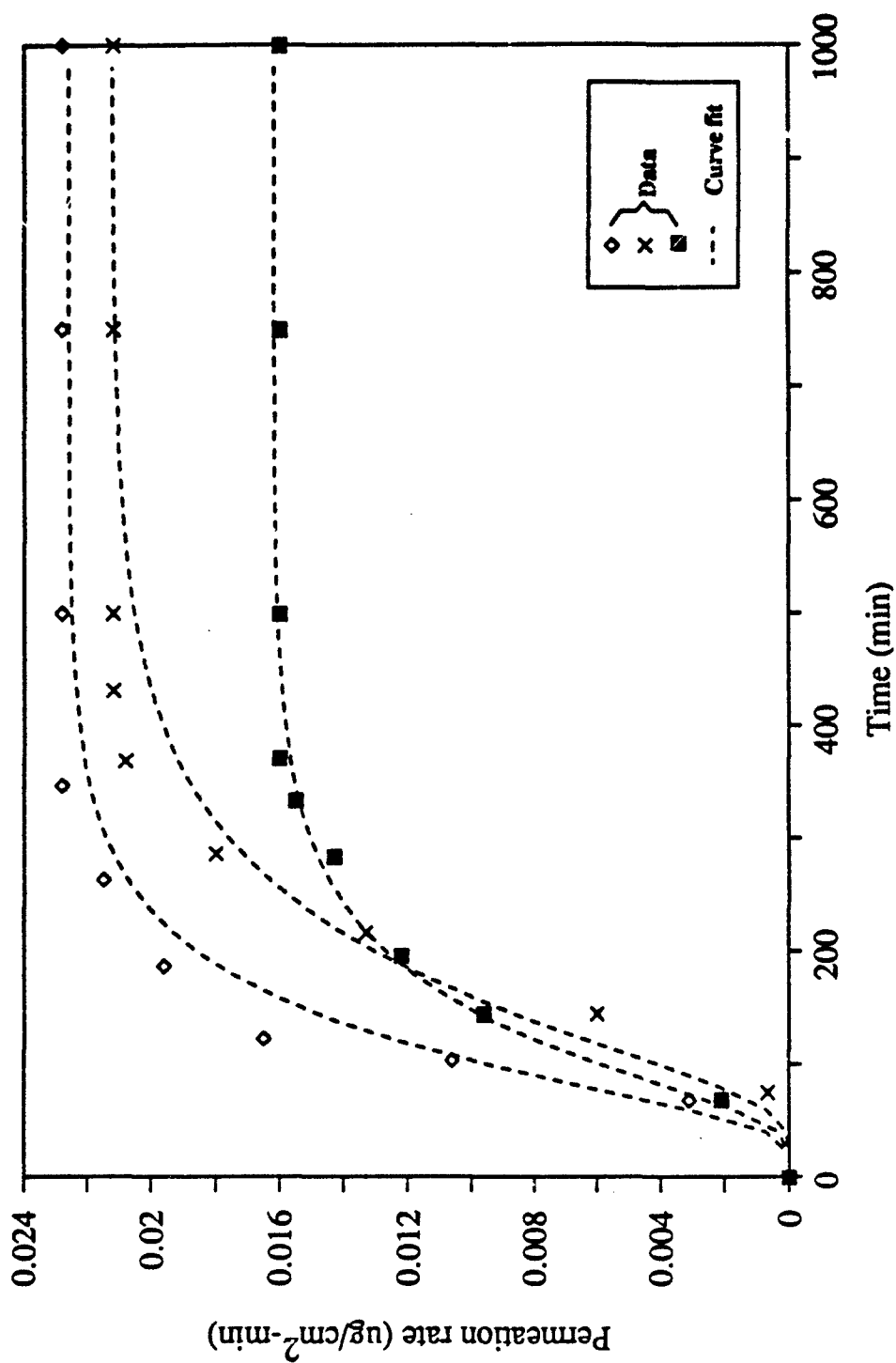


Figure 1. Fick's law curve fit for dichloromethane permeation through Challenge 5100 at 25°C. ( $D_{\text{ave}} = 1.1 \times 10^{-9} \text{ cm}^2/\text{s}$ ,  $S_{\text{ave}} = 2.4 \times 10^{-3} \text{ g/cm}^3$ ,  $l = 0.008 \text{ cm}$ )

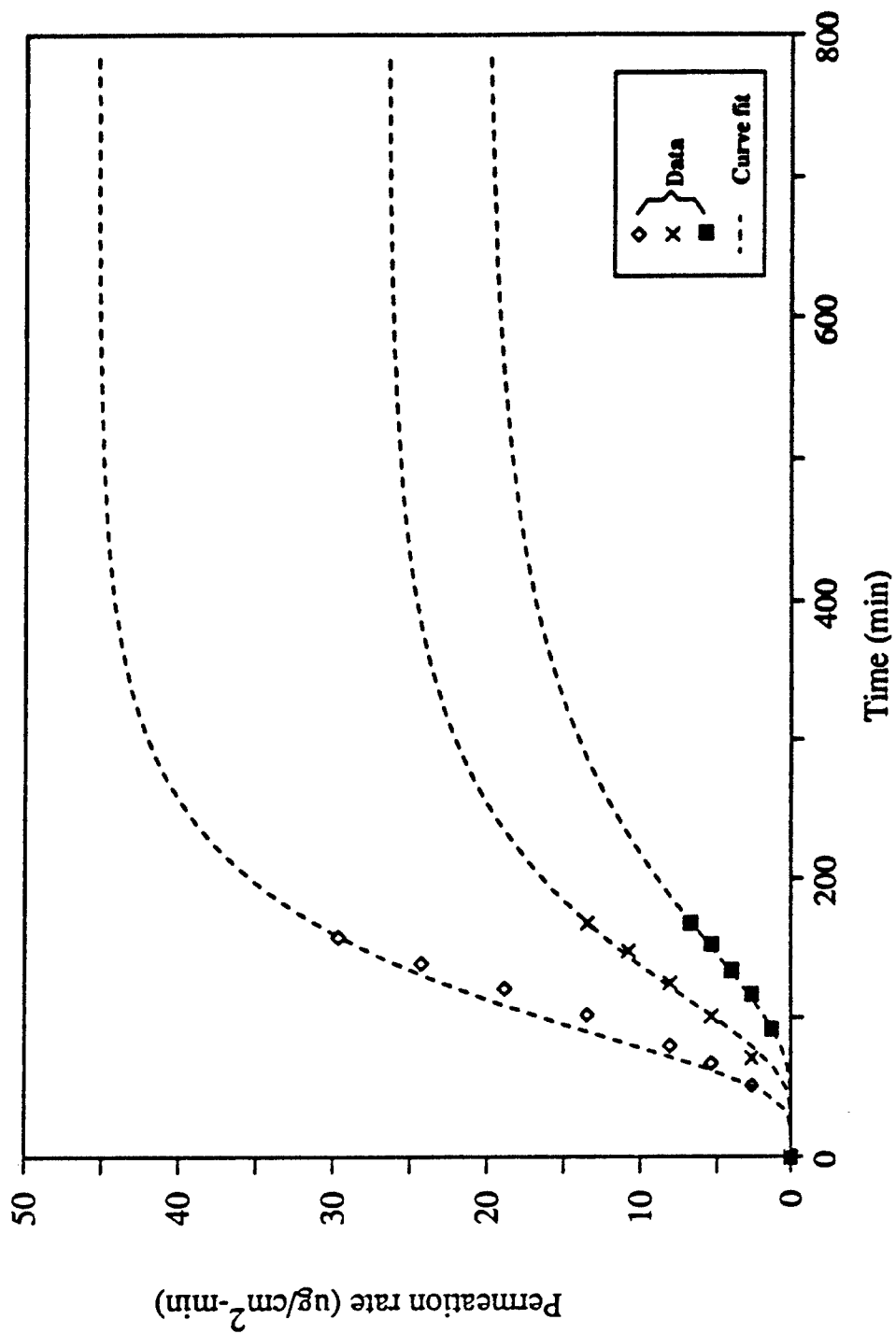


Figure 2. Fick's law curve fit for vinyl methyl ether permeation through Challenge 5200 at 25°C. ( $D_{\text{ave}} = 9.2 \times 10^{-10} \text{ cm}^2/\text{s}$ ,  $S_{\text{ave}} = 4.4 \text{ g}/\text{cm}^3$ ,  $l = 0.008 \text{ cm}$ )

TABLE 9. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE 5100 AT 25°C

| Chemical          | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|-------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Allyl Chloride    | 136         | 0.010                                                        | $2.2 \times 10^{-10}$           | $2.7 \times 10^{-10}$                      | $4.6 \times 10^{-2}$            | $3.8 \times 10^{-2}$                       | 0.073                                                                          |
|                   | 116         | 0.021                                                        | $3.6 \times 10^{-10}$           |                                            | $1.8 \times 10^{-2}$            |                                            | 0.049                                                                          |
|                   | 176         | 0.007                                                        | $2.2 \times 10^{-10}$           |                                            | $4.9 \times 10^{-2}$            |                                            | 0.070                                                                          |
| Carbon Disulfide  | 166         | 0.010                                                        | $1.8 \times 10^{-10}$           | $1.8 \times 10^{-10}$                      | $7.7 \times 10^{-3}$            | $7.7 \times 10^{-3}$                       | 0.010                                                                          |
|                   | 18          | 0.043                                                        | $3.0 \times 10^{-9}$            | $2.8 \times 10^{-9}$                       | $1.9 \times 10^{-3}$            | $2.7 \times 10^{-3}$                       | 0.043                                                                          |
|                   | 21          | 0.061                                                        | $3.9 \times 10^{-9}$            |                                            | $2.1 \times 10^{-3}$            |                                            | 0.061                                                                          |
|                   | 22          | 0.046                                                        | $1.5 \times 10^{-9}$            |                                            | $4.0 \times 10^{-3}$            |                                            | 0.046                                                                          |
| Chloroprene       | 192         | 0.003                                                        | $5.7 \times 10^{-10}$           | $5.8 \times 10^{-10}$                      | $6.2 \times 10^{-4}$            | $1.1 \times 10^{-3}$                       | 0.003                                                                          |
|                   | 184         | 0.003                                                        | $6.4 \times 10^{-10}$           |                                            | $7.0 \times 10^{-4}$            |                                            | 0.003                                                                          |
|                   | 160         | 0.009                                                        | $5.3 \times 10^{-10}$           |                                            | $2.1 \times 10^{-3}$            |                                            | 0.008                                                                          |
|                   | 21          | 0.14                                                         | $1.8 \times 10^{-9}$            | $1.6 \times 10^{-9}$                       | $9.3 \times 10^{-3}$            | $1.1 \times 10^{-2}$                       | 0.12                                                                           |
| Dichloroethylene  | 24          | 0.12                                                         | $1.3 \times 10^{-9}$            |                                            | $1.3 \times 10^{-2}$            |                                            | 0.12                                                                           |
| Dichloromethane   | 47          | 0.023                                                        | $1.3 \times 10^{-9}$            | $1.1 \times 10^{-9}$                       | $2.3 \times 10^{-3}$            | $2.4 \times 10^{-3}$                       | 0.023                                                                          |
|                   | 50          | 0.016                                                        | $1.2 \times 10^{-9}$            |                                            | $1.8 \times 10^{-3}$            |                                            | 0.016                                                                          |
|                   | 55          | 0.021                                                        | $8.9 \times 10^{-10}$           |                                            | $3.2 \times 10^{-3}$            |                                            | 0.021                                                                          |
| Ethyl Ether       | 88          | 0.006                                                        | $3.8 \times 10^{-10}$           | $3.9 \times 10^{-10}$                      | $2.4 \times 10^{-2}$            | $2.0 \times 10^{-2}$                       | 0.069                                                                          |
|                   | 84          | 0.008                                                        | $3.8 \times 10^{-10}$           |                                            | $3.1 \times 10^{-2}$            |                                            | 0.089                                                                          |
|                   | 104         | 0.001                                                        | $4.0 \times 10^{-10}$           |                                            | $4.5 \times 10^{-3}$            |                                            | 0.013                                                                          |
|                   | 148         | 0.004                                                        | $8.9 \times 10^{-10}$           | $1.3 \times 10^{-9}$                       | $1.2 \times 10^{-1}$            | $1.1 \times 10^{-1}$                       | 0.77                                                                           |
| Ethyl Vinyl Ether | 92          | 0.012                                                        | $1.7 \times 10^{-9}$            |                                            | $1.0 \times 10^{-1}$            |                                            | 1.3                                                                            |
|                   | 100         | 0.008                                                        | $1.4 \times 10^{-9}$            |                                            | $1.0 \times 10^{-1}$            |                                            | 1.1                                                                            |

(continued)

TABLE 9. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE 5100 AT 25°C

| Chemical             | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{h}$ ) | Average<br>D<br>( $\text{cm}^2/\text{h}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|----------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Methyl Bromide (Gas) | 6           | ul 0.0002                                                    | $2.5 \times 10^{-9}$            | $2.1 \times 10^{-9}$                       | $1.2 \times 10^{-5}$            | $2.9 \times 10^{-5}$                       | 0.0002                                                                         |
|                      | 11          | 0.0005                                                       | $1.8 \times 10^{-9}$            |                                            | $3.4 \times 10^{-5}$            |                                            | 0.001                                                                          |
|                      | 12          | 0.0005                                                       | $1.9 \times 10^{-9}$            |                                            | $4.1 \times 10^{-5}$            |                                            | 0.001                                                                          |
| Propylene (Gas)      | 60          | 0.0002                                                       | $1.7 \times 10^{-9}$            | $1.8 \times 10^{-9}$                       | $2.2 \times 10^{-5}$            | $2.7 \times 10^{-5}$                       | 0.0003                                                                         |
|                      | 48          | 0.001                                                        | $2.0 \times 10^{-9}$            |                                            | $3.8 \times 10^{-5}$            |                                            | 0.001                                                                          |
|                      | 76          | 0.0002                                                       | $1.7 \times 10^{-9}$            |                                            | $2.2 \times 10^{-5}$            |                                            | 0.0006                                                                         |
| Propylene Oxide      | 170         | 0.018                                                        | $2.9 \times 10^{-10}$           | $2.9 \times 10^{-10}$                      | $1.1 \times 10^{-2}$            | $1.1 \times 10^{-2}$                       | 0.024                                                                          |
| Trichloroethylene    | 143         | 0.034                                                        | $4.2 \times 10^{-10}$           | $4.1 \times 10^{-10}$                      | $1.1 \times 10^{-2}$            | $1.0 \times 10^{-2}$                       | 0.034                                                                          |
|                      | 156         | 0.027                                                        | $3.9 \times 10^{-10}$           |                                            | $9.4 \times 10^{-3}$            |                                            | 0.027                                                                          |
| Vinyl Acetate        | 74          | 0.055                                                        | $5.6 \times 10^{-10}$           | $5.1 \times 10^{-10}$                      | $1.3 \times 10^{-2}$            | $1.6 \times 10^{-2}$                       | 0.055                                                                          |
|                      | 137         | 0.062                                                        | $4.6 \times 10^{-10}$           |                                            | $1.8 \times 10^{-2}$            |                                            | 0.062                                                                          |
| Vinyl Methyl Ether   | 60          | 3.6                                                          | $7.8 \times 10^{-10}$           | $8.3 \times 10^{-10}$                      | 1.4                             | $8.3 \times 10^{-1}$                       | 8.1                                                                            |
|                      | 60          | 2.4                                                          | $7.7 \times 10^{-10}$           |                                            | $9.2 \times 10^{-1}$            |                                            | 5.3                                                                            |
|                      | 60          | 0.78                                                         | $9.3 \times 10^{-10}$           |                                            | $1.8 \times 10^{-1}$            |                                            | 1.3                                                                            |
| Vinylidene Chloride  | 52          | 0.012                                                        | $6.2 \times 10^{-10}$           | $6.3 \times 10^{-10}$                      | $7.6 \times 10^{-3}$            | $1.2 \times 10^{-2}$                       | 0.036                                                                          |
|                      | 52          | 0.011                                                        | $6.2 \times 10^{-10}$           |                                            | $7.6 \times 10^{-3}$            |                                            | 0.036                                                                          |
|                      | 48          | 0.043                                                        | $6.4 \times 10^{-10}$           |                                            | $2.2 \times 10^{-2}$            |                                            | 0.11                                                                           |

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE S200 AT 25°C

| Chemical            | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|---------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Allyl Chloride      | 68          | 0.29                                                         | $5.9 \times 10^{-10}$           | $5.3 \times 10^{-10}$                      | $1.5 \times 10^{-1}$            | $2.8 \times 10^{-1}$                       | 0.69                                                                           |
|                     | 64          | 0.15                                                         | $4.5 \times 10^{-10}$           |                                            | $2.5 \times 10^{-1}$            |                                            | 0.87                                                                           |
|                     | 36          | 0.41                                                         | $5.5 \times 10^{-10}$           |                                            | $4.2 \times 10^{-1}$            |                                            | 1.7                                                                            |
| Ammonia (Gas)       | 36          | 0.078                                                        | $2.4 \times 10^{-9}$            | $3.2 \times 10^{-9}$                       | $4.3 \times 10^{-3}$            | $4.6 \times 10^{-3}$                       | 0.076                                                                          |
|                     | 24          | 0.16                                                         | $3.6 \times 10^{-9}$            |                                            | $5.7 \times 10^{-3}$            |                                            | 0.16                                                                           |
|                     | 32          | 0.11                                                         | $3.6 \times 10^{-9}$            |                                            | $3.7 \times 10^{-3}$            |                                            | 0.099                                                                          |
|                     | 32          | $\mu\text{L}$ 0.12                                           | $1.7 \times 10^{-9}$            | $1.8 \times 10^{-9}$                       | $1.4 \times 10^{-2}$            | $1.6 \times 10^{-2}$                       | 0.17                                                                           |
|                     | 32          | 0.22                                                         | $1.8 \times 10^{-9}$            |                                            | $2.2 \times 10^{-2}$            |                                            | 0.29                                                                           |
|                     | 32          | 0.11                                                         | $1.9 \times 10^{-9}$            |                                            | $1.3 \times 10^{-2}$            |                                            | 0.19                                                                           |
| Bromochloromethane  | 93          | 0.019                                                        | $6.2 \times 10^{-10}$           | $5.8 \times 10^{-10}$                      | $5.0 \times 10^{-3}$            | $5.5 \times 10^{-3}$                       | 0.023                                                                          |
|                     | 109         | 0.015                                                        | $5.2 \times 10^{-10}$           |                                            | $5.0 \times 10^{-3}$            |                                            | 0.019                                                                          |
|                     | 93          | 0.023                                                        | $6.0 \times 10^{-10}$           |                                            | $6.4 \times 10^{-3}$            |                                            | 0.029                                                                          |
| Bromoethane         | 144         | 0.024                                                        | $2.9 \times 10^{-10}$           | $4.1 \times 10^{-10}$                      | $1.5 \times 10^{-1}$            | $8.9 \times 10^{-2}$                       | 0.032                                                                          |
|                     | 84          | 0.032                                                        | $5.8 \times 10^{-10}$           |                                            | $2.8 \times 10^{-2}$            |                                            | 0.12                                                                           |
|                     | 132         | 0.027                                                        | $3.5 \times 10^{-10}$           |                                            | $8.8 \times 10^{-2}$            |                                            | 0.23                                                                           |
| 1,3-Butadiene (Gas) | 24          | $\mu\text{L}$ 0.13                                           | $1.1 \times 10^{-9}$            | $1.2 \times 10^{-9}$                       | $2.4 \times 10^{-2}$            | $1.3 \times 10^{-2}$                       | 0.20                                                                           |
|                     | 24          | 0.070                                                        | $1.1 \times 10^{-9}$            |                                            | $1.1 \times 10^{-2}$            |                                            | 0.097                                                                          |
|                     | 24          | 0.038                                                        | $1.3 \times 10^{-9}$            |                                            | $4.9 \times 10^{-3}$            |                                            | 0.048                                                                          |
|                     | 8           | 0.024                                                        | $9.8 \times 10^{-10}$           | $1.0 \times 10^{-9}$                       | $4.1 \times 10^{-3}$            | $6.2 \times 10^{-3}$                       | 0.030                                                                          |
|                     | 4           | 0.038                                                        | $9.5 \times 10^{-10}$           |                                            | $6.8 \times 10^{-3}$            |                                            | 0.048                                                                          |
|                     | 4           | 0.055                                                        | $1.1 \times 10^{-9}$            |                                            | $7.6 \times 10^{-3}$            |                                            | 0.062                                                                          |

(continued)

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE 5200 AT 25°C

| Chemical                   | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|----------------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| 1-Chloropropane            | 269         | 0.24                                                         | $2.1 \times 10^{-10}$           | $2.4 \times 10^{-10}$                      | $8.6 \times 10^{-1}$            | $6.8 \times 10^{-1}$                       | 1.3                                                                            |
|                            | 225         | 0.33                                                         | $2.7 \times 10^{-10}$           |                                            | $4.9 \times 10^{-1}$            |                                            | 0.98                                                                           |
| cis-1,2-Dichloroethylene   | 56          | 0.22                                                         | $4.4 \times 10^{-10}$           | $3.6 \times 10^{-10}$                      | $5.3 \times 10^{-1}$            | $7.2 \times 10^{-1}$                       | 1.7                                                                            |
|                            | 80          | 0.097                                                        | $2.9 \times 10^{-10}$           |                                            | $9.4 \times 10^{-1}$            |                                            | 2.0                                                                            |
|                            | 72          | 0.15                                                         | $3.4 \times 10^{-10}$           |                                            | $6.8 \times 10^{-1}$            |                                            | 1.7                                                                            |
| trans-1,2-Dichloroethylene | 19          | 1.4                                                          | $9.8 \times 10^{-10}$           | $1.1 \times 10^{-9}$                       | $2.2 \times 10^{-1}$            | $2.0 \times 10^{-1}$                       | 1.6                                                                            |
|                            | 19          | 1.5                                                          | $1.1 \times 10^{-9}$            |                                            | $2.0 \times 10^{-1}$            |                                            | 1.6                                                                            |
|                            | 19          | 1.3                                                          | $1.1 \times 10^{-9}$            |                                            | $1.7 \times 10^{-1}$            |                                            | 1.4                                                                            |
| Dichloromethane            | 68          | 0.23                                                         | $5.4 \times 10^{-10}$           | $5.7 \times 10^{-10}$                      | $2.2 \times 10^{-1}$            | $2.3 \times 10^{-1}$                       | 0.90                                                                           |
|                            | 52          | 0.37                                                         | $6.7 \times 10^{-10}$           |                                            | $1.8 \times 10^{-1}$            |                                            | 0.94                                                                           |
|                            | 72          | 0.19                                                         | $4.9 \times 10^{-10}$           |                                            | $2.6 \times 10^{-1}$            |                                            | 0.95                                                                           |
| (27°C)                     | 84          | 4.0                                                          | $4.9 \times 10^{-10}$           | $5.1 \times 10^{-10}$                      | 5.8                             | 5.3                                        | 21.1                                                                           |
|                            | 88          | 3.0                                                          | $5.7 \times 10^{-10}$           |                                            | 3.5                             |                                            | 14.9                                                                           |
|                            | 76          | 4.0                                                          | $4.5 \times 10^{-10}$           |                                            | 6.7                             |                                            | 22.5                                                                           |
| Dimethyl Sulfide           | 116         | 0.0005                                                       | $3.5 \times 10^{-10}$           | $4.8 \times 10^{-10}$                      | 10.2                            | 4.8                                        | 26.1                                                                           |
|                            | 76          | 0.0005                                                       | $4.8 \times 10^{-10}$           |                                            | 3.0                             |                                            | 10.5                                                                           |
|                            | 92          | 0.0005                                                       | $6.0 \times 10^{-10}$           |                                            | 1.3                             |                                            | 5.8                                                                            |

(continued)

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE S200 AT 25°C

| Chemical               | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|------------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Ethylene Oxide (Gas)   | 68          | 0.83                                                         | $7.1 \times 10^{-10}$           | $9.0 \times 10^{-10}$                      | $4.1 \times 10^{-1}$            | $2.7 \times 10^{-1}$                       | 2.0                                                                            |
|                        | 60          | 0.85                                                         | $7.8 \times 10^{-10}$           |                                            | $3.3 \times 10^{-1}$            |                                            | 1.8                                                                            |
|                        | 44          | 0.50                                                         | $1.2 \times 10^{-9}$            |                                            | $7.2 \times 10^{-2}$            |                                            | 0.66                                                                           |
| Ethyl Ether            | 20          | 0.14                                                         | $1.7 \times 10^{-9}$            | $1.5 \times 10^{-9}$                       | $1.1 \times 10^{-2}$            | $1.4 \times 10^{-2}$                       | 0.14                                                                           |
|                        | 24          | 0.17                                                         | $1.5 \times 10^{-9}$            |                                            | $1.9 \times 10^{-2}$            |                                            | 0.14                                                                           |
|                        | 32          | 0.12                                                         | $1.4 \times 10^{-9}$            |                                            | $1.2 \times 10^{-2}$            |                                            | 0.13                                                                           |
|                        | 104         | 0.41                                                         | $3.8 \times 10^{-10}$           | $3.4 \times 10^{-10}$                      | $1.3 \times 10^{-1}$            | $1.4 \times 10^{-1}$                       | 0.36                                                                           |
| Ethyl Vinyl Ether      | 136         | 0.30                                                         | $3.2 \times 10^{-10}$           |                                            | $1.3 \times 10^{-1}$            |                                            | 0.31                                                                           |
|                        | 140         | 0.42                                                         | $3.3 \times 10^{-10}$           |                                            | $1.5 \times 10^{-1}$            |                                            | 0.65                                                                           |
|                        | 40          | 0.39                                                         | $5.0 \times 10^{-10}$           | $5.3 \times 10^{-10}$                      | $4.8 \times 10^{-1}$            | $6.4 \times 10^{-1}$                       | 1.8                                                                            |
|                        | 8           | 0.55                                                         | $4.6 \times 10^{-10}$           |                                            | $7.9 \times 10^{-1}$            |                                            | 2.7                                                                            |
| Hydrogen Sulfide (Gas) | 20          | 1.1                                                          | $6.4 \times 10^{-10}$           |                                            | $6.6 \times 10^{-1}$            |                                            | 3.2                                                                            |
|                        | 8           | $\mu\text{L}$ 0.0055                                         | $4.7 \times 10^{-9}$            | $5.0 \times 10^{-9}$                       | $1.5 \times 10^{-4}$            | $1.7 \times 10^{-4}$                       | 0.0054                                                                         |
|                        | 8           | 0.0077                                                       | $6.0 \times 10^{-9}$            |                                            | $1.7 \times 10^{-4}$            |                                            | 0.0076                                                                         |
| Isoprene               | 8           | 0.0068                                                       | $4.3 \times 10^{-9}$            |                                            | $2.0 \times 10^{-4}$            |                                            | 0.0066                                                                         |
|                        | 8           | 0.062                                                        | $4.2 \times 10^{-9}$            | $4.6 \times 10^{-9}$                       | $8.6 \times 10^{-2}$            | $5.1 \times 10^{-2}$                       | 2.7                                                                            |
|                        | 8           | 0.13                                                         | $8.2 \times 10^{-9}$            |                                            | $3.2 \times 10^{-2}$            |                                            | 1.9                                                                            |
| Methyl Acetate         | 12          | 0.36                                                         | $1.5 \times 10^{-9}$            |                                            | $3.4 \times 10^{-2}$            |                                            | 3.8                                                                            |
|                        | 84          | 0.007                                                        | $4.8 \times 10^{-10}$           | $5.0 \times 10^{-10}$                      | $1.2 \times 10^{-2}$            | $8.7 \times 10^{-3}$                       | 0.040                                                                          |
|                        | 144         | 0.004                                                        | $4.2 \times 10^{-10}$           |                                            | $1.0 \times 10^{-2}$            |                                            | 0.028                                                                          |
|                        | 108         | 0.005                                                        | $6.0 \times 10^{-10}$           |                                            | $4.2 \times 10^{-3}$            |                                            | 0.018                                                                          |

(continued)

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE 5200 AT 25°C

| Chemical               | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|------------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Methyl Bromide (Gas)   | 20          | $\mu\text{L}$ 0.005                                          | $1.7 \times 10^{-9}$            | $1.7 \times 10^{-9}$                       | $4.1 \times 10^{-4}$            | $5.3 \times 10^{-4}$                       | 0.006                                                                          |
|                        | 20          | 0.007                                                        | $1.9 \times 10^{-9}$            |                                            | $5.6 \times 10^{-4}$            |                                            | 0.008                                                                          |
|                        | 20          | 0.007                                                        | $1.5 \times 10^{-9}$            |                                            | $6.3 \times 10^{-4}$            |                                            | 0.007                                                                          |
|                        | 20          | 0.037                                                        | $2.3 \times 10^{-9}$            | $2.2 \times 10^{-9}$                       | $2.5 \times 10^{-3}$            | $2.5 \times 10^{-3}$                       | 0.042                                                                          |
|                        | 20          | 0.037                                                        | $2.1 \times 10^{-9}$            |                                            | $2.6 \times 10^{-3}$            |                                            | 0.041                                                                          |
|                        | 20          | 0.031                                                        | $2.1 \times 10^{-9}$            |                                            | $2.3 \times 10^{-3}$            |                                            | 0.036                                                                          |
| Methyl Iodide          | 32          | 27.0                                                         | $1.0 \times 10^{-9}$            | $8.2 \times 10^{-10}$                      | 4.8                             | 5.1                                        | 35.3                                                                           |
|                        | 32          | 10.8                                                         | $6.7 \times 10^{-10}$           |                                            | 6.0                             |                                            | 21.7                                                                           |
|                        | 32          | 13.9                                                         | $8.0 \times 10^{-10}$           |                                            | 4.6                             |                                            | 43.4                                                                           |
| Methyl Isocyanate      | 96          | 0.021                                                        | $2.1 \times 10^{-9}$            | $2.0 \times 10^{-9}$                       | $1.4 \times 10^{-3}$            | $1.4 \times 10^{-3}$                       | 0.022                                                                          |
|                        | 72          | 0.019                                                        | $2.0 \times 10^{-9}$            |                                            | $1.3 \times 10^{-3}$            |                                            | 0.019                                                                          |
|                        | 108         | 0.021                                                        | $1.9 \times 10^{-9}$            |                                            | $1.6 \times 10^{-3}$            |                                            | 0.023                                                                          |
| Nitrogen Dioxide (Gas) | 4           | $\mu\text{L}$ 5.3                                            | $5.5 \times 10^{-9}$            | $4.0 \times 10^{-9}$                       | $1.2 \times 10^{-1}$            | $1.8 \times 10^{-1}$                       | 5.0                                                                            |
|                        | 4           | 6.4                                                          | $3.3 \times 10^{-9}$            |                                            | $2.7 \times 10^{-1}$            |                                            | 6.7                                                                            |
|                        | 4           | 3.3                                                          | $3.1 \times 10^{-9}$            |                                            | $1.4 \times 10^{-1}$            |                                            | 3.3                                                                            |
| Propylene Oxide        | 96          | 0.00008                                                      | $4.2 \times 10^{-10}$           | $5.3 \times 10^{-10}$                      | $2.1 \times 10^{-4}$            | $1.3 \times 10^{-4}$                       | 0.00064                                                                        |
|                        | 96          | 0.00007                                                      | $5.4 \times 10^{-10}$           |                                            | $6.1 \times 10^{-5}$            |                                            | 0.00025                                                                        |
|                        | 76          | 0.0002                                                       | $6.2 \times 10^{-10}$           |                                            | $1.3 \times 10^{-4}$            |                                            | 0.00061                                                                        |
| Trichloroethylene      | 52          | 0.20                                                         | $4.3 \times 10^{-10}$           | $3.6 \times 10^{-10}$                      | $3.5 \times 10^{-1}$            | $7.2 \times 10^{-1}$                       | 1.1                                                                            |
|                        | 56          | 0.16                                                         | $2.9 \times 10^{-10}$           |                                            | $6.2 \times 10^{-1}$            |                                            | 1.3                                                                            |
|                        | 40          | 0.22                                                         | $3.6 \times 10^{-10}$           |                                            | 1.2                             |                                            | 3.2                                                                            |

(continued)

TABLE 10. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE 5200 AT 25°C

| Chemical             | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|----------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Vinyl Acetate        | 65          | 50.0                                                         | $4.9 \times 10^{-10}$           | $4.7 \times 10^{-10}$                      | 74.8                            | 80.3                                       | 271.1                                                                          |
|                      | 85          | 35.0                                                         | $3.8 \times 10^{-10}$           |                                            | 136.7                           |                                            | 392.9                                                                          |
|                      | 69          | 29.0                                                         | $5.4 \times 10^{-10}$           |                                            | 29.3                            |                                            | 117.3                                                                          |
| Vinyl Chloride (Gas) | 72          | 25.2                                                         | $2.2 \times 10^{-10}$           | $2.2 \times 10^{-10}$                      | 2354.1                          | 1084.9                                     | 3824.4                                                                         |
|                      | 132         | 2.2                                                          | $2.2 \times 10^{-10}$           |                                            | 203.2                           |                                            | 330.1                                                                          |
|                      | 124         | 6.4                                                          | $2.2 \times 10^{-10}$           |                                            | 697.3                           |                                            | 1045.9                                                                         |
|                      | 12          | $\mu\text{L}$ 0.15                                           | $2.7 \times 10^{-9}$            | $1.9 \times 10^{-9}$                       | $9.0 \times 10^{-1}$            | 1.4                                        | 18.1                                                                           |
| Vinyl Methyl Ether   | 12          | 0.16                                                         | $1.7 \times 10^{-9}$            |                                            | 1.6                             |                                            | 20.5                                                                           |
|                      | 12          | 0.12                                                         | $1.4 \times 10^{-9}$            |                                            | 1.7                             |                                            | 17.6                                                                           |
|                      | 36          | 7.7                                                          | $6.8 \times 10^{-10}$           | $9.2 \times 10^{-10}$                      | 4.0                             | 4.4                                        | 19.8                                                                           |
|                      | 24          | 35.1                                                         | $1.2 \times 10^{-9}$            |                                            | 5.1                             |                                            | 45.3                                                                           |
| Vinylidene Chloride  | 24          | 14.6                                                         | $8.9 \times 10^{-10}$           |                                            | 4.0                             |                                            | 26.5                                                                           |
|                      | 120         | 1.5                                                          | $5.0 \times 10^{-10}$           | $4.5 \times 10^{-10}$                      | 2.1                             | 2.6                                        | 7.7                                                                            |
|                      | 120         | 0.88                                                         | $4.0 \times 10^{-10}$           |                                            | 4.0                             |                                            | 11.6                                                                           |
|                      | 132         | 0.89                                                         | $4.4 \times 10^{-10}$           |                                            | 1.8                             |                                            | 5.7                                                                            |
|                      | 64          | 0.057                                                        | $5.0 \times 10^{-10}$           | $5.4 \times 10^{-10}$                      | $8.3 \times 10^{-2}$            | $9.0 \times 10^{-2}$                       | 0.31                                                                           |
|                      | 60          | 0.090                                                        | $6.0 \times 10^{-10}$           |                                            | $7.0 \times 10^{-2}$            |                                            | 0.30                                                                           |
|                      | 60          | 0.10                                                         | $5.2 \times 10^{-10}$           |                                            | $1.2 \times 10^{-1}$            |                                            | 0.48                                                                           |

TABLE 11 SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE 5200 AT 35°C

| Chemical            | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|---------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Acetone             | 32          | 0.016                                                        | $7.5 \times 10^{-10}$           | $6.6 \times 10^{-10}$                      | $4.4 \times 10^{-3}$            | $5.3 \times 10^{-3}$                       | 0.025                                                                          |
|                     | 80          | 0.014                                                        | $6.1 \times 10^{-10}$           |                                            | $5.8 \times 10^{-3}$            |                                            | 0.026                                                                          |
|                     | 88          | 0.014                                                        | $6.1 \times 10^{-10}$           |                                            | $5.8 \times 10^{-3}$            |                                            | 0.026                                                                          |
| Acrylonitrile       | 93          | 0.085                                                        | $7.0 \times 10^{-10}$           | $5.8 \times 10^{-10}$                      | $4.5 \times 10^{-2}$            | $6.0 \times 10^{-2}$                       | 0.24                                                                           |
|                     | 117         | 0.067                                                        | $5.4 \times 10^{-10}$           |                                            | $6.2 \times 10^{-2}$            |                                            | 0.25                                                                           |
|                     | 121         | 0.060                                                        | $5.0 \times 10^{-10}$           |                                            | $7.3 \times 10^{-2}$            |                                            | 0.28                                                                           |
|                     |             |                                                              |                                 |                                            |                                 |                                            |                                                                                |
| Carbon Disulfide    | 12          | 0.61                                                         | $2.1 \times 10^{-9}$            | $2.2 \times 10^{-9}$                       | $4.0 \times 10^{-2}$            | $3.3 \times 10^{-2}$                       | 0.62                                                                           |
|                     | 16          | 0.64                                                         | $2.5 \times 10^{-9}$            |                                            | $3.4 \times 10^{-2}$            |                                            | 0.65                                                                           |
|                     | 20          | 0.44                                                         | $2.0 \times 10^{-9}$            |                                            | $2.6 \times 10^{-2}$            |                                            | 0.38                                                                           |
|                     |             |                                                              |                                 |                                            |                                 |                                            |                                                                                |
| Dichloromethane     | 44          | 0.22                                                         | $1.1 \times 10^{-9}$            | $1.2 \times 10^{-9}$                       | $3.7 \times 10^{-2}$            | $3.1 \times 10^{-2}$                       | 0.32                                                                           |
|                     | 40          | 0.18                                                         | $1.3 \times 10^{-9}$            |                                            | $2.4 \times 10^{-2}$            |                                            | 0.24                                                                           |
|                     | 44          | 0.17                                                         | $1.1 \times 10^{-9}$            |                                            | $3.3 \times 10^{-2}$            |                                            | 0.28                                                                           |
|                     |             |                                                              |                                 |                                            |                                 |                                            |                                                                                |
| Ethyl Acetate       | 152         | 0.004                                                        | $5.6 \times 10^{-10}$           | $5.8 \times 10^{-10}$                      | $1.3 \times 10^{-3}$            | $1.2 \times 10^{-3}$                       | 0.005                                                                          |
|                     | 204         | 0.003                                                        | $4.6 \times 10^{-10}$           |                                            | $1.5 \times 10^{-3}$            |                                            | 0.005                                                                          |
|                     | 180         | 0.004                                                        | $7.3 \times 10^{-10}$           |                                            | $8.0 \times 10^{-4}$            |                                            | 0.004                                                                          |
| Propylene Oxide     | 88          | 0.060                                                        | $7.8 \times 10^{-10}$           | $6.2 \times 10^{-10}$                      | $2.3 \times 10^{-2}$            | $4.6 \times 10^{-2}$                       | 0.13                                                                           |
|                     | 124         | 0.040                                                        | $4.5 \times 10^{-10}$           |                                            | $9.5 \times 10^{-2}$            |                                            | 0.32                                                                           |
|                     | 120         | 0.030                                                        | $6.4 \times 10^{-10}$           |                                            | $1.9 \times 10^{-2}$            |                                            | 0.091                                                                          |
|                     |             |                                                              |                                 |                                            |                                 |                                            |                                                                                |
| Tetrachloroethylene | 236         | 0.058                                                        | $6.0 \times 10^{-10}$           | $6.8 \times 10^{-10}$                      | $2.3 \times 10^{-2}$            | $1.9 \times 10^{-2}$                       | 0.10                                                                           |
|                     | 236         | 0.072                                                        | $8.5 \times 10^{-10}$           |                                            | $1.6 \times 10^{-2}$            |                                            | 0.10                                                                           |
|                     | 236         | 0.043                                                        | $6.0 \times 10^{-10}$           |                                            | $1.7 \times 10^{-2}$            |                                            | 0.076                                                                          |

(continued)

TABLE 11. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE 5200 AT 35°C

| Chemical          | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|-------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Trichloroethylene | 68          | 0.33                                                         | $3.4 \times 10^{-10}$           | $3.9 \times 10^{-10}$                      | 1.6                             | 1.2                                        | 4.2                                                                            |
|                   | 84          | 0.48                                                         | $3.8 \times 10^{-10}$           |                                            | 1.2                             |                                            | 3.5                                                                            |
|                   | 76          | 0.35                                                         | $4.6 \times 10^{-10}$           |                                            | $6.9 \times 10^{-1}$            |                                            | 2.4                                                                            |
| Vinyl Acetate     | 52          | 0.64                                                         | $7.9 \times 10^{-10}$           | $7.3 \times 10^{-10}$                      | $1.6 \times 10^{-1}$            | $1.7 \times 10^{-1}$                       | 0.95                                                                           |
|                   | 52          | 0.84                                                         | $7.7 \times 10^{-10}$           |                                            | $2.3 \times 10^{-1}$            |                                            | 1.3                                                                            |
|                   | 76          | 0.36                                                         | $6.2 \times 10^{-10}$           |                                            | $1.2 \times 10^{-1}$            |                                            | 0.56                                                                           |

TABLE 12. SOLUBILITIES AND DIFFUSION COEFFICIENTS FOR  
CHALLENGE 5200 AT 40°C

| Chemical            | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | Average<br>D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Average<br>S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|---------------------|-------------|--------------------------------------------------------------|---------------------------------|--------------------------------------------|---------------------------------|--------------------------------------------|--------------------------------------------------------------------------------|
| Allyl Chloride      | 64          | 0.55                                                         | $1.0 \times 10^{-9}$            | $8.6 \times 10^{-10}$                      | $1.1 \times 10^{-1}$            | $1.4 \times 10^{-1}$                       | 0.86                                                                           |
|                     | 88          | 0.52                                                         | $8.3 \times 10^{-10}$           |                                            | $1.5 \times 10^{-1}$            |                                            | 0.95                                                                           |
|                     | 84          | 0.47                                                         | $7.6 \times 10^{-10}$           |                                            | $1.6 \times 10^{-1}$            |                                            | 0.90                                                                           |
| Epichlorohydrin     | 132         | 0.25                                                         | $3.7 \times 10^{-10}$           | $3.4 \times 10^{-10}$                      | 1.2                             | 1.3                                        | 3.2                                                                            |
|                     | 140         | 0.23                                                         | $3.7 \times 10^{-10}$           |                                            | $9.1 \times 10^{-1}$            |                                            | 2.5                                                                            |
|                     | 176         | 0.19                                                         | $2.8 \times 10^{-10}$           |                                            | 1.9                             |                                            | 3.7                                                                            |
|                     |             |                                                              |                                 |                                            |                                 |                                            |                                                                                |
| Ethyl Chloroformate | 116         | 0.19                                                         | $4.4 \times 10^{-10}$           | $4.9 \times 10^{-10}$                      | $3.1 \times 10^{-1}$            | $2.5 \times 10^{-1}$                       | 1.0                                                                            |
|                     | 104         | 0.22                                                         | $5.1 \times 10^{-10}$           |                                            | $2.2 \times 10^{-1}$            |                                            | 0.84                                                                           |
|                     | 104         | 0.21                                                         | $5.1 \times 10^{-10}$           |                                            | $2.2 \times 10^{-1}$            |                                            | 0.84                                                                           |
|                     |             |                                                              |                                 |                                            |                                 |                                            |                                                                                |
| Dichloromethane     | 28          | 0.30                                                         | $1.6 \times 10^{-9}$            | $1.6 \times 10^{-9}$                       | $3.0 \times 10^{-2}$            | $2.7 \times 10^{-2}$                       | 0.35                                                                           |
|                     | 32          | 0.23                                                         | $1.5 \times 10^{-9}$            |                                            | $2.2 \times 10^{-2}$            |                                            | 0.25                                                                           |
|                     | 28          | 0.27                                                         | $1.6 \times 10^{-9}$            |                                            | $2.8 \times 10^{-2}$            |                                            | 0.33                                                                           |
|                     |             |                                                              |                                 |                                            |                                 |                                            |                                                                                |
| Trichloroethylene   | 68          | 0.45                                                         | $5.1 \times 10^{-10}$           | $4.8 \times 10^{-10}$                      | $1.2 \times 10^{-1}$            | $1.3 \times 10^{-1}$                       | 0.46                                                                           |
|                     | 80          | 0.57                                                         | $5.1 \times 10^{-10}$           |                                            | $1.4 \times 10^{-1}$            |                                            | 0.54                                                                           |
|                     | 96          | 0.41                                                         | $4.1 \times 10^{-10}$           |                                            | $1.4 \times 10^{-1}$            |                                            | 0.42                                                                           |
| Vinyl Acetate       | 68          | 0.24                                                         | $6.7 \times 10^{-10}$           | $6.5 \times 10^{-10}$                      | $4.6 \times 10^{-2}$            | $4.9 \times 10^{-2}$                       | 0.23                                                                           |
|                     | 64          | 0.34                                                         | $6.8 \times 10^{-10}$           |                                            | $6.0 \times 10^{-2}$            |                                            | 0.31                                                                           |
|                     | 76          | 0.18                                                         | $6.0 \times 10^{-10}$           |                                            | $4.0 \times 10^{-2}$            |                                            | 0.18                                                                           |

$10^{-8}$  to  $10^{-6}$  cm<sup>2</sup>/s. The range of values for the Challenge materials is fairly narrow but this is not unexpected because most of the chemicals analyzed are similar in size with molecular weights ranging from 50 to 150 daltons. The S values ranged from 0.0001 to 10 g/cm<sup>3</sup>, with most values within 0.001 to 0.1 g/cm<sup>3</sup>. Again, the majority of the S values are quite low compared to typical solubilities of these chemicals in rubber materials. Several S values, however, are surprisingly high (e.g., >1.0 g/cm<sup>3</sup>) and raise questions regarding the Fick's law curve fitting technique as well as the accuracy of certain data sets. Possibly some of the S values should be confirmed by long-term immersion tests.

An important consequence of the generally low D and S values (and the correspondingly low permeation rates), is that the chemicals permeate the fluoropolymer material with minimal effects on the material (e.g, swelling) so that the behavior can be accurately described by an ideal Fickian solution-diffusion model.

#### 4.1.2 Temperature Dependence

Knowledge of the effect of temperature on the permeation resistance of a protective material is critical, particularly regarding chemical protective clothing. Although permeation resistance is generally evaluated at 20-25°C, the clothing when worn will be exposed to body temperatures and environments that exceed 25°C. Some polymeric materials are relatively unaffected by temperature changes, while many are strongly affected and show a great decrease in barrier properties with small increases in temperature. Typically, the temperature dependence shows an Arrhenius relationship or exponential change with temperature. As reported in Table 2, permeation tests were conducted for several chemicals at 30°, 35°, and 40°C. The results of these tests are summarized in Table 13 using the average breakthrough times and the average reported permeation rates. Again, because of differences in MDKs and test durations, it is difficult to directly compare many of these results. General observations on the data follow. Some chemicals that were not detected to breakthrough at 25°C were found to permeate at the higher temperatures (e.g., acetone, ethyl acetate, ethyl chloroformate). There are several cases in which the breakthrough times are shorter and permeation rates higher as temperature was increased. However, there are also several cases in which the reported breakthrough times are longer and the permeation rates are lower at the higher temperatures. We know of no explanation for such data and recommend that the tests be repeated.

The effect of temperature on the permeation behavior can also be evaluated through comparison of the D, S, and calculated steady-state permeation rate values listed in Tables 9 through 12. Some of these values may eliminate some of the data set/test method inconsistencies. Table 14 summarizes the reported permeation data and the Fick's law parameters for the 6 chemicals that were tested at three or more temperatures. These data also indicate several temperature effects: in some cases the Fick's law parameters and calculated steady-state permeation rates increase with increasing temperature, several show little or no effect, and one (vinyl acetate) shows improved permeation resistance with increasing temperature. These results are illustrated in Figures 3 through 5, in which the logarithm of the values for D (Figure 3), S (Figure 4), and calculated steady-state rate (Figure 5) are plotted versus the inverse of the absolute temperature (K). If the data followed

TABLE 13. COMPARISON OF CHALLENGE 5200 PERMEATION DATA AS A FUNCTION OF TEMPERATURE

| Chemical               | 25°C   |               |                                                               |        | 30°C          |                                                             |        |               | 35°C                                                        |        |               |                                                             | 40°C |               |                                                             |                                                             |
|------------------------|--------|---------------|---------------------------------------------------------------|--------|---------------|-------------------------------------------------------------|--------|---------------|-------------------------------------------------------------|--------|---------------|-------------------------------------------------------------|------|---------------|-------------------------------------------------------------|-------------------------------------------------------------|
|                        | MDR*   | Ave. BT (min) | Ave. reported rate** ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | MDR    | Ave. BT (min) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | MDR    | Ave. BT (min) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | MDR    | Ave. BT (min) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | MDR  | Ave. BT (min) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
| Acetone                | 0.040  | >180          |                                                               | 0.0004 | >210          |                                                             | 0.0004 | 67            | 0.015 (4hr)                                                 |        |               |                                                             |      |               |                                                             |                                                             |
| Acrolein               |        |               |                                                               | 0.0077 | 56            | 0.095 (nc)                                                  | 0.0018 | 23            | 0.068 (4hr)                                                 |        |               |                                                             |      |               |                                                             |                                                             |
| Acrylonitrile          |        |               |                                                               | 0.0017 | 76            | 0.028 (nc)                                                  | 0.0086 | 110           | 0.071 (3hr)                                                 |        |               |                                                             |      |               |                                                             |                                                             |
| Allyl chloride         | 0.0019 | 56            | 0.28 (3hr)                                                    | 0.0031 | 56            | 0.035 (nc)                                                  | 0.0080 | 236           | 0.53 (7hr)                                                  | 0.0043 | 79            | 0.51 (3hr)                                                  |      |               |                                                             |                                                             |
| Carbon disulfide       | 0.0006 | 20            | 0.034 (3hr)                                                   | 0.0006 | 15            | 0.23 (nc)                                                   | 0.0006 | 16            | 0.56 (3hr)                                                  |        |               |                                                             |      |               |                                                             |                                                             |
| Dichloromethane (27°C) | 0.0003 | 64            | 0.26 (3hr)                                                    | 0.0007 | 43            | 0.037 (nc)                                                  | 0.0027 | 43            | 0.19 (3hr)                                                  | 0.0021 | 29            | 0.27 (3hr)                                                  |      |               |                                                             |                                                             |
| Diethylamine           |        |               |                                                               |        |               |                                                             |        |               |                                                             |        |               |                                                             |      |               |                                                             |                                                             |
| Dimethylformamide      |        |               |                                                               | 0.0024 | >1182         |                                                             | 0.0041 | >180          |                                                             |        |               |                                                             |      |               |                                                             |                                                             |
| Ethyl acetate          | 0.0007 | >180          |                                                               | 0.0012 | >240          |                                                             | 0.0006 | >180          |                                                             |        |               |                                                             |      |               |                                                             |                                                             |
| Ethyl chloroformate    | 0.018  | >180          |                                                               | 0.0014 | >300          |                                                             | 0.0007 | 179           | 0.003 (6hr)                                                 |        |               |                                                             |      |               |                                                             |                                                             |
| Hexane                 | 0.0070 | >300          |                                                               |        |               |                                                             |        |               |                                                             | 0.0009 | 108           | 0.26 (3hr)                                                  |      |               |                                                             |                                                             |
| Methanol               |        |               |                                                               | 0.0070 | >300          |                                                             | 0.0014 | >180          |                                                             |        |               |                                                             |      |               |                                                             |                                                             |
| Nitrobenzene           |        |               |                                                               | 0.0065 | >300          |                                                             | 0.016  | 88            | 0.063 (nc)                                                  |        |               |                                                             |      |               |                                                             |                                                             |
| Propylene oxide        |        |               |                                                               | 0.0099 | >180          |                                                             | 0.0070 | >180          |                                                             | 0.0020 | >180          |                                                             |      |               |                                                             |                                                             |
| Tetrachloroethylene    | 0.0005 | 89            | 0.001 (3hr)                                                   | 0.0005 | 115           | 0.003 (3hr)                                                 | 0.0028 | 111           | 0.043 (3hr)                                                 |        |               |                                                             |      |               |                                                             |                                                             |
| Tetrahydrofuran        |        |               |                                                               | 0.0013 | >240          |                                                             | 0.0013 | 236           | 0.058 (4hr)                                                 | 0.0013 | 201           | 0.097 (3hr)                                                 |      |               |                                                             |                                                             |
| Toluene                |        |               |                                                               | 0.011  | >276          |                                                             | 0.024  | >180          |                                                             |        |               |                                                             |      |               |                                                             |                                                             |
| Trichloroethylene      | 0.0011 | 49            | 0.19 (3hr)                                                    | 0.0007 | >300          |                                                             | 0.0007 | >180          |                                                             |        |               |                                                             |      |               |                                                             |                                                             |
|                        | 0.0011 | 72            | 0.003 (3hr)                                                   | 0.0011 | 84            | 0.14 (nc)                                                   | 0.0011 | 76            | 0.34 (3hr)                                                  | 0.0011 | 81            | 0.48 (ss)                                                   |      |               |                                                             |                                                             |

(continued)

TABLE 13. COMPARISON OF CHALLENGE S200 PERMEATION DATA AS A FUNCTION OF TEMPERATURE

| Chemical      | 25°C   |               |                                                               |        | 30°C          |                                                             |        |               | 35°C                                                        |        |               |                                                             | 40°C          |                                                             |     |               |
|---------------|--------|---------------|---------------------------------------------------------------|--------|---------------|-------------------------------------------------------------|--------|---------------|-------------------------------------------------------------|--------|---------------|-------------------------------------------------------------|---------------|-------------------------------------------------------------|-----|---------------|
|               | MDR*   | Ave. BT (min) | Ave. reported rate** ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | MDR    | Ave. BT (min) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | MDR    | Ave. BT (min) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | MDR    | Ave. BT (min) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Ave. BT (min) | Ave. reported rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | MDR | Ave. BT (min) |
| Vinyl acetate | 0.0030 | 73            | 38.0 (3hr)                                                    | 0.0021 | 101           | 0.089 (nc)                                                  | 0.0007 | 60            | 0.61 (4hr)                                                  | 0.0014 | 69            | 0.25 (8hr)                                                  |               |                                                             |     |               |
|               | 0.0030 | 109           | 11.3 (3hr)                                                    |        |               |                                                             |        |               |                                                             |        |               |                                                             |               |                                                             |     |               |
|               | 0.0014 | 69            | 0.25 (nc)                                                     |        |               |                                                             |        |               |                                                             |        |               |                                                             |               |                                                             |     |               |

\* Minimum detectable permeation rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ )

\*\* Reported rate is the rate at the conclusion of the permeation test or the maximum reached during the test. Test durations are noted in parenthesis, (ss) indicates steady-state permeation value, and (nc) indicates that no permeation time curve was provided.

TABLE 14. TEMPERATURE DEPENDENCE OF CHEMICAL PERMEATION  
THROUGH CHALLENGE 5200

| Chemical         | Temp.<br>(°C) | MDR<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|------------------|---------------|-------------------------------------------------|-------------|--------------------------------------------------------------|---------------------------------|---------------------------------|--------------------------------------------------------------------------------|
| Allyl Chloride   | 25            | 0.0019                                          | 56          | 0.28                                                         | $5.3 \times 10^{-10}$           | $2.8 \times 10^{-1}$            | 1.1                                                                            |
|                  | 30            | 0.0031                                          | 56          | 0.035                                                        | (nc)                            | (nc)                            | (nc)                                                                           |
|                  | 35            | 0.0080                                          | 236         | 0.53                                                         |                                 |                                 |                                                                                |
|                  | 40            | 0.0043                                          | 79          | 0.51                                                         | $8.6 \times 10^{-10}$           | $1.4 \times 10^{-1}$            | 0.90                                                                           |
| Carbon Disulfide | 25            | 0.0006                                          | 20          | 0.034                                                        |                                 |                                 |                                                                                |
|                  | 30            | 0.0006                                          | 15          | 0.23                                                         | (nc)                            | (nc)                            | (nc)                                                                           |
|                  | 35            | 0.0006                                          | 16          | 0.56                                                         | $2.2 \times 10^{-9}$            | $3.3 \times 10^{-2}$            | 0.55                                                                           |
|                  | 25            | 0.0003                                          | 64          | 0.26                                                         | $5.7 \times 10^{-10}$           | $2.3 \times 10^{-1}$            | 0.93                                                                           |
| Dichloromethane  | 27            | 0.0005                                          | 83          | 3.7                                                          | $5.1 \times 10^{-10}$           | 5.3                             | 19.5                                                                           |
|                  | 30            | 0.0007                                          | 43          | 0.037                                                        | (nc)                            | (nc)                            | (nc)                                                                           |
|                  | 30            | 0.0021                                          | 52          | 0.072                                                        | (nc)                            | (nc)                            | (nc)                                                                           |
|                  | 35            | 0.0027                                          | 43          | 0.19                                                         | $1.2 \times 10^{-9}$            | $3.1 \times 10^{-2}$            | 0.28                                                                           |
|                  | 40            | 0.0021                                          | 29          | 0.27                                                         | $1.6 \times 10^{-9}$            | $2.7 \times 10^{-2}$            | 0.31                                                                           |
|                  | 27            | 0.0005                                          | 89          | 0.0007                                                       | $5.3 \times 10^{-10}$           | $1.3 \times 10^{-4}$            | 0.0005                                                                         |
| Propylene Oxide  | 30            | 0.0005                                          | 115         | 0.0031                                                       | $2.9 \times 10^{-10}$           | $6.7 \times 10^{-2}$            | 0.13                                                                           |
|                  | 30            | 0.0019                                          | 108         | 0.0084                                                       | (nc)                            | (nc)                            | (nc)                                                                           |
|                  | 35            | 0.0028                                          | 111         | 0.043                                                        | $6.2 \times 10^{-10}$           | $4.6 \times 10^{-2}$            | 0.18                                                                           |

(continued)

TABLE 14. TEMPERATURE DEPENDENCE OF CHEMICAL PERMEATION  
THROUGH CHALLENGE 5200

| Chemical          | Temp.<br>(°C) | MDR<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min) | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | D<br>( $\text{cm}^2/\text{s}$ ) | S<br>( $\text{g}/\text{cm}^3$ ) | Calculated<br>steady-state<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
|-------------------|---------------|-------------------------------------------------|-------------|--------------------------------------------------------------|---------------------------------|---------------------------------|--------------------------------------------------------------------------------|
| Trichloroethylene | 25            | 0.0011                                          | 49          | 0.19                                                         | $3.6 \times 10^{-10}$           | $7.2 \times 10^{-1}$            | 1.9                                                                            |
|                   | 27            | 0.0011                                          | 72          | 0.0028                                                       | (nc)                            | (nc)                            | (nc)                                                                           |
|                   | 30            | 0.0011                                          | 34          | 0.14                                                         | (nc)                            | (nc)                            | (nc)                                                                           |
|                   | 35            | 0.0011                                          | 76          | 0.34                                                         | $3.9 \times 10^{-10}$           | 1.2                             | 3.4                                                                            |
|                   | 40            | 0.0011                                          | 81          | 0.48                                                         | $4.8 \times 10^{-10}$           | $1.3 \times 10^{-1}$            | 0.47                                                                           |
| Vinyl Acetate     | 25            | 0.0014                                          | 69          | 0.25                                                         | (nc)                            | (nc)                            | (nc)                                                                           |
|                   | 25            | 0.0003                                          | 73          | 38.0                                                         | $4.7 \times 10^{-10}$           | 80.3                            | 260.4                                                                          |
|                   | 25            | 0.0003                                          | 109         | 11.3                                                         | $2.2 \times 10^{-10}$           | 1084.9                          | 1733                                                                           |
|                   | 30            | 0.0021                                          | 101         | 0.089                                                        | (nc)                            | (nc)                            | (nc)                                                                           |
|                   | 35            | 0.0007                                          | 60          | 0.61                                                         | $7.3 \times 10^{-10}$           | $1.7 \times 10^{-1}$            | 0.94                                                                           |
|                   | 40            | 0.0014                                          | 69          | 0.25                                                         | $6.5 \times 10^{-10}$           | $4.9 \times 10^{-2}$            | 0.24                                                                           |

• (nc) indicates no permeation-time curve was provided.

Figure 3. Temperature Dependence of Diffusion Coefficient Values

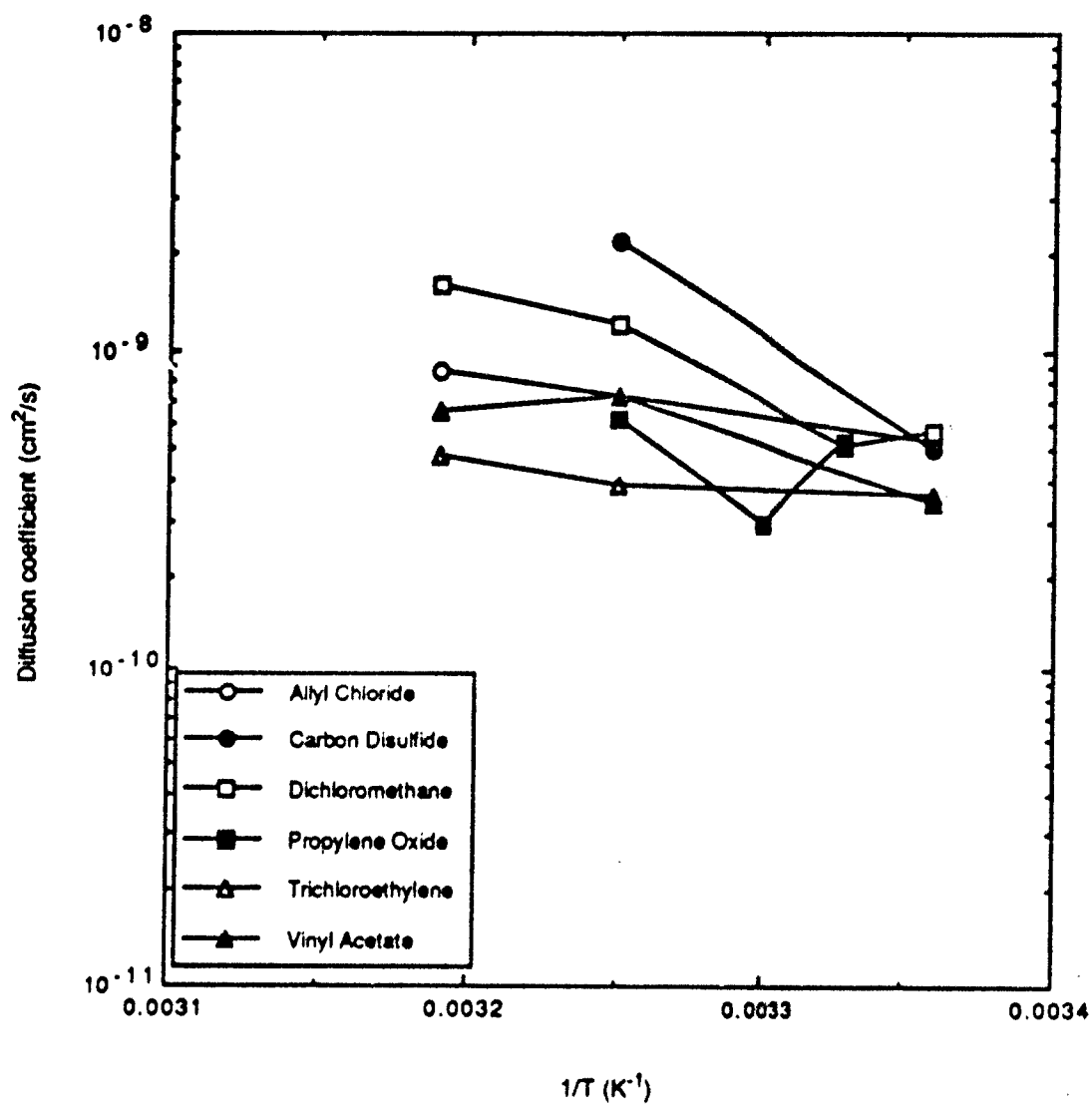


Figure 4. Temperature Dependence of Solubility Values

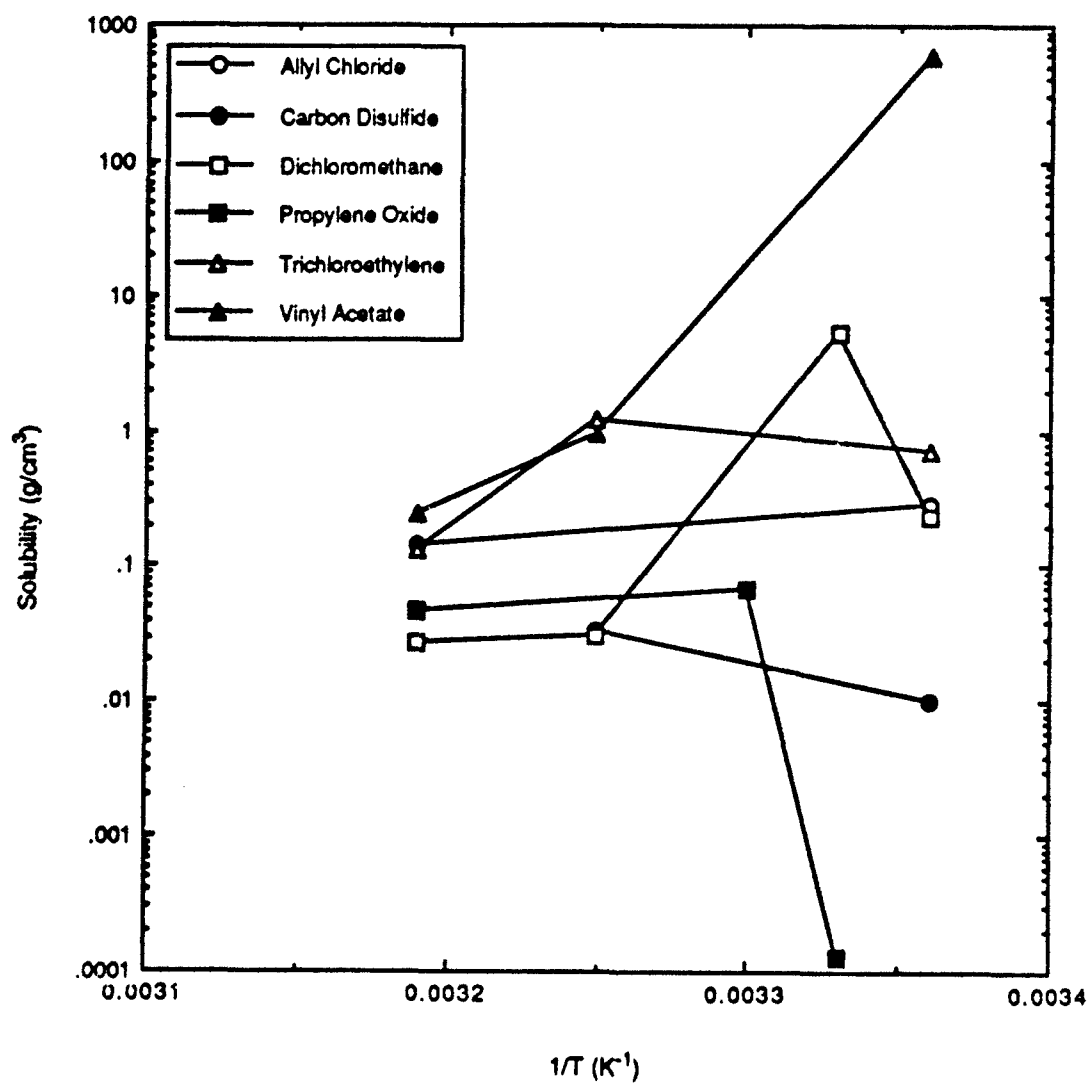
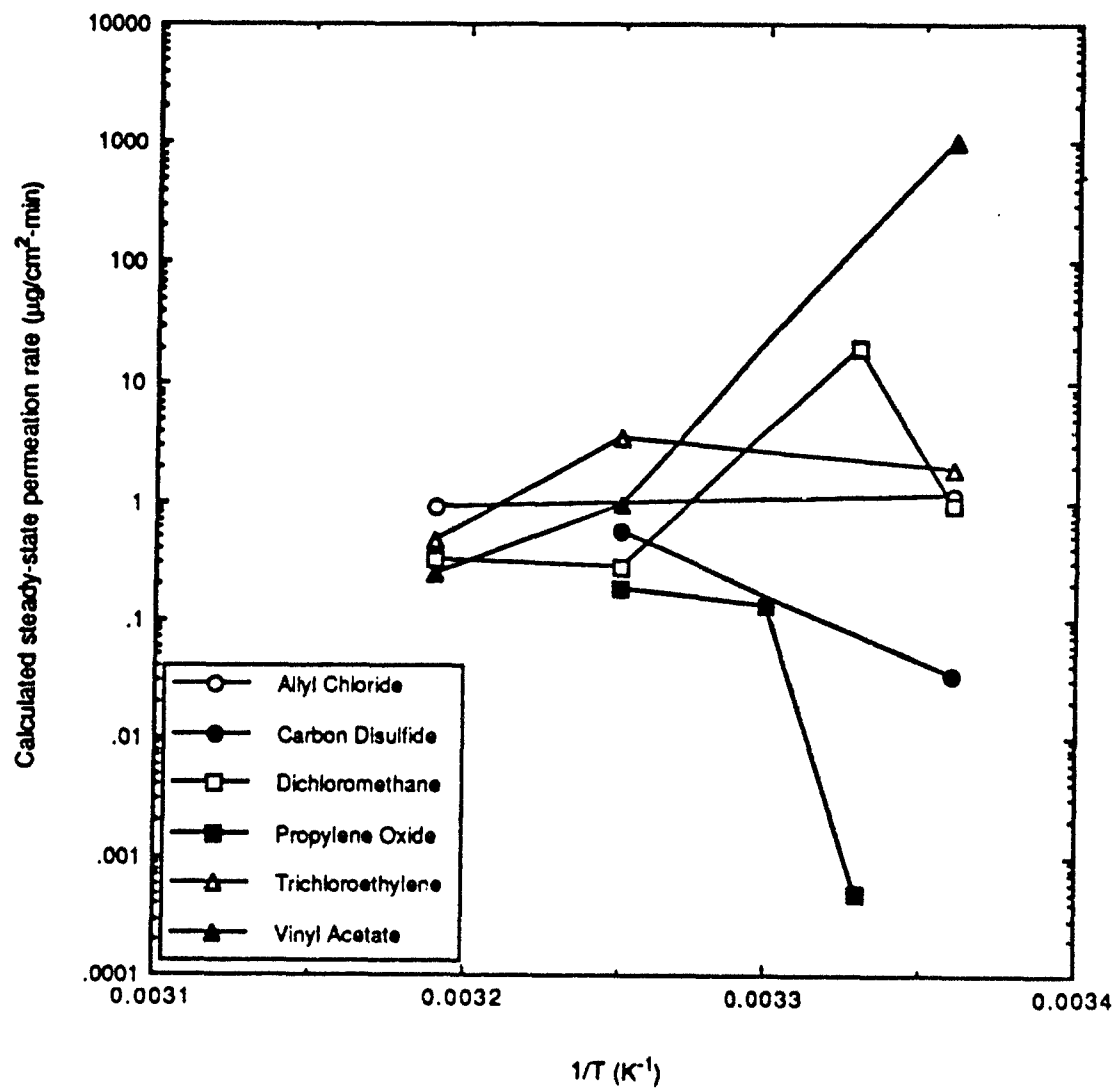


Figure 5. Temperature Dependence of Calculated Steady-State Permeation Rates



an Arrhenius relationship, such graphs would display a linear relationship between the logarithm of the parameter and the inverse temperature. For this data set, no consistent relationships are apparent, although the D values appear to show a small increase with temperature (i.e., decrease with increasing inverse temperature). Consequently, reliable conclusions regarding the temperature dependence of the barrier properties of the Challenge materials are not possible. The testing laboratory that generated the data could not provide insight into the cause for the inconsistencies. In order to achieve a better understanding of the temperature dependence, the tests should be repeated under better controlled test conditions.

#### 4.1.3 Prediction of D and S Values

To extend the above analysis to develop a Fick's law-based predictive model for the data set at 25°C, one must develop techniques to predict D and S from basic properties of a chemical of interest. Several approaches to predicting these parameters have been developed although not for fluoropolymer-based materials [12,13]. Historically, the approaches have involved theoretical, empirical, and statistical correlations with properties of the chemical and polymer material and often depend on the type and size of database available.

Using the small set of values reported above, we briefly explored approaches to correlate/predict D and S. For D, we explored correlations with chemical properties that are representative of its size. We expected that fairly good correlations would be possible because, unlike the elastomers studied elsewhere [12,13], the fluoropolymer materials exhibit very little swelling and diffusion of the chemical through the polymer matrix might truly be controlled by molecular size considerations. Also, some preliminary work by the Coast Guard indicated that molecular size/minimum cross section of the permeant was an important variable in the permeation process [14]. Initial attempts at correlations are shown in Figure 6, in which the calculated values for D are plotted versus the permeant molecular weight, and in Figure 7, in which the D values are plotted versus permeant molar volume (liquid permeants only.) In both figures, however, the data show no definitive relation although there may be a trend of decreasing D with increasing molecular size.

Solubility prediction approaches generally involve correlations of properties that describe a chemical and material's interaction potential: solubility parameters, chemical interaction parameters, dipole moments, and state variables (EOS approaches). Others involve specific consideration of the chemical and polymer structure and use group-contribution approaches to describe the interactions of various structural groups and their contribution to chemical solubility in a polymer matrix. One such group-contribution approach, UNIFAP, has been applied with success to predict the solubilities of chemicals in rubbery polymers [12,15]. However, for fluoropolymer materials, the required group interaction parameters are only available for two chemical class types: hydrocarbons and fluorocarbons (saturated). Because permeation data were not available for these types of compounds, equilibrium solubility data from the literature were used to evaluate this technique [16]. Table 15 reports solubilities for several chemicals in polytetrafluoroethylene and predicted values using the UNIFAP technique. While there is good agreement for the hydrocarbon values, the predictions for the perfluorocarbon compounds greatly exceed the measured values.

Figure 6. Diffusion Coefficients versus Permeant Molecular Weight

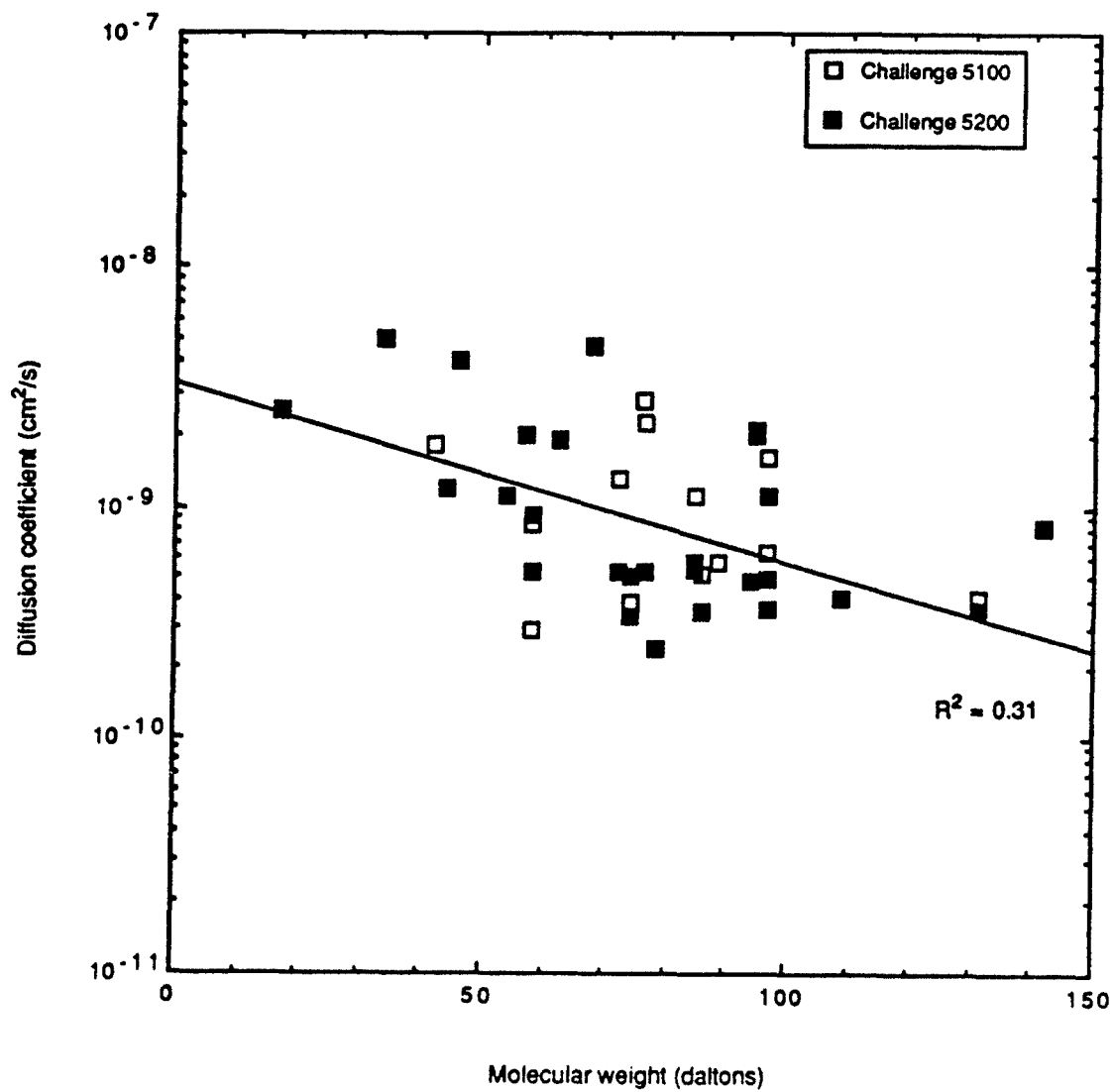


Figure 7. Diffusion Coefficients versus Permeant Molar Volume

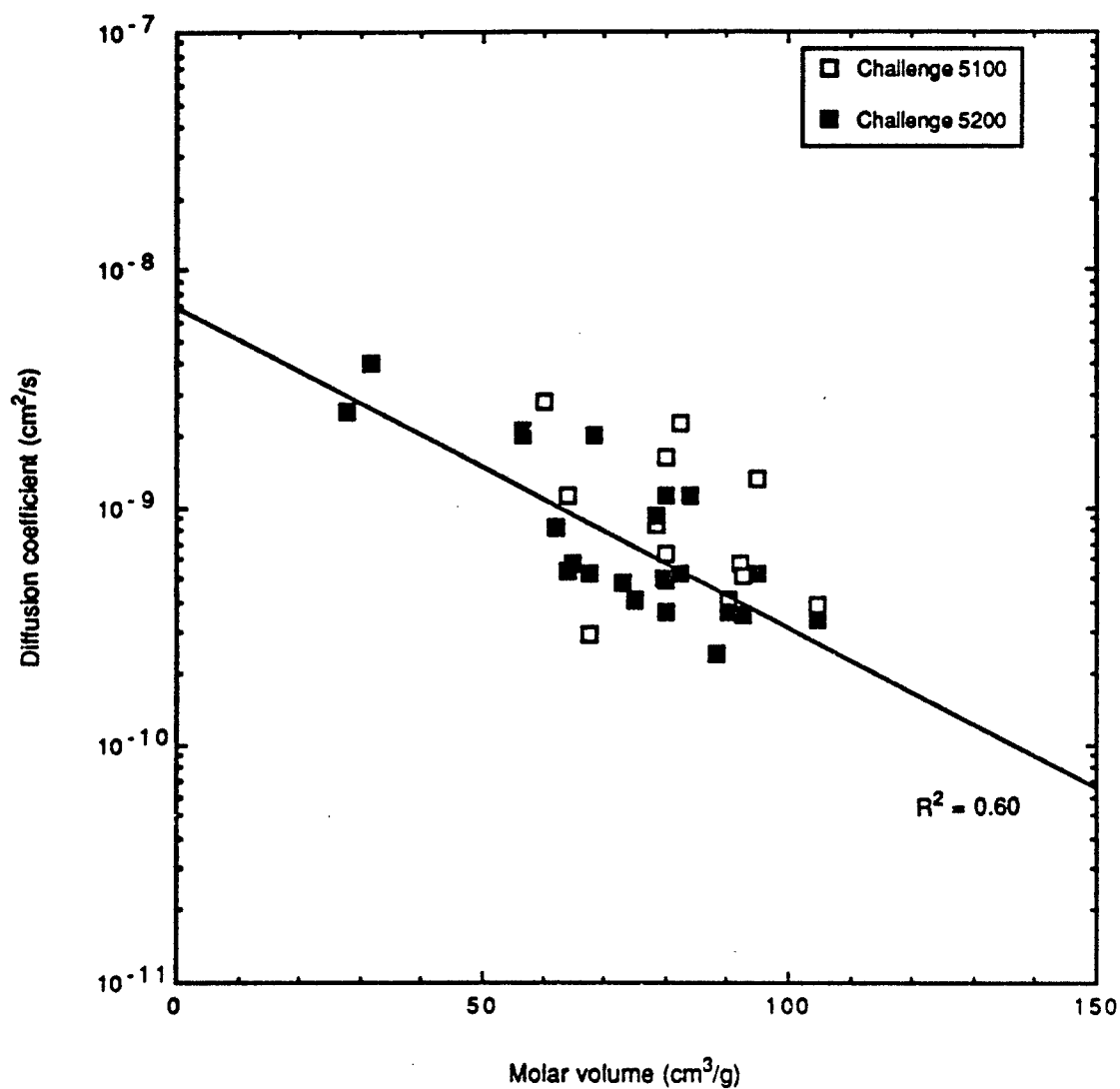


TABLE 15. SOLUBILITY PREDICTION FOR  
POLY(TETRAFLUOROETHYLENE) USING UNIFAP APPROACH

| Chemical                     | Literature Data* |                                    | Predicted<br>S<br>(g/cm <sup>3</sup> ) |
|------------------------------|------------------|------------------------------------|----------------------------------------|
|                              | Wt. gain<br>(%)  | Solubility<br>(g/cm <sup>3</sup> ) |                                        |
| HYDROCARBONS                 |                  |                                    |                                        |
| Cyclohexane                  | 1.1              | 0.023                              | 0.071                                  |
| Heptane                      |                  |                                    | 0.029                                  |
| Hexane                       | 0.7              | 0.015                              | 0.039                                  |
| Octane                       | 0.8              | 0.018                              | 0.022                                  |
| Pentane                      |                  |                                    | 0.048                                  |
| PERFLUOROCARBONS             |                  |                                    |                                        |
| Perfluorodimethylcyclohexane | 10.1             | 0.23                               |                                        |
| Perfluorocyclohexane         |                  |                                    | 11.9                                   |
| Perfluoroethane              |                  |                                    | 9.4                                    |
| Perfluoropropane             |                  |                                    | 10.1                                   |
| 1,1,1-Trifluoroethane        |                  |                                    | 5.7                                    |

\* Results reported by Starkweather [16]. Equilibrium weight gains were converted to solubilities using poly(tetrafluoroethylene) density = 2.1 g/cm<sup>3</sup>.

One other approach that was considered to predict S was using solubility parameters. Based on prior work by Hansen performed under contract to the Coast Guard [17-21], we evaluated the use of solubility parameters, both total and three-dimensional, to correlate the available S values. However, no correlations were identified. Other efforts regarding the use of solubility parameters are discussed in Section 4.2.

These efforts concluded our attempts to pursue a Fick's-law based predictive model. Because of our lack of success in predicting values for D and S, we abandoned our attempt to develop a quantitative model to predict permeation behavior as a function of time. Alternatively, we pursued empirical approaches to correlate the detection of permeation within 3 hours directly with properties descriptive of the permeating chemical: size, shape, and structure.

## 4.2 EMPIRICAL APPROACHES

### 4.2.1 Solubility Parameters

Solubility parameter approaches to predict chemical interactions have been pursued for several decades [22-24]. Much of this work was pioneered by Hansen, particularly regarding the application of three-dimensional solubility parameters [22,25]. In the past decade, solubility parameter correlations have been pursued to predict permeation of protective clothing materials and, since 1988, Hansen has been applying his three-dimensional solubility parameter approach to the Challenge material data set under contract to the Coast Guard. Although not pursued in our model development efforts, Hansen's findings are summarized briefly here because we applied solubility parameter considerations when selecting chemicals for our chemical mixture permeation tests as reported in Section 5.

Preliminary reports from 1988 describe efforts by Hansen to establish three-dimensional solubility parameter values for Challenge 5100 and to predict the Challenge 5100 data set [18-20]. The approach involved a combination of solubility parameter and molecular size considerations. A three-dimensional solubility parameter for Challenge 5100 was proposed and used to define the Relative Energy Difference (RED), a dimensionless parameter that describes the distance of a chemical from the center of a solubility parameter sphere divided by the sphere radius. The distance of the chemical from the sphere's center is calculated from the chemical's ( $\delta_{d,c}$ ,  $\delta_{p,c}$ ,  $\delta_{h,c}$ ) and polymer's ( $\delta_{d,p}$ ,  $\delta_{p,p}$ ,  $\delta_{h,p}$ ) three-dimensional solubility parameters as follows:

$$Distance = \sqrt{4(\delta_{d,c} - \delta_{d,p})^2 + (\delta_{p,c} - \delta_{p,p})^2 + (\delta_{h,c} - \delta_{h,p})^2} \quad \text{Eq. (3)}$$

The RED is calculated using the following equation and a value for the radius established by Hansen:

The preliminary values reported by Hansen for Challenge 5100 were:

- $\delta_{d,p} = 17.1 \text{ (J/cm}^3\text{)}^{1/2}$
- $\delta_{p,p} = 8.1 \text{ (J/cm}^3\text{)}^{1/2}$
- $\delta_{h,p} = 1.3 \text{ (J/cm}^3\text{)}^{1/2}$
- Radius = 4.7

The predictive model proposed was that chemicals (or mixtures) with calculated RED values less than 1 (or 2 in some cases) and with molar volumes less than  $103 \text{ cm}^3/\text{g}$  would permeate Challenge 5100. Based on this preliminary finding, Hansen proposed several chemicals and chemical mixtures as priorities for testing by the Coast Guard. These tests were conducted through mid-1989. We also used this preliminary solubility parameter model when selecting the chemical mixtures for testing by Arthur D. Little in April 1989. The chemical mixture permeation test results and analysis are described in Section 5.

The preliminary model by Hansen demonstrated moderate success in predicting pure chemical permeation through the Challenge materials but little success in predicting chemical mixture permeation. Several of the Challenge 5100 permeation test results, however, could not be predicted with this model. Through analysis of the additional test results through mid-1989, Hansen proposed revised Challenge 5100 solubility parameter values, new Challenge 5200 solubility parameter values, and a refined model for permeation prediction [21]. These were:

- Challenge 5100
  - $\delta_{d,p} = 16.6 \text{ (J/cm}^3\text{)}^{1/2}$
  - $\delta_{p,p} = 5.4 \text{ (J/cm}^3\text{)}^{1/2}$
  - $\delta_{h,p} = 4.0 \text{ (J/cm}^3\text{)}^{1/2}$
  - Radius = 3.3
- Challenge 5200
  - $\delta_{d,p} = 16.6 \text{ (J/cm}^3\text{)}^{1/2}$
  - $\delta_{p,p} = 6.0 \text{ (J/cm}^3\text{)}^{1/2}$
  - $\delta_{h,p} = 4.8 \text{ (J/cm}^3\text{)}^{1/2}$
  - Radius = 3.7
- Predictive model
  - Monomers: permeation will occur if RED < 1 and molar volume <  $100 \text{ cm}^3/\text{g}$
  - Other chemicals: permeation will occur if RED < 1 and molar volume <  $75 \text{ cm}^3/\text{g}$

The revised solubility parameter values and model provided a better fit to the data set although several outlier predictions remain. As noted in Section 3, some outliers may be the

result of discrepancies within the data set itself. The prediction of chemical mixture behavior is still not successful using the revised model.

In summary, the solubility parameter approach has demonstrated success in describing the present data set in terms of whether individual chemicals will permeate the Challenge materials within 3 hours. The empirical model can be used to predict whether permeation will occur for untested chemicals if a value for the three-dimensional solubility parameter is available for the chemical of interest. Another important finding by Hansen was that molecular size, in addition to solubility parameter, was a critical variable controlling the permeation behavior.

#### 4.2.2 Molecular Modeling

Molecular modeling was pursued by us as an aid to developing an empirical model to predict permeation of the Challenge fabrics. Our specific goal was to explore molecular size and shape considerations reported earlier by Bentz *et al.* [14] as important parameters. Molecular modelling software (Alchemy®, Tripos Associates) was used to examine the role of molecular size. Models were drawn of both permeating and non-permeating chemicals. Two aspects of size were considered: physical size (cross-sectional area and total volume), and molecular weight. Physical size was found to be more important than molecular weight in predicting permeation behavior.

With one exception (methyl acrylate), no chemical tested having greater than five non-hydrogen atoms permeates either fabric under the test conditions. This indicates that the molecular volume of five non-hydrogen atoms appears to be too large to enable permeation through the materials.

In general, chemicals tested with three or less non-hydrogen atoms permeate the materials under the test conditions. Only very polar compounds of this size such as inorganic acids and ionic compounds were not observed to permeate.

For chemicals of intermediate size (i.e., four or five non-hydrogen atoms), the electronic surface appears to be a more important determinant of permeation than absolute molecular size. Two molecules of identical size can have very different permeation characteristics. Neither very non-polar (butane) nor very polar (acetic acid) molecules permeate the materials. A necessary requirement for permeation appears to be the presence of functional groups of intermediate polarizability. These functional groups include carbon-carbon double bonds and halogen atoms. These groups have approximately the same degree of polarizability as the functional groups of the fluoropolymer barrier films in the Challenge fabrics. This observation is consistent with the identified solution-diffusion mechanism of permeation. Materials of like polarizability are most likely to be mutually soluble.

Attempts were made to correlate these observations with a physical property or properties of the chemicals, however, no correlation that adequately predicted the entire data set was identified. We found that the simplest and most accurate approach to predict the permeation data set was an empirical model that considered molecular structure, addressing both size and the presence of certain functional groups.

#### 4.3 EMPIRICAL MODEL TO PREDICT PURE CHEMICAL PERMEATION

Based on the above observations, a series of rules was developed to aid in predicting which compounds might permeate the Challenge materials. The set of rules predict whether permeation of Challenge 5100 or Challenge 5200 will occur within 3 hours at 25°C at a detection sensitivity of 0.05  $\mu\text{g}/\text{cm}^2\text{-min}$ . This detection sensitivity was selected because it approximates the average detection sensitivity reported in the permeation test program. However, as noted in Section 3, there was a wide range in the detection sensitivities used in the testing which complicated direct comparison of many of the results provided for this model development effort.

The initial set of rules, proposed in late-1988, was able to correctly predict the permeation behavior of 94% of the chemicals tested by that time. Based on these rules, priority chemicals were identified for future testing to evaluate the prediction accuracy of the rule set. These tests (and others) were conducted by the Coast Guard through 1989 and the results were compared to the predictions of the initial rule set. The rule set predicted correctly for 76% of the compounds. Many of these compounds were deliberately selected to test the limits of the rule set and, thus, aided in refining the rules.

On the basis of the expanded data set, the rules were modified slightly. The revised set correctly predicts the permeation behavior for 88 to 93% of the chemicals in the full data set. The final set of rules to predict permeation of Challenge 5100 or Challenge 5200 within 3 hours at 25°C and a detection sensitivity of 0.05  $\mu\text{g}/\text{cm}^2\text{-min}$  is as follows:

A. Compounds Containing Three (3) or Less Non-Hydrogen Atoms:

1. Acidic compounds ( $\text{pK}_a < 3$ ) will not permeate (e.g., inorganic acids such as hydrochloric).
2. Ionic compounds will not permeate.
3. All other compounds will permeate.

B. Compounds Containing Four (4) or Five (5) Non-Hydrogen Atoms:

1. If the compound does not contain either a carbon-carbon double bond or a halogen atom, it will not permeate.
2. Inorganic compounds will not permeate.

3. If the compound contains four (4) or more saturated (tetrasubstituted) carbon atoms, it will not permeate.
4. If the compound contains four (4) or more halogen atoms, it will not permeate.
5. If the compound has two (2) or more non-halogen substituents on a carbon-carbon double bond, it will not permeate.
6. If the compound contains any of the following polar functional groups, it will not permeate.
  - Alcohol
  - Aldehyde
  - Amine
  - Carboxylic acid
  - Ketone
  - Nitro
  - Nitroso
  - Any sulfur containing group
7. All other compounds will permeate.

C. Compounds Containing Six (6) or Greater Non-Hydrogen Atoms:

1. The compound will not permeate.

This revised rule set was used to predict permeation for the full data set to evaluate its accuracy. In total, predictions were made for 262 chemicals. The permeation data reported for nine of these 262 chemicals, however, indicated conflicting results so that determination of a "correct" prediction could not be made. These chemicals are listed in Table 16 and were not considered in judging the accuracy of the rule set. Of the remaining 253 chemicals, incorrect predictions were found for 30 chemicals (12%). However, several of these incorrect predictions can be resolved when the MDR values reported for the various tests are considered.

For example, Table 17 reports the 10 chemicals for which the model predicts no permeation should occur (within three hours at 25°C at an MDR of 0.05  $\mu\text{g}/\text{cm}^2\text{-min}$ ) but the test results indicate that permeation was observed. For nine of these chemicals, however, the reported MDRs were at least one order of magnitude lower than the target MDR for the model prediction. Table 18 identifies the remaining 20 chemicals for which the model predicts permeation but test results indicate that no permeation was observed. For four of these chemicals, as noted in the table, the reported MDRs were higher than the target MDR for the model, so these tests were less sensitive than most considered in the model development. If these 13 chemicals with MDR considerations are not counted, the chemicals with incorrect predictions drop to 17 of 253 (7%).

TABLE 16. PERMEATION MODEL PREDICTIONS FOR CHEMICALS WITH  
CONFLICTING PERMEATION TEST RESULTS

| Chemical            | Model* | Data** | MDR<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Comments                                               |
|---------------------|--------|--------|-------------------------------------------------|--------------------------------------------------------|
| Acetone             | N      | Y/N    | 0.00004<br>0.040                                | Permeation only at 27°C<br>or higher                   |
| Ammonia gas         | Y      | Y/N    | 0.0005<br>0.001                                 |                                                        |
| Ammonium hydroxide  | Y      | Y/N    | 0.0071<br>0.057                                 |                                                        |
| Freon 12            | N      | Y/N    | 0.0098<br>0.34                                  | Permeation detected in<br>only 1 of 6 replicates       |
| Ethyl ether         | N      | Y/N    | 0.0006<br>0.0078                                | Permeation only at low<br>MDR and/or 27°C              |
| Methyl acrylate     | N      | Y/N    | 0.0083<br>0.49                                  | Permeation not detected at<br>lower MDR                |
| Tetrachloroethylene | N      | Y/N    | 0.0001<br>0.015                                 | Permeation detected in 1<br>of 4 replicates            |
| Trimethylamine      | N      | Y/N    | 0.0007<br>0.007                                 | Permeation not detected at<br>lower MDR in repeat test |
| Vinylidene fluoride | Y      | Y/N    | 0.0021<br>0.036                                 | Permeation detected at<br>lower MDR in repeat test     |

\* Model prediction as to whether permeation will occur within 180 minutes at 25°C at a detection limit of 0.05  $\mu\text{g}/\text{cm}^2\text{-min}$ : Y = Yes, N = No.

\*\* Permeation test results indicating whether permeation was detected: Y = Yes, N = No, Y/N = Multiple or replicate tests indicate that permeation both was and was not detected.

TABLE 17. CHEMICALS FOR WHICH THE MODEL PREDICTS PERMEATION  
BUT TESTS INDICATE NO PERMEATION

| Chemical              | Model <sup>*</sup> | Data <sup>**</sup> | MDR<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Comments                      |
|-----------------------|--------------------|--------------------|-------------------------------------------------|-------------------------------|
| Acetaldehyde          | Y                  | N                  | Not reported                                    |                               |
| Acetonitrile          | Y                  | N                  | 0.033;0.066                                     |                               |
| Allyl bromide         | Y                  | N                  | 0.0010                                          |                               |
| Bromine               | Y                  | N                  | 0.068                                           | High MDR                      |
| Cyanogen bromide      | Y                  | N                  | 0.086                                           | High MDR                      |
| Cyanogen chloride     | Y                  | N                  | 0.025                                           |                               |
| Dibromomethane        | Y                  | N                  | 0.0070;0.0042                                   |                               |
| 1,3-Dichloropropene   | Y                  | N                  | 0.015                                           |                               |
| Ethane                | Y                  | N                  | 0.024                                           |                               |
| Ethanol               | Y                  | N                  | 0.11                                            | High MDR                      |
| Ethylamine            | Y                  | N                  | 0.027                                           |                               |
| Ethyleneimine         | Y                  | N                  | 0.00040                                         |                               |
| Ethylene sulfide      | Y                  | N                  | 0.015                                           |                               |
| Ethylene              | Y                  | N                  | 0.0020                                          |                               |
| Formaldehyde solution | Y                  | N                  | Not reported                                    |                               |
| Hydrazine hydrate     | Y                  | N                  | 0.023                                           | Prediction based on hydrazine |
| Hydrogen peroxide     | Y                  | N                  | 0.017                                           |                               |
| Methanol              | Y                  | N                  | 0.11                                            | High MDR                      |
| Methylamine           | Y                  | N                  | 0.0050                                          |                               |
| Propane               | Y                  | N                  | 0.00040                                         |                               |

\* Model prediction as to whether permeation will occur within 180 minutes at 25°C at a detection limit of 0.05  $\mu\text{g}/\text{cm}^2\text{-min}$ ; Y = Yes, N = No.

\*\* Permeation test results indicating whether permeation was detected; Y = Yes, N = No.

TABLE 18. CHEMICALS FOR WHICH THE MODEL PREDICTS NO PERMEATION  
BUT TESTS INDICATE PERMEATION

| Chemical             | Model* | Data** | MDR<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Comments      |
|----------------------|--------|--------|-------------------------------------------------|---------------|
| Acrolein             | N      | Y      | 0.0054                                          | Low MDR       |
| 2-Butene             | N      | Y      | 0.0018                                          | 27°C, low MDR |
| Cyanogen             | N      | Y      | 0.021                                           |               |
| Isoprene             | N      | Y      | 0.00050                                         | Low MDR       |
| Methyl acetate       | N      | Y      | 0.0012                                          | Low MDR       |
| Methyl chloroformate | N      | Y      | 0.0038                                          | Low MDR       |
| Methyl isocyanate    | N      | Y      | 0.00050                                         | Low MDR       |
| Nitrogen tetroxide   | N      | Y      | 0.0059                                          | Low MDR       |
| Phosgene             | N      | Y      | 0.5 ppm                                         | 27°C, Low MDR |
| Propylene oxide      | N      | Y      | 0.0005;0.008                                    | Low MDR       |

\* Model prediction as to whether permeation will occur within 180 minutes at 25°C at a detection limit of  $0.05 \mu\text{g}/\text{cm}^2\text{-min}$ ; Y = Yes, N = No.

\*\* Permeation test results indicating whether permeation was detected; Y = Yes, N = No, Y/N = Multiple or replicate tests indicate that permeation both was and was not detected.

This prediction accuracy of 88 to 93% is quite good considering the lack of consistency in portions of the data set, particularly regarding the MDRs. Possibly, some of the chemicals for which incorrect predictions were found should be retested.

These rules were organized into a decision tree in the form of a series of questions with yes or no answers regarding the chemical's structure that leads to a Yes/No prediction of permeation. One benefit of this approach is that no information other than the structure of a chemical is required to make a prediction. In most applications, information on a chemical's structure can be readily obtained. The rules/decision tree questions are illustrated in flowcharts in Appendix F. The rules/decision tree were also computerized as described in Section 6 to simplify the use of this empirical model by Coast Guard field personnel.

## SECTION 5

### DEVELOPMENT OF MODEL TO PREDICT CHEMICAL MIXTURE PERMEATION

#### 5.1 ANALYSIS OF CHEMICAL MIXTURE DATA

##### 5.1.1 TRI Mixture Permeation Test Results

The results of the permeation tests with 29 chemical mixtures conducted by TRI are summarized in Appendix C. The mixtures span a range of chemical classes and include both two- and three-component mixtures. Also, the mixtures include combinations of chemicals in which only one component was known to permeate as well as those in which both (or all three) components were known to permeate. Only the breakthrough times were reported for these tests, no permeation rates were measured. Although individual MDRs and breakthrough times are reported for each mixture component in most of the Challenge 5100 tests, the results for the Challenge 5200 tests were reported only as generic breakthrough times without identifying the permeating species. These results are noted in Appendix C.

The results are summarized and compared in Table 19 for both Challenge 5100 and Challenge 5200. The table combines and reports the results alphabetically by mixture component. Each chemical tested in a mixture is listed separately in the table. Thus, for each chemical, the results of all mixture tests with that chemical are listed as well as any pure chemical test results. In all cases, the results for the pure chemical are listed in the first row (or rows). Subsequent rows list the results of all mixture tests involving that chemical. For example, Table 19 begins with acetone and reports the average results of the pure chemical tested against Challenge 5100 and Challenge 5200. The table then lists the results of all mixture permeation tests in which acetone was a component. In this case, there were eight such tests performed. For these tests, the table lists the reported breakthrough times for each mixture component. Because of this format, the results of each mixture test are reported multiple times, once for each component in the mixture in alphabetical order. This format was selected because it simplifies comparison of the results and facilitates comparison with the pure chemical results.

Review of this table indicates that, in essentially all cases, the permeation of the chemicals from the various chemical mixtures can be predicted directly from the behavior when tested as a pure chemical. If a mixture component was found to permeate when tested as a pure chemical, it was found to permeate from the mixture and at approximately the same or slightly longer breakthrough time. If a mixture component did not permeate when tested as a pure chemical, it also was not found to permeate from a mixture. Two exceptions to this rule exist: acetonitrile and nitromethane. In the case of acetonitrile, permeation was not detected when tested as a pure chemical at MDLs of 1.0 and 2.0 ppm. In the mixture tests, acetonitrile permeation was detected but at an MDL of 0.02 ppm. In the other case, the MDLs for nitromethane were similar in the various tests, however, permeation was detected in one pure chemical test with Challenge 5200 but not in the test with Challenge 5100 or the

TABLE 19. COMPARISON OF CHEMICAL MIXTURE PERMEATION TEST RESULTS (TRI)

| Mixture            |              | Component #1 |           | Component #2 |          | Component #3 |          |
|--------------------|--------------|--------------|-----------|--------------|----------|--------------|----------|
| Component #1       | Component #2 | MDL (ppm)    | BT (min)  | MDL (ppm)    | BT (min) | MDL (ppm)    | BT (min) |
| Acetone            | -            | 1.20         | > 210     | -            | -        | -            | -        |
| -                  | -            | 1.00         | > 180     | -            | -        | -            | -        |
| Chlorobenzene      | -            | 0.10         | > 180     | -            | -        | -            | -        |
| 1,2-Dichloroethane | -            | 0.82         | > 180     | 0.10         | > 180    | -            | -        |
| Epichlorohydrin    | -            | 0.14         | > 180     | 0.82         | > 180    | -            | -        |
| Nitrobenzene       | -            | 0.02         | > 180     | 0.14         | > 180    | -            | -        |
| Toluene            | -            | 0.01         | > 180     | 0.02         | > 180    | -            | -        |
| Toluene            | -            | 0.01         | > 180     | 0.01         | > 180    | -            | -        |
| Toluene            | -            | 0.02         | > 180     | 0.01         | > 180    | -            | -        |
| Vinyl Acetate      | -            | 0.01         | > 180     | 0.02         | > 180    | -            | -        |
| Acetonitrile       | -            | 1.00         | > 180     | -            | -        | -            | -        |
| -                  | -            | 2.00         | > 180     | -            | -        | -            | -        |
| Chlorobenzene      | -            | 0.02         | 93        | -            | -        | -            | -        |
| 1,2-Dichloroethane | -            | 0.02         | 85, > 180 | -            | -        | -            | -        |
| Nitrobenzene       | -            | 0.02         | 80        | -            | -        | -            | -        |
| Chlorobenzene      | -            | 0.02         | 80        | -            | -        | -            | -        |
| Acrylonitrile      | -            | 0.46         | 65        | -            | -        | -            | -        |
| Trichloroethylene  | -            | 0.01         | 120-140   | -            | -        | -            | -        |
| Benzene            | -            | 0.05         | > 192     | -            | -        | -            | -        |
| Dimethyl Sulfoxide | -            | 0.01         | > 180     | -            | -        | -            | -        |
| Dimethyl Sulfoxide | -            | 0.01         | > 180     | -            | -        | -            | -        |
| Carbon Disulfide   | -            | 0.10         | 20        | -            | -        | -            | -        |
| -                  | -            | 0.01         | 20        | -            | -        | -            | -        |
| Dichloromethane    | -            | 0.02         | 12        | -            | -        | -            | -        |

(Continued)

TABLE 19. COMPARISON OF CHEMICAL MIXTURE PERMEATION TEST RESULTS (TRI)

| Mixture                  |                    |                    | Component #1 |           |          | Component #2 |          |           | Component #3 |           |          |
|--------------------------|--------------------|--------------------|--------------|-----------|----------|--------------|----------|-----------|--------------|-----------|----------|
| Component #1             | Component #2       | Component #3       | Material     | MDL (ppm) | BT (min) | MDL (ppm)    | BT (min) | MDL (ppm) | BT (min)     | MDL (ppm) | BT (min) |
| Carbon Disulfide (cont.) | Dichloromethane    | (50%)              | 5100         | **        | 0.55     | 17           | 0.55     | 17        |              |           |          |
|                          | Dichloromethane    | (25%)              | 5100         | **        | 0.03     | 16           | 0.03     | 16        |              |           |          |
|                          | Dimethylformamide  |                    | 5100         |           | 0.01     | 12           | 0.01     | > 180     |              |           |          |
| Chlorobenzene            | --                 |                    | 5100         |           | 0.20     | > 180        |          |           |              |           |          |
|                          | Acetone            |                    | 5200         | *         | 0.01     | > 180        | 0.01     | > 180     |              |           |          |
|                          | Acetonitrile       |                    | 5100         |           | 0.01     | > 180        | 0.02     | 93        |              |           |          |
|                          | Acetonitrile       | Nitrobenzene       | 5100         |           | 0.01     | > 180        | 0.02     | 80        |              | 0.01      | > 180    |
|                          | Dichloromethane    |                    | 5100         |           | 0.01     | > 180        | 0.02     | 81        |              |           |          |
| Chloroform               | --                 |                    | 5100         |           | 0.19     | > 216        |          |           |              |           |          |
|                          | Dimethylformamide  |                    | 5200         | *         | 0.07     | > 180        | 0.07     | > 180     |              |           |          |
|                          | Dimethyl Sulfoxide |                    | 5200         | *         | 0.01     | > 180        | 0.01     | > 180     |              |           |          |
|                          | Nitromethane       |                    | 5200         | *         | 0.55     | > 180        | 0.55     | > 180     |              |           |          |
| 1,2-Dichloroethane       | --                 |                    | 5100         |           | 0.09     | > 342        |          |           |              |           |          |
|                          | Acetone            |                    | 5200         | *         | 0.82     | > 180        | 0.82     | > 180     |              |           |          |
|                          | Acetonitrile       |                    | 5100         |           | 0.01     | > 180        | 0.02     | 85, > 180 |              |           |          |
|                          | Benzene            | Dimethyl Sulfoxide | 5200         | *         | 0.01     | > 180        | 0.01     | > 180     |              | 0.01      | > 180    |
| Dichloromethane          | --                 |                    | 5103         |           | 0.27     | 51           |          |           |              |           |          |
|                          | --                 |                    | 5200         |           | 0.01     | 83           |          |           |              |           |          |
|                          | Carbon Disulfide   | (75%)              | 5100         | **        | 0.03     | 16           | 0.03     | 16        |              |           |          |
|                          | Carbon Disulfide   | (50%)              | 5100         | **        | 0.55     | 17           | 0.55     | 17        |              |           |          |
|                          | Carbon Disulfide   | (25%)              | 5100         | **        | 0.02     | 12           | 0.02     | 12        |              |           |          |
|                          | Chlorobenzene      |                    | 5100         |           | 0.02     | 81           | 0.01     | > 180     |              |           |          |
|                          | Nitrobenzene       |                    | 5100         |           | 0.02     | 56           | 0.01     | > 180     |              |           |          |
|                          | Trichloroethylene  | (75%)              | 5100         | **        | 0.06     | 47           | 0.06     | 47        |              |           |          |

(Continued)

TABLE 19. COMPARISON OF CHEMICAL MIXTURE PERMEATION TEST RESULTS (TRI)

| Component #1            | Mixture           |                    | Material | Component #1 |          |       | Component #2 |          |  | Component #3 |          |  |
|-------------------------|-------------------|--------------------|----------|--------------|----------|-------|--------------|----------|--|--------------|----------|--|
|                         | Component #1      | Component #2       |          | MDL (ppm)    | BT (min) |       | MDL (ppm)    | BT (min) |  | MDL (ppm)    | BT (min) |  |
| Dichloromethane (cont.) | Trichloroethylene | (50%)              | --       | 5100 **      | 0.03     | 68    | 0.03         | 68       |  | 0.01         | > 180    |  |
|                         | Trichloroethylene | (25%)              | --       | 5100 **      | 0.05     | 105   | 0.05         | 105      |  | 0.01         | > 180    |  |
| Dimethylformamide       | --                | --                 | --       | 5100         | nd       | > 192 |              |          |  |              |          |  |
|                         | Carbon Disulfide  | --                 | --       | 5100         | 0.01     | > 180 | 0.01         | 12       |  |              |          |  |
|                         | Chloroform        | --                 | --       | 5200 *       | 0.07     | > 180 | 0.07         | > 180    |  |              |          |  |
| Dimethyl Sulfoxide      | --                | --                 | --       | 5200         | 0.01     | > 180 |              |          |  |              |          |  |
|                         | Benzene           | --                 | --       | 5200 *       | 0.01     | > 180 | 0.01         | > 180    |  |              |          |  |
|                         | Benzene           | 1,2-Dichloroethane | --       | 5200 *       | 0.01     | > 180 | 0.01         | > 180    |  | 0.01         | > 180    |  |
|                         | Chloroform        | --                 | --       | 5200 *       | 0.01     | > 180 | 0.01         | > 180    |  | 0.01         | > 180    |  |
| Epichlorohydrin         | --                | --                 | --       | 5100         | 0.75     | > 180 |              |          |  |              |          |  |
|                         | Acetone           | --                 | --       | 5200 *       | 0.14     | > 180 | 0.14         | > 180    |  |              |          |  |
| Methyl Ethyl Ketone     | --                | --                 | --       | 5100         | 0.65     | > 180 |              |          |  |              |          |  |
|                         | Acetone           | Toluene            | --       | 5200 *       | 0.01     | > 180 | 0.01         | > 180    |  | 0.01         | > 180    |  |
|                         | 2-Nitropropane    | Toluene            | --       | 5200 *       | 0.82     | > 180 | 0.82         | > 180    |  | 0.82         | > 180    |  |
| Nitrobenzene            | --                | --                 | --       | 5100         | 0.08     | > 180 |              |          |  |              |          |  |
|                         | Acetone           | --                 | --       | 5200 *       | 0.02     | > 180 | 0.02         | > 180    |  |              |          |  |
|                         | Acetone           | Toluene            | --       | 5200 *       | 0.02     | > 180 | 0.02         | > 180    |  | 0.02         | > 180    |  |
|                         | Acetonitrile      | --                 | --       | 5100         | 0.01     | > 180 | 0.02         | 80       |  |              |          |  |
|                         | Acetonitrile      | Chlorobenzene      | --       | 5100         | 0.01     | > 180 | 0.02         | 80       |  | 0.01         | > 180    |  |
|                         | Dichloromethane   | --                 | --       | 5100         | 0.01     | > 180 | 0.02         | 56       |  |              |          |  |
|                         | Toluene           | --                 | --       | 5200 *       | 0.01     | > 180 | 0.01         | > 180    |  | 0.01         | > 180    |  |
| Nitromethane            | --                | --                 | --       | 5100         | 0.26     | > 180 |              |          |  |              |          |  |

(Continued)

TABLE 19. COMPARISON OF CHEMICAL MIXTURE PERMEATION TEST RESULTS (TRI)

| Component #1         | Mixture             |                     | Material | Component #1 |          | Component #2 |          | Component #3 |          |
|----------------------|---------------------|---------------------|----------|--------------|----------|--------------|----------|--------------|----------|
|                      | Component #1        | Component #2        |          | MDL (ppm)    | BT (min) | MDL (ppm)    | BT (min) | MDL (ppm)    | BT (min) |
| Nitromethane (cont.) | --                  | --                  | 5200     | 0.73         | 168      |              |          |              |          |
|                      | --                  | --                  | 5200     | 0.70         | > 180    |              |          |              |          |
|                      | Chloroform          | --                  | 5200 *   | 0.55         | > 180    | 0.55         | > 180    |              |          |
| 2-Nitropropane       | --                  | --                  | 5100     | 0.59         | > 180    |              |          |              |          |
|                      | Methyl Ethyl Ketone | Toluene             | 5200 *   | 0.82         | > 180    | 0.82         | > 180    | 0.82         | > 180    |
| Toluene              | --                  | --                  | 5100     | 0.06         | > 180    |              |          |              |          |
|                      | Acetone             | --                  | 5200 *   | 0.01         | > 180    |              |          |              |          |
|                      | Acetone             | Methyl Ethyl Ketone | 5200 *   | 0.01         | > 180    | 0.01         | > 180    | 0.01         | > 180    |
|                      | Acetone             | Nitrobenzene        | 5200 *   | 0.02         | > 180    | 0.02         | > 180    | 0.02         | > 180    |
|                      | Methyl Ethyl Ketone | 2-Nitropropane      | 5200 *   | 0.82         | > 180    | 0.82         | > 180    | 0.82         | > 180    |
|                      | Nitrobenzene        | --                  | 5200 *   | 0.01         | > 180    | 0.01         | > 180    | 0.01         | > 180    |
| Trichloroethylene    | --                  | --                  | 5100     | 0.07         | 143      |              |          |              |          |
|                      | --                  | --                  | 5200     | 0.01         | 61       |              |          |              |          |
|                      | Acrylonitrile       | --                  | 5100     | 0.01         | 60-80    | 0.01         | 120-140  |              |          |
|                      | Dichloromethane     | (75%)               | 5100 **  | 0.05         | 105      | 0.05         | 105      |              |          |
|                      | Dichloromethane     | (50%)               | 5100 **  | 0.03         | 68       | 0.03         | 68       |              |          |
|                      | Dichloromethane     | (25%)               | 5100 **  | 0.06         | 47       | 0.06         | 47       |              |          |
| Vinyl Acetate        | --                  | --                  | 5100     | 0.21         | 106      |              |          |              |          |
|                      | --                  | --                  | 5200     | 0.01         | 84       |              |          |              |          |
|                      | Acetone             | --                  | 5100     | 0.01         | 120      | 0.01         | > 180    |              |          |

\* Reported MDL values did not indicate whether they were for specific mixture components or generic values for the mixture.

\*\* Reported MDL values are generic values for the mixture. The breakthrough times report the time at which some component was detected but the specific component was not identified.

repeat test with Challenge 5200. No permeation was detected prior to concluding the one mixture test at 180 minutes. In the pure chemical test in which permeation was detected, the breakthrough time, 168 minutes, approaches the test termination time so the apparent discrepancy is not surprising.

Because no synergistic effects were observed, the results could be interpreted as further support of a solution-diffusion mechanism with the mixture components behaving independently. This is usually not the case for elastomeric protective clothing materials, in which swelling and chemical synergies produce unexpected and non-ideal behavior [26,27]. To further explore the mixture permeation behavior, supplementary tests were conducted by Arthur D. Little as described below.

#### 5.1.2 Supplementary Tests to Explore Behavior as Function of Time

We conducted a series of tests that involved two- and three-component mixtures of three chemicals: carbon disulfide, vinyl acetate, and ethanol. Mixtures of various combinations and concentrations were tested to explore the effect of concentration on the permeation behavior. Permeation rates as a function of time were measured. Pure chemical tests were also conducted for baseline values. Carbon disulfide was selected because of its fast breakthrough and high permeation rate. Vinyl acetate was selected for its intermediate permeation properties. Ethanol was selected because it did not permeate (within three hours.) These chemicals were also selected to test the solubility parameter approach proposed by Hansen to predict permeation behavior. Table 20 identifies the mixtures that were tested and lists the RED values calculated for these chemicals. At the time the mixtures were selected only the preliminary solubility parameter values for Challenge 5100 were available and thus were used. Because both carbon disulfide and vinyl acetate were known to permeate, mixtures at several concentrations of these two compounds were selected to study the effect of concentration. The remaining mixtures involved ethanol, a chemical not detected to permeate, in an attempt to produce mixtures that would increase ethanol permeation or "carry" ethanol through the material.

The detailed results of these tests are reported in Appendix D. A summary of the results is provided in Table 21. In general, the breakthrough times for the mixture components were relatively constant for that component in each mixture compared to the value measured as a pure chemical. Note that in these tests, ethanol was detected to permeate but at very long times, almost 6 hours. The permeation rates of the mixture components, however, were often reduced relative to those measured as pure compounds in proportion to their concentration in the mixture (i.e., as the concentration was decreased, the steady-state permeation rate decreased although not in a direct proportion). The behavior of the carbon disulfide/vinyl acetate mixture behavior as a function of time and concentration is shown in Figures 8 and 9. Figure 8 illustrates the permeation of carbon disulfide and Figure 9 illustrates the permeation of vinyl acetate at the various mixture concentrations. The permeation of the carbon disulfide had the smallest concentration effect (i.e., reduction in permeation rate as the concentration was reduced) and, for mixtures with ethanol, the carbon disulfide permeation rates measured were similar to that for the pure compound.

TABLE 20. SUPPLEMENTARY CHEMICAL MIXTURE TESTED AND HANSEN  
SOLUBILITY PARAMETERS

| Test<br># | Component(s)                           | Comp.<br>(vol. %) | Solubility Parameters<br>(J/cm <sup>3</sup> ) <sup>1/2</sup> |       |      | RED*     |        |
|-----------|----------------------------------------|-------------------|--------------------------------------------------------------|-------|------|----------|--------|
|           |                                        |                   | Disp.                                                        | Polar | Hyd. | C-5100-p | C-5200 |
| 1         | Carbon Disulfide                       | 100               | 19.9                                                         | 5.8   | 0.6  | 1.3      | 2.1    |
| 2         | Vinyl Acetate                          | 100               | 16.0                                                         | 7.2   | 5.9  | 1.1      | 0.5    |
| 3         | Ethanol                                | 100               | 15.8                                                         | 8.8   | 19.4 | 3.9      | 4.0    |
| 4         | Carbon Disulfide/Vinyl Acetate         | 90/10             | 19.5                                                         | 5.9   | 1.1  | 1.1      | 1.9    |
| 5         | Carbon Disulfide/Vinyl Acetate         | 50/50             | 18.0                                                         | 6.5   | 3.3  | 0.6      | 0.9    |
| 6         | Carbon Disulfide/Vinyl Acetate         | 10/90             | 16.4                                                         | 7.1   | 5.4  | 0.9      | 0.3    |
| 7         | Carbon Disulfide/Ethanol               | 50/50             | 17.9                                                         | 7.3   | 10.0 | 1.9      | 1.6    |
| 8         | Vinyl Acetate/Ethanol                  | 50/50             | 15.9                                                         | 8.0   | 12.7 | 2.5      | 2.2    |
| 9         | Carbon Disulfide/Vinyl Acetate/Ethanol | 45/45/10          | 17.7                                                         | 6.7   | 4.9  | 0.9      | 0.6    |
| 10        | Carbon Disulfide/Vinyl Acetate/Ethanol | 25/25/50          | 16.9                                                         | 7.7   | 11.3 | 2.1      | 1.8    |

\* RED calculated using Eq. (4) and solubility parameter values reported by Hansen for Challenge materials: C-5100-p uses preliminary values reported for Challenge 5100 in 1988, C-5200 uses values reported for Challenge 5200 in 1989.

TABLE 21. CHEMICAL MIXTURE PERMEATION RESULTS FOR CHALLENGE 5200  
Temperature = 23-26°C

| Chemical Challenge                                | Average*<br>breakthrough (min)** |                  |         | Average*<br>steady-state rate ( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |                  |         |
|---------------------------------------------------|----------------------------------|------------------|---------|------------------------------------------------------------------------|------------------|---------|
|                                                   | Carbon<br>Disulfide              | Vinyl<br>Acetate | Ethanol | Carbon<br>Disulfide                                                    | Vinyl<br>Acetate | Ethanol |
| Carbon Disulfide                                  | 46                               | --               | --      | 0.58                                                                   | --               | --      |
| Vinyl Acetate                                     | --                               | 37               | --      | --                                                                     | 0.060            | --      |
| Ethanol                                           | --                               | --               | 277     | --                                                                     | --               | 0.0037  |
| Carbon Disulfide/Vinyl Acetate (90/10) +          | 43                               | 124              | --      | 0.52                                                                   | 0.018            | --      |
| Carbon Disulfide/Vinyl Acetate (50/50)            | 57                               | 87               | --      | 0.46                                                                   | 0.042            | --      |
| Carbon Disulfide/Vinyl Acetate (10/90)            | 75                               | 61               | --      | 0.30                                                                   | 0.058            | --      |
| Carbon Disulfide/Ethanol (50/50)                  | 37                               | --               | 349     | 0.74                                                                   | --               | NR++    |
| Vinyl Acetate/Ethanol (50/50)                     | --                               | 71               | >450    | --                                                                     | 0.025            | ND++    |
| Carbon Disulfide/Vinyl Acetate/Ethanol (45/45/10) | 41                               | 71               | 393     | 0.65                                                                   | 0.052            | NR      |
| Carbon Disulfide/Vinyl Acetate/Ethanol (25/25/50) | 48                               | 96               | 444     | 0.52                                                                   | 0.035            | NR      |

\* Average of three replicate tests

\*\* Breakthrough was detected at the following minimum detectable permeation rates: Carbon Disulfide:  $0.060 \mu\text{g}/\text{cm}^2\text{-min}$ ;  
Vinyl Acetate:  $0.0020 \mu\text{g}/\text{cm}^2\text{-min}$ ; Ethanol:  $0.0020 \mu\text{g}/\text{cm}^2\text{-min}$ .

+ Percents by volume

++ NR: Steady-state not reached, ND: None detected

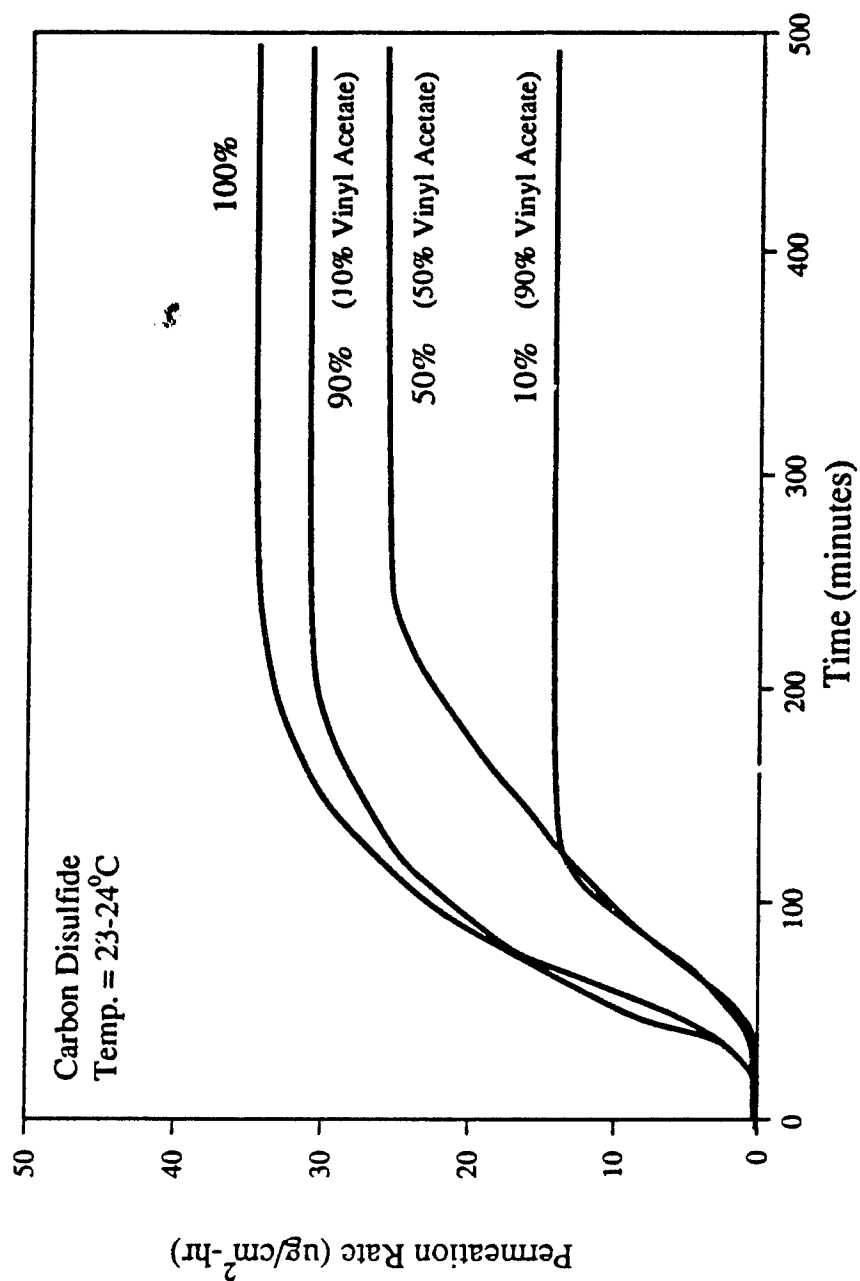


Figure 8. Permeation of carbon disulfide from carbon disulfide/vinyl acetate mixtures through Challenge 5200

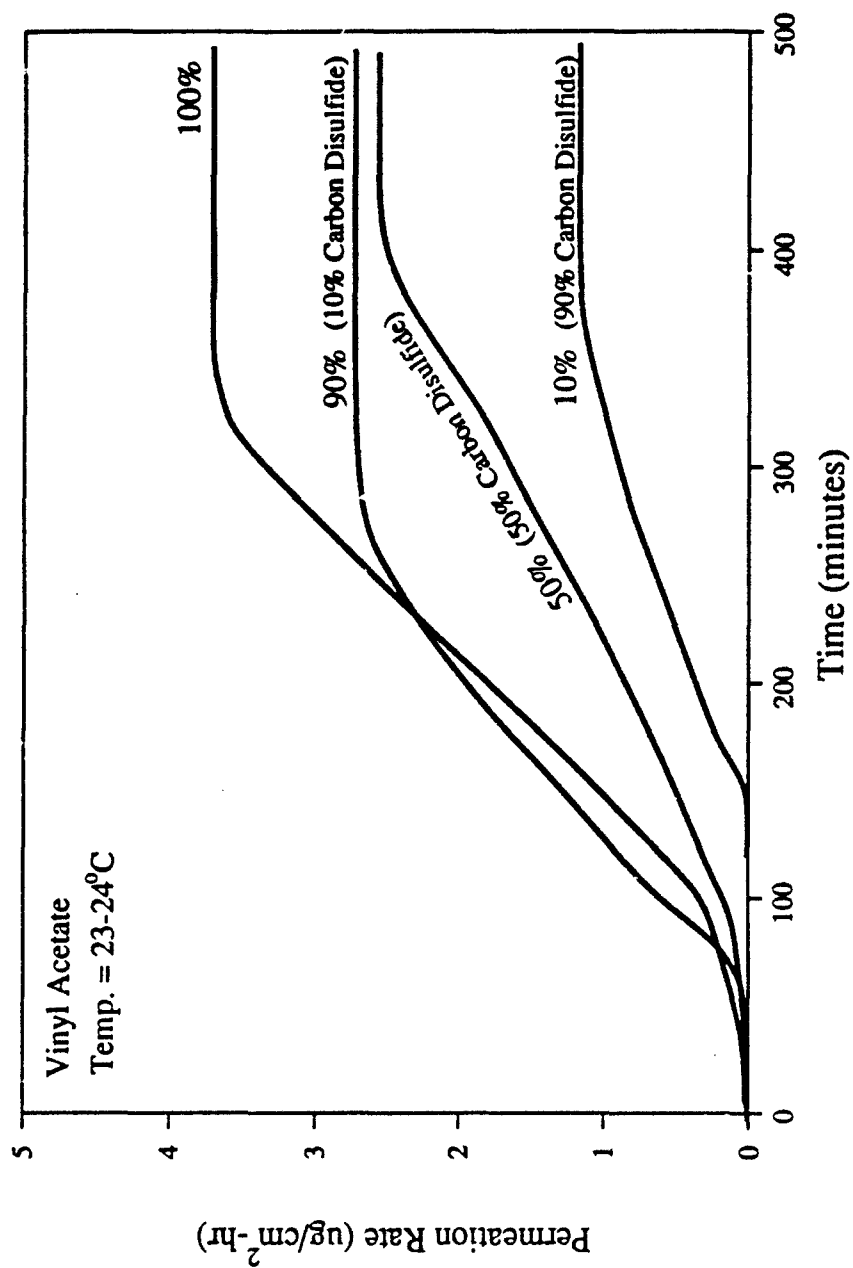


Figure 9. Permeation of vinyl acetate from carbon disulfide/vinyl acetate mixtures through Challenge 5200

## 5.2 EMPIRICAL MODEL TO PREDICT CHEMICAL MIXTURE PERMEATION

Although the supporting data base is small, a general rule is proposed to predict chemical mixture permeation through the Challenge materials, again at 25°C and within three hours at a representative detection sensitivity of 0.05  $\mu\text{g}/\text{cm}^2\text{-min}$ :

- If the chemical permeates in pure form, it will permeate from a mixture at a rate proportional to its concentration in the mixture, and
- If the chemical does not permeate in pure form, it will not permeate from a mixture.

Additional permeation tests with selected chemical mixtures should be conducted to further test this proposed rule.

## SECTION 6

### COMPUTERIZED DATABASE AND MODEL FOR PERMEATION PREDICTION

#### 6.1 DESCRIPTION

A computerized version of the permeation database and empirical prediction model was developed for Macintosh computers using SuperCard 1.5 (Silicon Beach Software). The computer system was developed for use by Coast Guard personnel with some basic training in chemistry. In addition to storing the existing Challenge material permeation test results, the computer system allows users to generate predictions using the empirical model described in Section 4.

The system was developed to run on Macintosh Plus and all later versions of Macintosh computers with at least 1 megabyte of RAM. The screen display area has been sized for the Macintosh Plus/SE monitor. The only software requirement is System 6.0.4 or later (available from any Apple dealer). SuperCard is not needed to run the database. The system is divided into two parts: a control program and a data file. The control program is provided in two formats: the master version which allows modification of the data, and the field version which allows "browsing" only. The data file is designed to work with both versions of the control program with no modifications.

##### 6.1.1 Database Structure and Card Format

Each entry in the database is stored on a "card." Thus, for every chemical in the database, there is one card that stores information on the chemical identity, permeation data if available, and permeation model prediction if generated. The card format, illustrated in Figure 10, is segmented into three parts. The first part provides chemical identity information. The second segment provides a permeation data summary using a standard, tabular format. The third segment reports the permeation model prediction, if generated and stored, also using a standard format. Data for all replicates and other temperatures are entered on the Expanded Data segment of the card shown in Figure 11. The Expanded Data segment of the card is accessed from the permeation data summary segment of the card.

Information available for each chemical stored in the database will vary. For example, some chemicals have permeation data for both Challenge 5100 and Challenge 5200 and at several temperatures, while others may have data for only one material at one temperature. Also, some chemicals will have both permeation data and a model prediction, others may have only model predictions. All available information has been included (i.e., no data were excluded as apparent outliers or because of conflicting results) and reported using the standard card format.

|                                                 |                       |                          |  |
|-------------------------------------------------|-----------------------|--------------------------|--|
| <b>Name: Carbon disulfide; Carbon bisulfide</b> |                       |                          |  |
| <b>CHRIS Code: CBB</b>                          | <b>CAS #: 75-15-0</b> | <b>ASTM Class #: 502</b> |  |

| <b>Permeation Data Summary</b> |                         |                                                          | <b>View Expanded Data</b> |
|--------------------------------|-------------------------|----------------------------------------------------------|---------------------------|
| Challenge Material             | Breakthrough Time (min) | Rate at 3 Hours ( $\mu\text{g}/\text{cm}^2/\text{min}$ ) | ND = Not Detected         |
| 5100                           | 18                      | 0.061                                                    |                           |
| 5200                           | 20                      | 0.050                                                    |                           |

|                                                                           |              |                                                     |               |
|---------------------------------------------------------------------------|--------------|-----------------------------------------------------|---------------|
| <b>Detection Limit (<math>\mu\text{g}/\text{cm}^2/\text{min}</math>):</b> | 0.006;0.0006 | <b>Temperature (<math>^{\circ}\text{C}</math>):</b> | 25 $^{\circ}$ |
|---------------------------------------------------------------------------|--------------|-----------------------------------------------------|---------------|

|                                                                                                                                                                                                                                                                                                            |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Model Prediction</b><br><br>Permeation predicted within 180 minutes at 25 $^{\circ}\text{C}$ at a detection limit of 0.05 $\mu\text{g}/\text{cm}^2/\text{min}$ .<br><br>Use caution when basing courses of action on model predictions.<br>See report for discussion of model accuracy and limitations. |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

Figure 10. Example of permeation model and database card format.

# Carbon disulfide; Carbon bisulfide

## Permeation Data

Return

| Challenge Material | Temp (°C) | BT (min) | Rate at 3 Hours (µg/cm²/min) | Det Limit (µg/cm²/min) |
|--------------------|-----------|----------|------------------------------|------------------------|
| 5100               | 25        | 18       | 0.043                        | 0.0061                 |
|                    |           | 21       | 0.061                        | 0.0061                 |
|                    |           | 22       | 0.046                        | 0.0061                 |
| 5200               | 25        | 20       | 0.050                        | 0.00061                |
|                    |           | 20       | 0.021                        | 0.00061                |
|                    |           | 20       | 0.030                        | 0.00061                |
| 5200               | 30        | 12       | 0.29                         | 0.00061                |
|                    |           | 16       | 0.18                         | 0.00061                |
|                    |           | 16       | 0.23                         | 0.00061                |
| 5200               | 35        | 12       | 0.61                         | 0.00061                |
|                    |           | 16       | 0.64                         | 0.00061                |
|                    |           | 16       | 0.44                         | 0.00061                |

ND: Not Detected

Figure 11. Example of expanded data card format.

### 6.1.2 System Operation

System features include capabilities to search the database, run the permeation prediction model, enter data or model predictions into the database (access to this feature is restricted), and print entries from the database. Standard Macintosh procedures are followed to select options from the menu list provided across the top of the screen display area. The menu options include:

- FILE - to print a single entry, to print the all database entries, and to quit from the system
- EDIT - to create/edit a new entry and to delete an existing entry (access to this option is limited)
- SEARCH - to search the database by chemical name or partial name, by CHRIS code, or by CAS number
- MODEL - to run permeation prediction model
- HELP - to access help information on operation of the data base system

### 6.1.3 Information Required to Run the Model

The computerized model was developed to be easy to use but does require basic chemistry training for proper use. As described in Section 4, the empirical model involves a set of rules or questions regarding the structure and size of the chemical. Therefore, before running the model, the structure of the chemical must be known so that the functional groups present and the number of atoms in the structure can be identified.

The computer system asks a series of questions regarding the chemical structure which the user answers by selecting from the options provided on screen. Most questions involve a Yes or No answer. As each question is answered, the computer selects the next question to ask based on the previous answer. The permeation prediction model ultimately leads to one of two predictions. If permeation is predicted to occur, the following message will be displayed:

*Permeation predicted  
within 180 minutes at 25°C at a detection limit of 0.05  $\mu\text{g}/\text{cm}^2\text{-min}$ .*

If no permeation is predicted to occur, the message below will be displayed:

*No permeation predicted  
within 180 minutes at 25°C at a detection limit of 0.05  $\mu\text{g}/\text{cm}^2\text{-min}$ .*

The master version of the computer system then provides the option to save the model prediction. Access to this capability is prevented in the field version.

## 6.2 APPLICABILITY AND LIMITATIONS

It is important to recognize that the permeation model predictions are intended only as guidance. As described throughout this report, the model was developed using the available data set and should be refined as new permeation data become available. Caution should be used when relying solely on permeation model predictions. If there are concerns regarding potential exposures to a specific chemical, permeation testing should be performed.

## SECTION 7

### CONCLUSIONS AND RECOMMENDATIONS

The permeation resistance of Challenge 5100 and Challenge 5200 has been widely tested and the results indicate that these materials are effective barriers to a broad range of chemicals and chemical mixtures. The materials appear to provide comparable barriers although the Challenge 5100 material may be a slightly better barrier. When permeation was observed, it was shown to follow a simple Fickian diffusion mechanism with a constant diffusion coefficient. However, no quantitative predictive model based on the Fick's law approach was developed however. Also, no definitive conclusions could be reached regarding the effect of temperature on the permeation resistance of the Challenge materials based on the limited data set available.

An empirical model or rule system was developed that enables predictions as to whether permeation will be detected within three hours at 25°C based on the structure and size of the chemical of interest. Based on a smaller set of data, the permeation of mixtures or the components thereof was found to behave similarly to the results for the chemicals tested individually. If a chemical permeates the Challenge material as a pure chemical then it will permeate from a mixture. Conversely, if a chemical does not permeate in pure form then it will not permeate from a mixture.

A computerized version of the permeation data base and prediction model was developed for use by personnel with minimal permeation or chemistry training. The computer system should facilitate thorough and efficient reviews of existing data and assessments of probable permeation behavior by field (or other) users who must make clothing selection decisions. Although use of the model was targeted as an aid for making clothing selection decisions, it is also useful to focus decisions regarding priority chemicals and mixtures for future testing.

Further research should be undertaken to address some of the uncertainties in the data set, the predictive model described herein, and other approaches being evaluated to predict the permeation behavior. Specific recommendations include:

- A trial implementation of the computerized permeation database and predictive model should be undertaken in the field to evaluate the product's usefulness and identify ways to optimize the product to better meet Coast Guard's needs.
- Future permeation tests, if performed, should be conducted so that chemical breakthrough is determined at a single, normalized permeation detection rate, if feasible, as is now being proposed as a revision to ASTM Method F739. Use of a standard permeation detection rate would eliminate some of the difficulties in comparing the present data set.

- Permeation tests with additional chemical mixtures should be undertaken to further validate the mixture permeation rule. Validation of this rule is important because it would eliminate the need to test infinite numbers of chemical mixtures if the behavior can be predicted using only the pure chemical results.
- Selected permeation tests at elevated temperatures should be repeated to confirm the results reported to date and to better understand the effect of temperature on the permeation resistance of the Challenge materials.
- The computerized permeation database should be updated as more data are generated and the predictive model should be continually tested as new data become available to expand and improve the prediction accuracy. Also, further development of a Fick's law based model should be pursued if a quantitative model to predict permeation as a function of time is desired.
- In the long term, similar computer databases and predictive models could be developed to address other important components of the Coast Guard CRS (e.g., glove materials, faceshield material) or alternative materials for the encapsulating suit fabric that may be adopted at a later date. Development of such databases and models provide a better understanding of the barrier properties of critical materials and help to focus priorities for testing.

## REFERENCES

1. U.S. Coast Guard, Chemical Hazard Response Information System, U.S. Coast Guard Commandant's Instruction M16465.12A, Stock No. 050-012-00215-1, Government Printing Office, Washington, DC, 1984.
2. Friel, J.V., M.J. McGoff, and S.J. Rodgers, "Material Development Study for a Hazardous Chemical Protective Clothing Outfit," Technical Report CG-D-58-80, U.S. Coast Guard, Washington, DC, 1980. (NTIS Report No. AD A095 993)
3. Bentz, A.P., and V. Mann, "Critical Variables Regarding Permeability of Materials for Totally Encapsulating Suits," Proceedings, Scandinavian Symposium on Protective Clothing Against Chemicals, Copenhagen, Denmark, 1984.
4. Stull, J.O., "Early Development of a Hazardous Chemical Protective Ensemble," Technical Report CG-D-24-86, U.S. Coast Guard, Washington, DC, 1986.
5. Hendrick, M.S., and C.B. Billing, Jr., "Selection of Priority Chemicals for Permeation Testing and Hazardous Chemical Spill Detection and Analysis," Technical Report CG-D-22-86, U.S. Coast Guard, Washington, DC, 1986. (NTIS Report No. AD A172 370)
6. Stull, J.O., "Development of the U.S. Coast Guard Chemical Response Suit," Technical Report CG-D-16-87, U.S. Coast Guard, Washington, DC, 1987.
7. Texas Research International, Chemical Resistance Testing of Protective Clothing Materials, work in progress under U.S. Coast Guard Contract, internal progress reports to U.S. Coast Guard, 1987-90.
8. Verschoor, K.L., L.N. Britton, and E.D. Golla, "Innovative Method for Determining Minimum Detectable Limits in Permeation Testing," Performance of Protective Clothing: Second Symposium, ASTM STP 989, S.Z. Mansdorf, R. Sager, and A.P. Nielsen, Eds., American Society for Testing and Materials, Philadelphia, pp. 252-256, 1988.
9. Schwope, A.D., R. Goydan, R.C. Reid, and S. Krishnamurthy, "State-of-the-Art Review of Permeation Testing and Interpretation of Its Results," Am. Ind. Hyg. Assoc. J., 49(11), 557-565, 1988.
10. Chemical Fabrics Corporation, Merrimack, NH, Challenge 5200 Product Information and Permeation Data, 1989.
11. Crank, J., The Mathematics of Diffusion, 2nd. Ed., Clarendon Press, Oxford, 1975.

12. Goydan, R., A.D. Schwope, T.R. Carroll, H.S. Tseng, and R.C. Reid, Development and Assessment of Methods for Estimating Protective Performance. EPA/600/2-87/104, U.S. Environmental Protection Agency, Cincinnati, Ohio, 1988.
13. Goydan, R., T.R. Carroll, A.D. Schwope, and R.C. Reid, Refinement of a Model to Predict the Chemical Permeation of Protective Clothing Materials. EPA/600/2-90/028, U.S. Environmental Protection Agency, Cincinnati, Ohio, 1990.
14. Bentz, A., and C.B. Billing, Jr., private communication, 1988.
15. Goydan, R., R.C. Reid, and H. Tseng, "Estimation of the Solubilities of Organic Compounds in Polymers by Group-Contribution Methods," *I&EC Research*, 28, 445-454, 1989.
16. Starkweather, H.W., Jr., "The Sorption of Chemicals by Perfluorocarbon Polymers," *Macromolecules*, 10, 1161, 1977.
17. Bentz, A.P., and C.B. Billing, Jr., "Determination of Solubility Parameters of New Suit Materials," Performance of Protective Clothing: Second Symposium, ASTM STP 989, S.Z. Mansdorf, R. Sager, and A.P. Nielsen, Eds., American Society for Testing and Materials, Philadelphia, pp.209-218, 1988.
18. Hansen, C.M., "Solubility Parameter for Teflon," Contract No. DTCG-88-P-0563, U.S. Coast Guard Research and Development Center internal report, May 1988.
19. Hansen, C.M., "Chemicals Pairs for Permeation Testing," Contract No. DTCG-88-P-0563, U.S. Coast Guard Research and Development Center internal report, May 1988.
20. Hansen, C.M., "Chemicals for Permeation Testing," Contract No. DTCG-88-P-0563, U.S. Coast Guard Research and Development Center internal report, September 1988.
21. Hansen, C.M., "Selection of Chemicals for Permeation Testing based on New Solubility Parameter Models for Challenge 5100 and Challenge 5200," Contract No. DTCG50-89-P-0333, U.S. Coast Guard Research and Development Center internal report, June 1989.
22. Hansen, C.M., doctoral thesis, Technical University of Denmark, Danish Technical Press, Copenhagen, Denmark, 1967.
23. Hansen, C.M., and A. Beerbower, "Solubility Parameters," in Encyclopedia of Chemical Technology, Supplementary Volume, 2nd ed., Wiley, New York, pp. 889-910, 1971.
24. Barton, A.F.M., Handbook of Solubility Parameters and Other Cohesion Parameters, CRC Press, Inc., Boca Raton, FL, 1983.

25. Hansen, C.M., and K.M. Hansen, "Solubility Parameter Prediction of the Barrier Properties of Chemical Protective Clothing," Performance of Protective Clothing: Second Symposium, ASTM STP 989, S.Z. Mansdorf, R. Sager, and A.P. Nielsen, Eds., American Society for Testing and Materials, Philadelphia, pp.197-208, 1988.
26. Nelson, G.O., B.Y. Lum, G.J. Carlson, C.M. Wong, and J.S. Johnson, "Glove Permeation by Organic Solvents," Am. Ind. Hyg. Assoc. J., 42, 217-225, 1981.
27. Mickelsen, R.L., M.M. Roder, and S.P. Berardinelli, "Permeation of Chemical Protective Clothing by Three Binary Solvent Mixtures," Am. Ind. Hyg. Assoc. J., 47, 236-240, 1986.

**APPENDIX A**

**CHALLENGE 5100 AND CHALLENGE 5200  
PERMEATION TEST RESULTS AT 25°C**

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

| Chemical +               | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|--------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                          |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Acetaldehyde             | ND            | ND                                | >           | 180                                             | >            |                                               |              |                                               |              |                                               |
| Acetic Acid              | 35.460        | 1.7178                            | >           | 240                                             | >            |                                               |              |                                               |              |                                               |
| Acetic Anhydride         | 0.570         | 0.0396                            | >           | 180                                             | >            |                                               |              |                                               |              |                                               |
| Acetone                  | 1.160         | 0.0469                            | >           | 210                                             | >            |                                               |              |                                               |              |                                               |
| Acetone (27C) +          | 0.001         | 0.00004                           |             |                                                 |              |                                               |              |                                               |              |                                               |
| Acetone Cyanohydrin      | 2.740         | 0.1881                            | >           | 192                                             |              | 1.630 (3hr)                                   | 44           | 1.3000                                        | 104          | 1.2000                                        |
| Acetonitrile             | ND            | ND                                | >           | 270                                             |              |                                               |              |                                               | 64           | 2.4000                                        |
| Acetonitrile +           | 1.000         | 0.0331                            | >           | 180                                             |              |                                               |              |                                               |              |                                               |
| Acetophenone (USCG R&DC) | ND            | ND                                | >           | 5520                                            |              |                                               |              |                                               |              |                                               |
| Acetyl Bromide           | 0.200         | 0.0198                            | >           | 282                                             |              |                                               |              |                                               |              |                                               |
| Acetyl Chloride          | 35.460        | 2.2455                            | >           | 186                                             |              |                                               |              |                                               |              |                                               |
| Acrolein                 | 0.120         | 0.0054                            |             | 41                                              |              | 0.033 (ss)                                    | 44           | 0.0395                                        | 38           | 0.0268                                        |
| Acrylic Acid             | 0.860         | 0.0500                            | >           | 180                                             |              |                                               |              |                                               |              |                                               |
| Acrylonitrile            | 0.460         | 0.0049                            |             | 65                                              |              |                                               | 54           |                                               | 76           | 0.0143                                        |
| Adiponitrile             | 0.300         | 0.0261                            | >           | 186                                             |              |                                               |              |                                               |              |                                               |
| Allyl Alcohol            | 1.130         | 0.0529                            | >           | 840                                             |              |                                               |              |                                               |              |                                               |
| Allyl Amine              | 0.800         | 0.0368                            | >           | 210                                             |              |                                               |              |                                               |              |                                               |
| Allyl Bromide            | 0.010         | 0.0010                            | >           | 240                                             |              |                                               |              |                                               |              |                                               |
| Allyl Chloride           | 0.160         | 0.0025                            |             | 134                                             |              |                                               | 102          | 0.0107                                        | 166          | 0.0103                                        |
| Allyl Chloride           | 0.060         | 0.0037                            |             | 143                                             |              |                                               | 136          | 0.0098                                        | 116          | 0.0210                                        |
| Allyl Cyanide            | 0.400         | 0.0216                            | >           | 240                                             |              |                                               |              |                                               | 176          | 0.0068                                        |
| Allyl Isothiocyanate     | 1.000         | 0.0800                            | >           | 258                                             |              |                                               |              |                                               |              |                                               |
| Allyl Mercaptan          | 0.020         | 0.0012                            | >           | 600                                             |              |                                               |              |                                               |              |                                               |
| Ammonia (Gas) +          | 0.040         | 0.0005                            | >           | 180                                             |              |                                               |              |                                               |              |                                               |
| Ammonium Hydroxide +     | 2.000         | 0.0565                            |             | 7                                               |              | (3hr)                                         | 30           | 26.6667                                       | >            | 180                                           |
| Ammonium Hydroxide +     | 7.200         | 0.2033                            | >           | 180                                             |              |                                               |              |                                               |              |                                               |
| Aniline                  | 0.460         | 0.0346                            | >           | 198                                             |              |                                               |              |                                               |              |                                               |
| Benzene                  | 0.050         | 0.0032                            | >           | 192                                             |              |                                               |              |                                               |              |                                               |
| Benzoyl Chloride         | 0.020         | 0.0023                            | >           | 960                                             |              |                                               |              |                                               |              |                                               |

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

| Chemical +                           | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|--------------------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                                      |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Benzyl Chloride                      | 0.110         | 0.0112                            | > 192       |                                                 |              |                                               |              |                                               |              |                                               |
| Bromine (Gas)                        | 0.530         | 0.0683                            | > 198       |                                                 |              |                                               |              |                                               |              |                                               |
| Butanol                              | 0.320         | 0.0191                            | > 936       |                                                 |              |                                               |              |                                               |              |                                               |
| 2-Butanol                            | 0.240         | 0.0144                            | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| t-Butanol                            | 0.200         | 0.0120                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 2-Butoxyethanol                      | 0.040         | 0.0038                            | > 258       |                                                 |              |                                               |              |                                               |              |                                               |
| Butyl Acetate                        | 0.250         | 0.0234                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Butyl Acrylate                       | 0.220         | 0.0227                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Butylamine                           | 0.320         | 0.0189                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Butyraldehyde                        | 0.290         | 0.0169                            | > 450       |                                                 |              |                                               |              |                                               |              |                                               |
| Carbon Disulfide                     | 0.100         | 0.0061                            | 20          | 0.050 (u)                                       | 22           | 0.0460                                        | 21           | 0.0608                                        | 18           | 0.0432                                        |
| Carbon Tetrachloride                 | 0.290         | 0.0360                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Chlordane, 25%                       | 0.260         | 0.0860                            | > 204       |                                                 |              |                                               |              |                                               |              |                                               |
| Chlorobenzene                        | 0.200         | 0.0182                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Chloroform                           | 0.190         | 0.0183                            | > 216       |                                                 |              |                                               |              |                                               |              |                                               |
| Chloropicrin (Trichloronitromethane) | 1.800         | 0.2387                            | > 186       |                                                 |              |                                               |              |                                               |              |                                               |
| Chloroprene (2-Chloro-1,3-Butadiene) | 0.030         | 0.0021                            | 179         |                                                 | 192          | 0.0025                                        | 184          | 0.0032                                        | 160          | 0.0087                                        |
| Chlorosulfonic Acid                  | 0.500         | 0.0470                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Creosote                             | 0.320         | *                                 | > 1086      |                                                 |              |                                               |              |                                               |              |                                               |
| m-Cresol                             | 0.030         | 0.0026                            | > 240       |                                                 |              |                                               |              |                                               |              |                                               |
| Crotonaldehyde                       | 0.620         | 0.0351                            | > 186       |                                                 |              |                                               |              |                                               |              |                                               |
| Cumene Hydroperoxide                 | 1.200         | 0.1471                            | > 210       |                                                 |              |                                               |              |                                               |              |                                               |
| Cyclohexane                          | 0.250         | 0.0170                            | > 204       |                                                 |              |                                               |              |                                               |              |                                               |
| Cyclohexanol                         | 0.040         | 0.0032                            | > 240       |                                                 |              |                                               |              |                                               |              |                                               |
| Cyclohexanone                        | 0.020         | 0.0016                            | > 210       |                                                 |              |                                               |              |                                               |              |                                               |
| Cyclohexylamine                      | 0.020         | 0.0016                            | > 240       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,2-Dibromoethane                    | 0.100         | 0.0152                            | > 204       |                                                 |              |                                               |              |                                               |              |                                               |
| Dibromomethane +                     | 0.050         | 0.0070                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Dibutyl Phthalate                    | 0.020         | 0.0045                            | > 288       |                                                 |              |                                               |              |                                               |              |                                               |

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

| Chemical +                    | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|-------------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                               |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| o-Dichlorobenzene             | 0.010         | 0.0012                            | > 870       |                                                 |              |                                               |              |                                               |              |                                               |
| p-Dichlorobenzene             | 0.020         | 0.0024                            | > 240       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,2-Dichloroethane            | 0.090         | 0.0072                            | > 342       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,2-Dichloroethylene          | 0.010         | 0.0008                            | 15          | 1.079 (ss)                                      | 20           | 0.1933                                        | 4            | 2.9333                                        | 20           | 0.1115                                        |
| 1,2-Dichloroethylene          | 0.010         | 0.0008                            | 23          | 0.130 (ss)                                      | 21           | 0.1417                                        | 24           | 0.1177                                        |              |                                               |
| 1,2-Dichloroethyl Ether       | ND            | ND                                | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Dichloromethane               | 0.270         | 0.0042                            | 51          | 0.020 (ss)                                      | 47           | 0.0228                                        | 50           | 0.2161                                        | 55           | 0.0212                                        |
| Dichloromethane (USCG R&DC)   | 0.030         | *                                 | 61          |                                                 | 54           |                                               | 65           |                                               | 63           |                                               |
| 1,2-Dichloropropane           | 0.310         | 0.0283                            | > 186       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,3-Dichloropropene           | 0.170         | 0.0152                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Diethanolamine                | ND            | ND                                | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Diethylamine (USCG R&DC)      | ND            | ND                                | > 270       |                                                 |              |                                               |              |                                               |              |                                               |
| Diethylenetriamine            | 0.900         | 0.749                             | > 1200      |                                                 |              |                                               |              |                                               |              |                                               |
| Diisopropylamine              | 0.390         | 0.0318                            | > 672       |                                                 |              |                                               |              |                                               |              |                                               |
| 2,3-Dimethyl-2-Butene         | 0.020         | 0.0014                            | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Dimethylformamide (USCG R&DC) | ND            | ND                                | > 192       |                                                 |              |                                               |              |                                               |              |                                               |
| Dimethyl sulfate              | 1.520         | 0.1547                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,4-Dioxane                   | 0.380         | 0.0270                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Di-n-Propylamine              | 0.220         | 0.0180                            | > 204       |                                                 |              |                                               |              |                                               |              |                                               |
| Epichlorohydrin               | 0.750         | 0.0560                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,2-Epoxy Butane              | 0.070         | 0.0041                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Ethanol                       | 2.860         | 0.1063                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Ethion 4                      | 0.030         | 0.0093                            | > 288       |                                                 |              |                                               |              |                                               |              |                                               |
| 2-Ethoxy Ethanol              | 0.050         | 0.0036                            | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Ethyl Acetate                 | 0.490         | 0.0348                            | > 258       |                                                 |              |                                               |              |                                               |              |                                               |
| Ethyl Acrylate                | 1.720         | 0.1389                            | > 1020      |                                                 |              |                                               |              |                                               |              |                                               |
| Ethylamine (70%)              | 0.740         | 0.0269                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Ethyl Benzene                 | 0.140         | 0.0120                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Ethylene +                    | 0.090         | 0.0020                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

| Chemical +                     | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                            | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|--------------------------------|---------------|-----------------------------------|-------------|------------------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                                |               |                                   | BT<br>(min) | Reported<br>rate <sup>a</sup><br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Ethylene Cyanohydrin           | 0.400         | 0.0229                            | >           | 228                                                        |              |                                               |              |                                               |              |                                               |
| Ethylene diamine               | 2.780         | 0.1348                            | >           | 192                                                        |              |                                               |              |                                               |              |                                               |
| Ethylene Glycol                | 2.630         | 0.1317                            | >           | 1008                                                       |              |                                               |              |                                               |              |                                               |
| Ethylene Sulfide               | 0.300         | 0.0145                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Ethyl Ether                    | 0.130         | 0.0078                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Ethyl Ether +                  | 0.010         | 0.0006                            | 92          | 0.005 (3hr)                                                | 88           | 0.0060                                        | 84           | 0.0078                                        | 104          | 0.0012                                        |
| Ethyl Ether (27C) +            | 0.006         | 0.0004                            | 117         | 1.070 (3hr)                                                | 124          | 1.4000                                        | 112          | 0.9000                                        | 116          | 0.9000                                        |
| Ethyl Vinyl Ether              | 0.030         | 0.0017                            | 113         | 0.008 (3hr)                                                | 148          | 0.0040                                        | 92           | 0.0117                                        | 100          | 0.0075                                        |
| Formaldehyde, 37%              | ND            | ND                                | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Formic Acid                    | 1.000         | 0.0371                            | >           | 1200                                                       |              |                                               |              |                                               |              |                                               |
| Freon 12 (Gas) +               | 3.500         | 0.3414 ul                         | ?           |                                                            | 160          | 0.0001                                        | >            | 180                                           | >            | 180                                           |
| Furfural                       | 0.080         | 0.0062                            | >           | 186                                                        | (3hr)        |                                               |              |                                               |              |                                               |
| Gasoline                       | 1.650         | 0.0347                            | >           | 894                                                        |              |                                               |              |                                               |              |                                               |
| Glutaraldehyde (sol'n)         | 0.430         | 0.0347                            | >           | 216                                                        |              |                                               |              |                                               |              |                                               |
| Heptane                        | 0.040         | 0.0032                            | >           | 240                                                        |              |                                               |              |                                               |              |                                               |
| Hexane                         | 0.250         | 0.0174                            | >           | 300                                                        |              |                                               |              |                                               |              |                                               |
| Hexylene Glycol                | 0.080         | 0.0076                            | >           | 198                                                        |              |                                               |              |                                               |              |                                               |
| Hydrazine Hydrate [10217-52-4] | 0.900         | 0.0233                            | >           | 192                                                        |              |                                               |              |                                               |              |                                               |
| Hydrochloric Acid              | 2.000         | 0.0588                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Hydrogen Peroxide, 30%         | 0.600         | 0.0165                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Isobutyl Acetate               | 0.030         | 0.0028                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Isobutanol +                   | 0.040         | 0.0024                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Isophorone                     | 0.030         | 0.0033                            | >           | 300                                                        |              |                                               |              |                                               |              |                                               |
| Isopropanol                    | 1.160         | 0.0562                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Isopropyl Acetate              | 0.100         | 0.0082                            | >           | 240                                                        |              |                                               |              |                                               |              |                                               |
| Isopropylamine                 | 1.570         | 0.0749                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Isopropyl Ether                | 0.010         | 0.0008                            | >           | 180                                                        |              |                                               |              |                                               |              |                                               |
| Malathion, 50%                 | 1.030         | 0.2745                            | >           | 186                                                        |              |                                               |              |                                               |              |                                               |
| Mesityl Oxide                  | 0.300         | 0.0238                            | >           | 240                                                        |              |                                               |              |                                               |              |                                               |

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

| Chemical +                    | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|-------------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                               |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Methacrylonitrile             | 0.290         | 0.0157                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Methanol                      | 4.070         | 0.1052                            | >           |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Acrylate               | 0.120         | 0.0083                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Bromide (Gas) +        | 0.010         | 0.0008 ul                         |             |                                                 |              |                                               |              |                                               |              |                                               |
| 2-Methyl-2-Butene             | 0.110         | 0.0062                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Ethyl Ketone           | 0.650         | 0.0378                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Isobutyl Ketone        | 3.900         | 0.3151                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Isocyanate (NIOSH)     | 0.260         | *                                 | 28          |                                                 | 28           |                                               |              |                                               |              |                                               |
| Methyl Methacrylate           | 0.190         | 0.0132                            | > 186       |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Parathion              | 0.150         | 0.0319                            | > 186       |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Vinyl Ketone           | 0.050         | 0.0028                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Morpholine                    | 0.020         | 0.0014                            | > 960       |                                                 |              |                                               |              |                                               |              |                                               |
| Naled                         | ND            | ND                                | > 204       |                                                 |              |                                               |              |                                               |              |                                               |
| Naphthalene                   | ND            | ND                                | > 792       |                                                 |              |                                               |              |                                               |              |                                               |
| Nephtha, Stoddard Solvent     | 0.040         | *                                 | > 480       |                                                 |              |                                               |              |                                               |              |                                               |
| Nitric Acid                   | 0.200         | 0.0102                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Nitrobenzene                  | 0.080         | 0.0079                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Nitromethane +                | 0.260         | 0.0128                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 2-Nitropropane                | 0.590         | 0.0424                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Oleum (Sulfuric Acid, Fuming) | 0.200         | 0.0158                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Parathion                     | 0.090         | 0.0211                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Petroleum Ether               | 4.550         | *                                 | > 204       |                                                 |              |                                               |              |                                               |              |                                               |
| Phenol                        | 0.030         | 0.0023                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Phosphoric Acid               | 0.500         | 0.0395                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Phosphorus Oxichloride        | 0.500         | 0.0619                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Phosphorus Trichloride        | 0.500         | 0.0554                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Polychlorinated Biphenyls     | 0.020         | *                                 | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Potassium Hydroxide           | 1.000         | 0.0453                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Propanol                      | 0.760         | 0.0368                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

| Chemical +                       | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|----------------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                                  |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Propionic Acid                   | 0.310         | 0.0185                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Propyl Acetate                   | 0.200         | 0.0165                            | > 240       |                                                 |              |                                               |              |                                               |              |                                               |
| Propylamine                      | 0.740         | 0.0353                            | > 612       |                                                 |              |                                               |              |                                               |              |                                               |
| Propylene (Gas) +                | 0.010         | 0.0003                            | 61          | 0.0003 (as)                                     | 60           | 0.0002                                        | 48           | 0.0005                                        | 76           | 0.0002                                        |
| Propylene Oxide                  | 0.680         | 0.0080                            | 154         | 0.021 (as)                                      | 137          | 0.0238                                        | 170          | 0.0182                                        |              |                                               |
| Pyridine                         | 0.020         | 0.0013                            | > 240       |                                                 |              |                                               |              |                                               |              |                                               |
| Silicon Tetrachloride            | 0.500         | 0.0685                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Sodium Hydroxide                 | 0.500         | 0.0226                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Sodium Hydroxide, 50% (USCG)     | ND            | ND                                | > 4260      |                                                 |              |                                               |              |                                               |              |                                               |
| Sodium Hydroxide, 50%            | 0.500         | 0.0161                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Styrene                          | 0.050         | 0.0042                            | > 240       |                                                 |              |                                               |              |                                               |              |                                               |
| Sulfuric Acid, 95%               | 0.200         | 0.0158                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Sulfur Monochloride              | 0.500         | 0.0545                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,1,2,2-Tetrachloroethane        | 0.230         | 0.0311                            | > 912       |                                                 |              |                                               |              |                                               |              |                                               |
| Tetrachloroethylene              | 0.110         | 0.0147                            | > 624       |                                                 |              |                                               |              |                                               |              |                                               |
| Tetrachloroethylene (USCG RADDC) | ND            | ND                                | 108         | (ac)                                            | 108          |                                               |              |                                               |              |                                               |
| Tetrachloroethylene (27C) +      | 0.001         | 0.0001                            | 7           | (3hr)                                           | 180          |                                               | 8            | 33.0000                                       | 44           | 3.0000                                        |
| Tetrahydrofuran (USCG RADDC)     | ND            | ND                                | > 330       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,1,1-Trichloroethane            | 0.600         | 0.0646                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Trichloroethylene                | 0.070         | 0.0017                            | 148         | 0.031 (as)                                      | 143          | 0.0340                                        | 156          | 0.0272                                        | 146          | 0.0318                                        |
| Trichloroethylene                | 0.010         | 0.0011                            | 138         | 0.031 (6hr)                                     | 155          | 0.0148                                        | 140          | 0.0233                                        | 120          | 0.0540                                        |
| Toluene                          | 0.060         | 0.0045                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Toluene-2,4-Diisocyanate         | 0.690         | 0.0969                            | > 198       |                                                 |              |                                               |              |                                               |              |                                               |
| o-Toluidine                      | 0.430         | 0.0372                            | > 198       |                                                 |              |                                               |              |                                               |              |                                               |
| Turpentine                       | 0.030         | *                                 | > 216       |                                                 |              |                                               |              |                                               |              |                                               |
| Vinyl Acetate                    | 0.210         | 0.0036                            | 106         | 0.059 (as)                                      | 74           | 0.0550                                        | 137          | 0.0622                                        |              |                                               |
| Vinyl Methyl Ether +             | 0.540         | 0.0253                            | 60          | 2.242 (3hr)                                     | 60           | 3.5833                                        | 60           | 2.3667                                        | 60           | 0.7750                                        |
| Vinylidene Chloride              | 0.490         | 0.0383                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Vinylidene Chloride +            | 0.010         | 0.0008                            | 51          | 0.022 (3hr)                                     | 52           | 0.0117                                        | 52           | 0.0110                                        | 48           | 0.0433                                        |

(Continued)

TABLE A-1. SUMMARY OF CHALLENGE 5100 PERMEATION TESTS RESULTS AT 25C

| Chemical +               | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average                                         |             | Replicate #1                                  |             | Replicate #2                                  |             | Replicate #3                                  |             |
|--------------------------|---------------|-----------------------------------|-------------------------------------------------|-------------|-----------------------------------------------|-------------|-----------------------------------------------|-------------|-----------------------------------------------|-------------|
|                          |               |                                   | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min) |
| Vinylidene Fluoride +    | 0.700         | 0.0361                            |                                                 | > 180       |                                               |             |                                               |             |                                               |             |
| Xylenes                  | 0.130         | 0.0111                            |                                                 | > 180       |                                               |             |                                               |             |                                               |             |
| Xylenol (Dimethylphenol) | ND            | ND                                |                                                 | > 198       |                                               |             |                                               |             |                                               |             |

+ Received after initial model development effort.

\* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area. Values entered as (°) could not be converted. ND indicates not determined.

Note: ul indicates that the MDR and the reported rate are reported in units of ul/cm<sup>2</sup>-min.

\*\* Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses when known. (ss) indicates a steady-state permeation rate value. (nc) indicates that no permeation time curve was available.

Source: U.S. Coast Guard Research and Development Center

Testing Laboratory: Texas Research International (unless otherwise noted)

TABLE A-2. SUMMARY OF CHALLENGE \$200 PERMEATION TESTS RESULTS AT 25C

| Chemical +                 | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|----------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                            |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Acetone                    | 1.000         | 0.0404                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Acetone (27C) +            | 0.010         | 0.0004                            | 116         | 0.0004 (3hr)                                    | 116          | 0.0002                                        | 116          | 0.0005                                        | 116          | 0.0005                                        |
| Acetone (27C) +            | 0.001         | 0.00004                           | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Acetone (ChemFab) +        | 0.100         | *                                 | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Acetonitrile               | 2.000         | 0.0662                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Acetonitrile (ChemFab) +   | 2.000         | *                                 | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Acetyl Chloride +          | 0.020         | 0.0013                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Allyl Chloride +           | 0.030         | 0.0019                            | 56          | 0.2833 (3hr)                                    | 68           | 0.2867                                        | 64           | 0.1498                                        | 36           | 0.4133                                        |
| Ammonia (Gas)              | 0.300         | 0.0041                            | 31          | 0.1144 (ss)                                     | 36           | 0.0783                                        | 24           | 0.1583                                        | 32           | 0.1067                                        |
| Ammonia (Gas) +            | 0.070         | 0.0010 ul                         | 25          | 0.2378 (3hr)                                    | 18           | 0.2683                                        | 23           | 0.2867                                        | 35           | 0.1583                                        |
| Ammonia (Gas) (27C) +      | 0.030         | 0.0004 ul                         | 32          | 0.1490 (ss)                                     | 32           | 0.1200                                        | 32           | 0.2183                                        | 32           | 0.1100                                        |
| Ammonia (Gas) (ChemFab) +  | 0.100         | *                                 | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Ammonium Hydroxide +       | 0.250         | 0.0071                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Ammonium Hydroxide (27C) + | 7.200         | 0.2033                            | 120         | 0.3390 (3hr)                                    | 120          | 0.2500                                        | 120          | 0.4500                                        | 120          | 0.3167                                        |
| Ammonium Sulfide, 20% +    | 1.000         | 0.0412                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Asphalt +                  | 1.000         | *                                 | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Benzaldehyde +             | 0.010         | 0.0009                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Benzonitrile +             | 0.010         | 0.0008                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Benzonitrile +             | 0.020         | 0.0017                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Benzyl Bromide +           | 0.010         | 0.0014                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Benzylamine +              | 0.010         | 0.0009                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Bromochloromethane         | 0.010         | 0.0009                            | 120         | 0.0281 (3hr)                                    | 144          | 0.0245                                        | 84           | 0.0325                                        | 132          | 0.0272                                        |
| 1,3-Butadiene (Gas)        | 0.030         | 0.0031                            | 98          | 0.0188 (7hr)                                    | 93           | 0.0188                                        | 109          | 0.0147                                        | 93           | 0.0230                                        |
| 1,3-Butadiene (Gas) +      | 0.068         | 0.0030                            | 5           | 0.0389 (5hr)                                    | 8            | 0.0240                                        | 4            | 0.0375                                        | 4            | 0.0552                                        |
| 1,3-Butadiene (Gas) +      | 0.010         | 0.0004 ul                         | 24          | 0.0795 (3hr)                                    | 24           | 0.1300                                        | 24           | 0.0700                                        | 24           | 0.0383                                        |
| Butane (Gas)               | 0.300         | 0.0141                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 2-Butene (Gas) (27C) +     | 0.040         | 0.0018                            | 55          | 0.1300 (3hr)                                    | 72           | 0.1000                                        | 36           | 0.2000                                        | 56           | 0.1000                                        |
| Butyl Chloride             | 0.070         | 0.0052                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Butylamine +               | 0.010         | 0.0006                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |

(Continue.)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

| Chemical +                        | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|-----------------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                                   |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| iso-Butyronitrile +               | 0.310         | 0.0173                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Carbon Disulfide                  | 0.010         | 0.0006                            | 20          | 0.0335 (3hr)                                    | 20           | 0.0497                                        | 20           | 0.0208                                        | 20           | 0.0300                                        |
| Carbon Disulfide (ChemFab) +      | 0.300         | *                                 | 143         | 0.0500 (ac)                                     |              |                                               |              |                                               |              |                                               |
| Cetyltrimethylammonium Chloride + | 0.100         | 0.0258                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Chlorine (Gas) +                  | 1.000         | 0.0572                            | 70          | 0.0182 (ac)                                     | 90           | 0.0138                                        | 60           | 0.0267                                        | 60           | 0.0143                                        |
| Chlorine (Gas) +                  | 38.000        | *                                 | 60          | 170.33 (ac)                                     | 30           | 320.00                                        | 90           | 140.00                                        | 60           | 51.0000                                       |
| Chlorine (Gas) (ChemFab) +        | 0.300         | *                                 | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Chloroacetone +                   | 0.010         | 0.0007                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Chloroacetyl Chloride +           | 0.020         | 0.0018                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 4-Chlorobutyronitrile +           | 0.030         | 0.0025                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Chloroethane +                    | 0.070         | 0.0036                            | 60          | 0.6330 (ac)                                     | 68           | 0.3667                                        | 52           | 1.2500                                        | 60           | 0.2833                                        |
| 2-Chloroethanol +                 | 0.020         | 0.0013                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Chloromethane (ChemFab) +         | 0.260         | *                                 | 21          | 0.7600 (ac)                                     |              |                                               |              |                                               |              |                                               |
| Chloromethyl Methyl Ether +       | 0.010         | 0.0006                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 1-Chloropropane                   | 2.000         | 0.1267                            | 260         | 0.2367 (7hr)                                    | 285          | 0.1433                                        | 269          | 0.2350                                        | 225          | 0.3317                                        |
| Chromyl Chloride +                | 0.100         | 0.0125                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Cresols +                         | 0.010         | 0.0009                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Cumene +                          | 0.010         | 0.0010                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Cyanogen (Gas) +                  | 0.500         | 0.0210                            | 30          | 0.0600 (ac)                                     |              |                                               |              |                                               |              |                                               |
| Cyanogen Bromide (Solid) +        | 1.000         | 0.0855                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Cyanogen Chloride (Gas) +         | 0.500         | 0.0248                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Cyclopropane (Gas) +              | 0.020         | 0.0007 al                         | 92          | 0.0008 (3hr)                                    | 96           | 0.0003                                        | 72           | 0.0015                                        | 108          | 0.0005                                        |
| Cyclopropane (Gas) (27C) +        | 0.002         | 0.0001                            | 78          | 0.0008 (3hr)                                    | 76           | 0.0008                                        | 80           | 0.0013                                        | 80           | 0.0002                                        |
| Decyl Aldehyde +                  | 0.010         | 0.0013                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Dibromomethane                    | 0.030         | 0.0042                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,3-Dichloro-2-Butene +           | 0.010         | 0.0010                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 1,2-Dichloroethylene +            | 0.010         | 0.0008                            | 24          | 0.3578 (ac)                                     | 28           | 0.2850                                        | 28           | 0.4050                                        | 16           | 0.3833                                        |
| cis-1,2-Dichloroethylene          | 0.010         | 0.0008                            | 69          | 0.1550 (3hr)                                    | 56           | 0.2200                                        | 80           | 0.0967                                        | 72           | 0.1483                                        |
| trans-1,2-Dichloroethylene +      | 0.010         | 0.0008                            | 19          | 1.3967 (ac)                                     | 19           | 1.4317                                        | 19           | 1.4700                                        | 19           | 1.2883                                        |

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE S200 PERMEATION TESTS RESULTS AT 25C

| Chemical +                          | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                     | Replicate #1 |                                   | Replicate #2 |                                   | Replicate #3 |                                   |
|-------------------------------------|---------------|-----------------------------------|-------------|-------------------------------------|--------------|-----------------------------------|--------------|-----------------------------------|--------------|-----------------------------------|
|                                     |               |                                   | BT<br>(min) | rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | rate<br>(ug/cm <sup>2</sup> -min) |
| Dichloromethane (27C) +             | 0.007         | 0.0005                            | 83          | 3.6700 (3hr)                        | 84           | 4.0000                            | 88           | 3.0000                            | 76           | 4.0000                            |
| Dichloromethane +                   | 0.005         | 0.0003                            | 64          | 0.2630 (3hr)                        | 68           | 0.2300                            | 52           | 0.3700                            | 72           | 0.1900                            |
| Dichloromethane (ChemFab) +         | 0.100         | *                                 | 64          | 0.1200 (ec)                         |              |                                   |              |                                   |              |                                   |
| Diethylamine (ChemFab) +            | 0.400         | *                                 | > 300       |                                     |              |                                   |              |                                   |              |                                   |
| Dimethyl Acetamide*                 | 0.010         | 0.0007                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Dimethylformamide (ChemFab) +       | 0.700         | *                                 | > 300       |                                     |              |                                   |              |                                   |              |                                   |
| Dimethylhydrazine +                 | 0.090         | 0.0044                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Dimethyl Sulfide (Methyl Sulfone) + | 0.010         | 0.0008                            | 95          | 0.0005 (3hr)                        | 116          | 0.0005                            | 76           | 0.0005                            | 92           | 0.0005                            |
| Dimethyl Sulfide (Methyl Sulfone) + | 0.010         | 0.0008                            | 48          | 0.0002 (3hr)                        | 60           | 0.0002                            | 40           | 0.0002                            | 44           | 0.0003                            |
| Dimethyl Sulfoxide                  | 0.010         | 0.0006                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Diphenyldichloroallene +            | 3.000         | 0.6123                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| 1-Dodecanethiol +                   | 1.000         | 0.1630                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Ethane +                            | 1.000         | 0.0243                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Ethanethiol +                       | 0.020         | 0.0010                            | 65          | 0.0028 (3hr)                        | 60           | 0.0030                            | 76           | 0.0025                            | 60           | 0.0030                            |
| Ethanethiol (27C) +                 | 0.003         | 0.0002                            | 83          | 15.3300 (3hr)                       | 88           | 4.0000                            | 88           | 16.0000                           | 72           | 26.0000                           |
| Ethyl Acetate                       | 0.010         | 0.0007                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Ethyl Acetate (ChemFab) +           | 0.100         | *                                 | > 300       |                                     |              |                                   |              |                                   |              |                                   |
| Ethyl Acrylate                      | 0.050         | 0.0040                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Ethyl Chloroformate +               | 0.200         | 0.0175                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Ethyl Ether (27C)                   | 0.010         | 0.0006                            | 127         | 0.3761 (20hr)                       | 104          | 0.4050                            | 136          | 0.3033                            | 140          | 0.4200                            |
| Ethyl Ether (27C) +                 | 0.010         | 0.0006                            | 92          | 0.0080 (3hr)                        | 92           | 0.0143                            | 96           | 0.0035                            | 88           | 0.0072                            |
| Ethyl Ether (27C) +                 | 0.003         | 0.0002                            | 149         | 2.1000 (3hr)                        | 144          | 4.9000                            | 156          | 0.9000                            | 148          | 0.5000                            |
| Ethyl Ether (27C) +                 | 0.010         | 0.0006                            | 40          | 173.33 (3hr)                        | 44           | 130.00                            | 36           | 220.00                            | 40           | 170.00                            |
| 2-Ethylhexanal +                    | 0.010         | 0.0010                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| 2-Ethylhexylacrylate +              | 0.010         | 0.0015                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Ethyl Methacrylate +                | 0.010         | 0.0009                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Ethyl Vinyl Ether                   | 0.020         | 0.0012                            | 23          | 0.6694 (3hr)                        | 40           | 0.3933                            | 8            | 0.5517                            | 20           | 1.0633                            |
| Ethyl Vinyl Ketone +                | 0.060         | 0.0041                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |
| Ethylencimine +                     | 0.020         | 0.0007                            | > 180       |                                     |              |                                   |              |                                   |              |                                   |

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE S200 PERMEATION TESTS RESULTS AT 25C

| Chemical +                          | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|-------------------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                                     |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Ethylene Oxide (Gas) +              | 3.000         | 0.1066                            | 57          | 0.7250 (3hr)                                    | 68           | 0.8250                                        | 60           | 0.8483                                        | 44           | 0.5017                                        |
| Ethylene Oxide (Gas) +              | 0.650         | 0.0231                            | 25          | 0.1420 (3hr)                                    | 20           | 0.1418                                        | 24           | 0.1683                                        | 32           | 0.1160                                        |
| Ethylene Oxide (Gas) (ChemFab) +    | 0.340         | *                                 | 64          | 0.7600 (ac)                                     |              |                                               |              |                                               |              |                                               |
| Freon 11 (Trichlorofluoromethane) + | 0.500         | 0.0554                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Freon 12 (Dichlorodifluoromethane)  | 0.100         | 0.0098                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Freon 21 (Dibromofluoromethane) +   | 3.000         | 0.2491                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Freon 22 (Chlorodifluoromethane) +  | 3.000         | 0.2093                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Gasoline JP-4 +                     | 0.100         | *                                 | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Hexanal +                           | 0.020         | 0.0016                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Hexane +                            | 0.100         | 0.0070                            | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Hexene +                            | 0.010         | 0.0007                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Hydrazine (ChemFab) +               | 0.760         | *                                 | > 480       |                                                 |              |                                               |              |                                               |              |                                               |
| Hydrobromic Acid (Gas) +            | 10.000        | 0.6527                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Hydrogen Chloride (Gas) (ChemFab)   | 0.040         | *                                 | > 480       |                                                 |              |                                               |              |                                               |              |                                               |
| Hydrogen Cyanide (Gas) (ChemFab)    | 0.050         | *                                 | > 480       |                                                 |              |                                               |              |                                               |              |                                               |
| Hydrogen Sulfide (Gas) +            | 0.030         | 0.0008 ul                         | 4           | 0.0028 (3hr)                                    | 4            | 0.0017                                        | 4            | 0.0005                                        | 4            | 0.0017                                        |
| Hydrogen Sulfide (27C) (Gas) +      | 0.010         | 0.0003 ul                         | 8           | 0.0070 (3hr)                                    | 8            | 0.0055                                        | 8            | 0.0077                                        | 8            | 0.0068                                        |
| Hydrogen Sulfide (Gas) +            | 0.030         | 0.0008 ul                         | 15          | 0.0078 (ac)                                     | 20           | 0.0017                                        | 12           | 0.0133                                        | 12           | 0.0083                                        |
| 2-Hydroxyethyl Acrylate +           | 0.120         | 0.0112                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Isobutylamine +                     | 0.030         | 0.0018                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Isobutyraldehyde +                  | 0.010         | 0.0006                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Isoprene                            | 0.010         | 0.0005                            | 9           | 0.1820 (3hr)                                    | 8            | 0.0615                                        | 8            | 0.1295                                        | 12           | 0.3550                                        |
| Isovaleraldehyde +                  | 0.010         | 0.0007                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Methane +                           | 1.000         | 0.0129                            | 7           | 18.0000 (ac)                                    | 7            | 16.0000                                       | 6            | 27.0000                                       | 8            | 11.0000                                       |
| Methanol (ChemFab) +                | 0.400         | *                                 | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Acetate +                    | 0.020         | 0.0012                            | 112         | 0.0053 (3hr)                                    | 84           | 0.0072                                        | 144          | 0.0042                                        | 108          | 0.0048                                        |
| Methyl Acrylate +                   | 7.000         | 0.4861                            | 7           | (3hr)                                           | 116          | 0.7683                                        | 112          | 0.7700                                        | > 180        |                                               |
| Methyl Bromide (Gas) +              | 0.400         | 0.0306                            | 21          | 0.0347 (3hr)                                    | 20           | 0.0367                                        | 20           | 0.0367                                        | 24           | 0.0308                                        |
| Methyl Bromide (Gas) +              | 0.020         | 0.0015 ul                         | 20          | 0.0065 (3hr)                                    | 20           | 0.0053                                        | 20           | 0.0073                                        | 20           | 0.0067                                        |

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 25C

| Chemical +                        | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|-----------------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                                   |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Methyl Chloride (Gas) (27C) +     | 0.060         | 0.0024 ul                         | 16          | 0.0020 (ss)                                     | 16           | 0.0020                                        | 16           | 0.0020                                        | 16           | 0.0020                                        |
| Methyl Chloroformate +            | 0.050         | 0.0038                            | 81          | 0.0120 (3hr)                                    | 76           | 0.0092                                        | 76           | 0.0198                                        | 92           | 0.0068                                        |
| Methyl Chloroformate (27C) +      | 0.100         | 0.0076                            | 95          | 0.9500 (3hr)                                    | 116          | 0.7500                                        | 72           | 1.2000                                        | 96           | 0.8900                                        |
| Methyl Ethyl Ketone (ChemFab) +   | 1.000         | *                                 | > 120       |                                                 |              |                                               |              |                                               |              |                                               |
| Methyl Iodide +                   | 0.370         | 0.0424                            | 32          | 17.2333 (3hr)                                   | 32           | 27.0000                                       | 32           | 10.8000                                       | 32           | 13.9000                                       |
| Methyl Isocyanate +               | 0.010         | 0.0005                            | 92          | 0.0202 (3hr)                                    | 96           | 0.0207                                        | 72           | 0.0188                                        | 108          | 0.0212                                        |
| Methyl Vinyl Ketone               | 0.010         | 0.0006                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Methylamine (Gas)                 | 0.200         | 0.0050                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Monoethanolamine +                | 0.010         | 0.0005                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Nicotine +                        | 1.000         | 0.1309                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Nitric Acid, Red Fuming (ChemFab) | 0.100         | *                                 | > 480       |                                                 |              |                                               |              |                                               |              |                                               |
| Nitric Oxide (Gas) +              | 1.000         | 0.0508 ul                         | 30          | 2.0000                                          |              |                                               |              |                                               |              |                                               |
| 2-Nitroaniline +                  | 0.100         | 0.0111                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 4-Nitroaniline +                  | 0.010         | 0.0011                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Nitrobenzene (ChemFab) +          | 1.000         | *                                 | > 300       |                                                 |              |                                               |              |                                               |              |                                               |
| Nitroethane +                     | 0.010         | 0.0006                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Nitrogen Dioxide (Gas) +          | 0.500         | 0.0186 ul                         | 4           | 4.9900 (ss)                                     | 4            | 5.3333                                        | 4            | 6.3500                                        | 4            | 3.2833                                        |
| Nitrogen Tetroxide (Gas) +        | 0.080         | 0.0059 ul                         | 15          | 13.7600 (ss)                                    | 24           | 16.2000                                       | 4            | 18.7000                                       | 16           | 6.4000                                        |
| Nitromethane                      | 0.730         | 0.0359                            | 168         | 0.0538 (ss)                                     | 168          | 0.0447                                        | 168          | 0.0630                                        | 168          | 0.0537                                        |
| Nitroethane +                     | 0.700         | 0.0345                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| o-Nitrotoluene +                  | 0.010         | 0.0011                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Nonyl Phenol +                    | 0.100         | 0.0177                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Pentachlorophenol +               | 1.000         | 0.2149                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Pentanedione +                    | 0.100         | 0.0081                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| 2,4-Pentanedione +                | 0.070         | 0.0057                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Pentene +                         | 0.010         | 0.0006                            | 81          | 0.0440 (ss)                                     | 88           | 0.0500                                        | 64           | 0.0500                                        | 92           | 0.0333                                        |
| Pentylchlorosilane +              | 0.010         | *                                 | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Perchloric Acid +                 | 0.350         | 0.0284                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Phenyldecane +                    | 1.000         | 0.1984                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE S200 PERMEATION TESTS RESULTS AT 25C

| Chemical +                      | MDL*<br>(ppm) | MDR*<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | Average     |                                                                | Replicate #1 |                                                              | Replicate #2 |                                                              | Replicate #3 |                                                              |
|---------------------------------|---------------|--------------------------------------------------|-------------|----------------------------------------------------------------|--------------|--------------------------------------------------------------|--------------|--------------------------------------------------------------|--------------|--------------------------------------------------------------|
|                                 |               |                                                  | BT<br>(min) | Reported<br>rate**<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) | BT<br>(min)  | Reported<br>rate<br>( $\mu\text{g}/\text{cm}^2\text{-min}$ ) |
| Phosgene (Gas) (27C) +          | 0.500         | *                                                | 60          | 0.2000 (ac)                                                    | 60           | 0.2000                                                       | 60           | 0.2000                                                       | 60           | 0.2000                                                       |
| Phosgene (Gas) (ChemFab) +      | 1.000         | *                                                | > 480       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Potassium Hydroxide +           | 0.500         | 0.0226                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Propane +                       | 0.010         | 0.0004                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| 1-Propanethiol +                | 0.050         | 0.0031                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| 2-Propanethiol +                | 0.010         | 0.0006                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Propylacetate +                 | 0.020         | 0.0012                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Propylene Oxide (27C) +         | 0.010         | 0.0005                                           | 89          | 0.0001 (3hr)                                                   | 96           | 0.0001                                                       | 96           | 0.0001                                                       | 76           | 0.0002                                                       |
| Sodium Hydroxide +              | 0.500         | 0.0161                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Sodium Hydroxide, 50% (ChemFab) | 0.200         | *                                                | > 300       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Sulfur Dioxide (Gas) +          | 47.000        | 2.4292 ml                                        | 60          | 0.0695 (3hr)                                                   | 60           | 0.0717                                                       | 60           | 0.1250                                                       | 60           | 0.0717                                                       |
| Sulfur Dioxide (Gas) +          | 1.000         | 0.0517 ml                                        | 40          | 2.3000 (ac)                                                    | 30           | 2.3000                                                       | 60           | 2.3000                                                       | 30           | 2.3000                                                       |
| Sulfuryl Chloride +             | 0.010         | 0.0011                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Tetrachloroethylene (ChemFab) + | 0.200         | *                                                | > 300       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Tetrachloroethylene +           | 1.000         | 0.1525                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Tetrahydrofuran (ChemFab) +     | 0.100         | *                                                | > 300       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Toluene (ChemFab) +             | 0.100         | *                                                | > 300       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| 1,1,2-Trichloroethane +         | 0.690         | 0.0743                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Trichloroethylene +             | 0.010         | 0.0011                                           | 49          | 0.1949 (3hr)                                                   | 52           | 0.2017                                                       | 56           | 0.1630                                                       | 40           | 0.2700                                                       |
| Trichloroethylene (27C) +       | 0.010         | 0.0011                                           | 72          | 0.0028 (3hr)                                                   | 80           | 0.0022                                                       | 76           | 0.0042                                                       | 60           | 0.0022                                                       |
| Trichlorobenzene +              | 0.010         | 0.0013                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Trichloromethane +              | 0.010         | 0.0012                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Trimethylamine +                | 0.150         | 0.0072                                           | 20          |                                                                | 20           |                                                              |              |                                                              |              |                                                              |
| Trimethylamine +                | 0.014         | 0.0007                                           | > 180       |                                                                |              |                                                              |              |                                                              |              |                                                              |
| Trimethylamine +                | 0.150         | 0.0072                                           | 25          |                                                                | 20           |                                                              | 24           |                                                              | 32           |                                                              |
| Vinyl Acetate                   | 0.020         | 0.0014                                           | 69          | 0.2522 (ac)                                                    | 68           | 0.2433                                                       | 64           | 0.3350                                                       | 76           | 0.1783                                                       |
| Vinyl Acetate +                 | 0.004         | 0.0003                                           | 73          | 38.0000 (3hr)                                                  | 65           | 50.0000                                                      | 85           | 35.0000                                                      | 69           | 29.0000                                                      |
| Vinyl Acetate +                 | 0.004         | 0.0003                                           | 109         | 11.2800 (3hr)                                                  | 77           | 25.2000                                                      | 132          | 2.1900                                                       | 124          | 6.4400                                                       |
| Vinyl Chloride (Gas) +          | 0.010         | 0.0005 ml                                        | 12          | 0.0840 (3hr)                                                   | 12           | 0.0860                                                       | 12           | 0.0952                                                       | 12           | 0.0715                                                       |

(Continued)

TABLE A-2. SUMMARY OF CHALLENGE S200 PERMEATION TESTS RESULTS AT 25C

| Chemical +                  | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average     |                                                 | Replicate #1 |                                               | Replicate #2 |                                               | Replicate #3 |                                               |
|-----------------------------|---------------|-----------------------------------|-------------|-------------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|--------------|-----------------------------------------------|
|                             |               |                                   | BT<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | BT<br>(min)  | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Vinyl Chloride (Gas) +      | 0.020         | 0.0010 ul                         | 7           | 0.0600 (3hr)                                    | 4            | 0.0800                                        | 8            | 0.0400                                        | 8            | 0.0400                                        |
| Vinyl Methyl Ether +        | 33.070        | 1.5448                            | 28          | 19.1000 (3hr)                                   | 36           | 7.6500                                        | 24           | 35.0500                                       | 24           | 14.6000                                       |
| Vinyl Sulfone +             | 0.010         | 0.0010                            | > 180       |                                                 |              |                                               |              |                                               |              |                                               |
| Vinylidene Chloride         | 0.490         | 0.0343                            | 124         | 1.0828 (3hr)                                    | 120          | 1.4800                                        | 120          | 0.8800                                        | 132          | 0.8883                                        |
| Vinylidene Chloride (27C) + | 0.010         | 0.0008                            | 40          | 0.0860 (3hr)                                    | 32           | 0.1570                                        | 40           | 0.0655                                        | 48           | 0.0352                                        |
| Vinylidene Chloride +       | 0.030         | 0.0023                            | 61          | 0.0822 (3hr)                                    | 64           | 0.0567                                        | 60           | 0.0900                                        | 60           | 0.1000                                        |
| Vinylidene Fluoride +       | 0.040         | 0.0021                            | 32          | 0.0760 (3hr)                                    | 32           | 0.0700                                        | 32           | 0.0900                                        | 32           | 0.0700                                        |

+ Received after initial model development effort.

\* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area. Values entered as (\*) could not be converted. ND indicates not determined.

Note: ul indicates MDR and reported rate are in units of ul/cm<sup>2</sup>-min, ml indicates MDR and reported rate are in units of ml/cm<sup>2</sup>-min.

\*\* Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses when known. (ns) indicates a steady-state permeation rate value. (ac) indicates that no permeation time curve was available.

Source: U.S. Coast Guard Research and Development Center

Testing Laboratory: Texas Research International (unless otherwise noted)

(USCG R&DC=U.S. Coast Guard Research and Development Center, ChemFab=Chemical Fabrics Corporation)

**APPENDIX B**

**CHALLENGE 5200 PERMEATION TEST RESULTS  
AT ELEVATED TEMPERATURES**

TABLE B-1. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 30C

| Chemical            | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average                 |                                                 | Replicate #1            |                                               | Replicate #2            |                                               | Replicate #3            |                                               |
|---------------------|---------------|-----------------------------------|-------------------------|-------------------------------------------------|-------------------------|-----------------------------------------------|-------------------------|-----------------------------------------------|-------------------------|-----------------------------------------------|
|                     |               |                                   | Break.<br>time<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Acetone             | 0.01          | 0.0004                            | > 210                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Acrolein            | 0.17          | 0.0077                            | 56                      | 0.095 (ac)                                      | 48                      | 0.102                                         | 60                      | 0.071                                         | 60                      | 0.112                                         |
| Acrylonitrile       | 0.04          | 0.0017                            | 76                      | 0.028 (ac)                                      | 84                      | 0.024                                         | 68                      | 0.032                                         | 76                      | 0.028                                         |
| Allyl Chloride      | 0.05          | 0.0031                            | 56                      | 0.035 (ac)                                      | 52                      | 0.030                                         | 56                      | 0.051                                         | 60                      | 0.024                                         |
| Carbon Disulfide    | 0.01          | 0.0006                            | 15                      | 0.234 (ac)                                      | 16                      | 0.178                                         | 16                      | 0.230                                         | 12                      | 0.293                                         |
| Dichloromethane     | 0.01          | 0.0007                            | 43                      | 0.037 (ac)                                      | 48                      | 0.028                                         | 36                      | 0.040                                         | 44                      | 0.043                                         |
| Dichloromethane     | 0.03          | 0.0021                            | 52                      | 0.072 (ac)                                      | 49                      | 0.091                                         | 53                      | 0.062                                         | 53                      | 0.063                                         |
| Diethylamine        | 0.04          | 0.0024                            | > 1182                  |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Dimethylformamide   | 0.02          | 0.0012                            | > 240                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Ethyl Acetate       | 0.02          | 0.0014                            | > 300                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Hexane              | 0.10          | 0.0070                            | > 300                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Methanol            | 0.25          | 0.0065                            | > 300                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Nitrobenzene        | 0.10          | 0.0099                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Propylene Oxide     | 0.04          | 0.0019                            | 108                     | 0.008 (ac)                                      | 108                     | 0.009                                         | 96                      | 0.013                                         | 120                     | 0.003                                         |
| Propylene Oxide     | 0.01          | 0.0005                            | 115                     | 0.003 (3hr)                                     | 108                     | 0.004                                         | 112                     | 0.004                                         | 124                     | 0.002                                         |
| Tetrachloroethylene | 0.01          | 0.0013                            | > 240                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Tetrahydrofuran     | 0.19          | 0.0111                            | > 276                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Toluene             | 0.01          | 0.0007                            | > 300                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Trichloroethylene   | 0.01          | 0.0011                            | 84                      | 0.139 (ac)                                      | 80                      | 0.126                                         | 80                      | 0.122                                         | 92                      | 0.168                                         |
| Vinyl Acetate       | 0.03          | 0.0021                            | 101                     | 0.089 (ac)                                      | 98                      | 0.104                                         | 98                      | 0.083                                         | 107                     | 0.080                                         |

\* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area.

\*\* Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses when known. (ac) indicates that no permeation-time curve was available.

Source: U.S. Coast Guard Research and Development Center  
Testing Laboratory: Texas Research International

TABLE B-2. SUMMARY OF CHALLENGE 5200 PERMEATION TESTS RESULTS AT 35C

| Chemical            | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average                 |                                                 | Replicate #1            |                                               | Replicate #2            |                                               | Replicate #3            |                                               |
|---------------------|---------------|-----------------------------------|-------------------------|-------------------------------------------------|-------------------------|-----------------------------------------------|-------------------------|-----------------------------------------------|-------------------------|-----------------------------------------------|
|                     |               |                                   | Break.<br>time<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Acetone             | 0.01          | 0.0004                            | 67                      | 0.015 (4hr)                                     | 32                      | 0.016                                         | 80                      | 0.014                                         | 88                      | 0.015                                         |
| Acrolein            | 0.04          | 0.0018                            | 23                      | 0.679 (4hr)                                     | 20                      | 0.258                                         | 22                      | 0.218                                         | 27                      | 1.562                                         |
| Acrylonitrile       | 0.20          | 0.0086                            | 110                     | 0.071 (3hr)                                     | 93                      | 0.085                                         | 117                     | 0.067                                         | 121                     | 0.060                                         |
| Allyl Chloride      | 0.13          | 0.0080                            | 236                     | 0.530 (7hr)                                     | 229                     | 0.648                                         | 237                     | 0.552                                         | 241                     | 0.390                                         |
| Carbon Disulfide    | 0.01          | 0.0006                            | 16                      | 0.559 (3hr)                                     | 12                      | 0.608                                         | 16                      | 0.635                                         | 20                      | 0.435                                         |
| Chloroform          | 0.02          | 0.0019                            | > 240                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Dichloromethane     | 0.04          | 0.0027                            | 43                      | 0.188 (3hr)                                     | 44                      | 0.220                                         | 40                      | 0.175                                         | 44                      | 0.170                                         |
| Diethylamine        | 0.07          | 0.0041                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Dimethylformamide   | 0.01          | 0.0006                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Ethyl Acetate       | 0.01          | 0.0007                            | 179                     | 0.003 (6hr)                                     | 152                     | 0.004                                         | 204                     | 0.003                                         | 180                     | 0.004                                         |
| Hexane              | 0.02          | 0.0014                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Methanol            | 0.61          | 0.0158                            | 88                      | 0.063 (pc)                                      | 72                      | 0.077                                         | 88                      | 0.070                                         | 104                     | 0.043                                         |
| Nitrobenzene        | 0.07          | 0.0070                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| n-Propylamine       | 0.83          | 0.0396                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Propylene Oxide     | 0.06          | 0.0028                            | 111                     | 0.043 (3hr)                                     | 88                      | 0.060                                         | 124                     | 0.040                                         | 120                     | 0.030                                         |
| Tetrachloroethylene | 0.01          | 0.0013                            | 236                     | 0.058 (4hr)                                     | 236                     | 0.058                                         | 236                     | 0.072                                         | 236                     | 0.043                                         |
| Tetrahydrofuran     | 0.42          | 0.0244                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Toluene             | 0.01          | 0.0007                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Trichloroethylene   | 0.01          | 0.0011                            | 76                      | 0.337 (3hr)                                     | 68                      | 0.325                                         | 84                      | 0.338                                         | 76                      | 0.348                                         |
| Vinyl Acetate       | 0.01          | 0.0007                            | 60                      | 0.614 (4hr)                                     | 52                      | 0.643                                         | 52                      | 0.842                                         | 76                      | 0.357                                         |

\* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area.

\*\* Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses when known. (pc) indicates that no permeation-time curve was available.

Source: U. S. Coast Guard Research and Development Center  
Testing Laboratory: Texas Research International

TABLE B-3. SUMMARY OF CHALLENGE S200 PERMEATION TESTS RESULTS AT 40C

| Chemical            | MDL*<br>(ppm) | MDR*<br>(ug/cm <sup>2</sup> -min) | Average                 |                                                 | Replicate #1            |                                               | Replicate #2            |                                               | Replicate #3            |                                               |
|---------------------|---------------|-----------------------------------|-------------------------|-------------------------------------------------|-------------------------|-----------------------------------------------|-------------------------|-----------------------------------------------|-------------------------|-----------------------------------------------|
|                     |               |                                   | Break.<br>time<br>(min) | Reported<br>rate**<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) | Break.<br>time<br>(min) | Reported<br>rate<br>(ug/cm <sup>2</sup> -min) |
| Allyl Chloride      | 0.07          | 0.0043                            | 79                      | 0.512 (3hr)                                     | 64                      | 0.548                                         | 88                      | 0.517                                         | 84                      | 0.470                                         |
| Dichloromethane     | 0.03          | 0.0021                            | 29                      | 0.269 (3hr)                                     | 28                      | 0.303                                         | 32                      | 0.230                                         | 28                      | 0.273                                         |
| Epichlorohydrin     | 0.18          | 0.0134                            | 149                     | 0.221 (3hr)                                     | 132                     | 0.247                                         | 140                     | 0.227                                         | 176                     | 0.188                                         |
| Ethyl Chloroformate | 0.01          | 0.0009                            | 108                     | 0.259 (3hr)                                     | 116                     | 0.725                                         | 104                     | 0.033                                         | 104                     | 0.018                                         |
| Methacrylonitrile   | 0.25          | 0.0135                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Nitrobenzene        | 0.02          | 0.0020                            | > 180                   |                                                 |                         |                                               |                         |                                               |                         |                                               |
| Tetrachloroethylene | 0.01          | 0.0013                            | 201                     | 0.097 (3hr)                                     | 164                     | 0.113                                         | 176                     | 0.125                                         | 263                     | 0.052                                         |
| Trichloroethylene   | 0.01          | 0.0011                            | 81                      | 0.477 (as)                                      | 68                      | 0.452                                         | 80                      | 0.567                                         | 96                      | 0.412                                         |
| Vinyl Acetate       | 0.02          | 0.0014                            | 69                      | 0.252 (8hr)                                     | 68                      | 0.243                                         | 64                      | 0.335                                         | 76                      | 0.178                                         |

\* MDL = Minimum detectable concentration determined by syringe pump calibration; MDR = Minimum detectable permeation rate calculated from the MDL (ppm), the open-loop carrier gas flow rate, and the clothing material surface area.

\*\* Reported rate is the permeation rate at the conclusion of the permeation test or the maximum rate measured during the test. Permeation test durations are indicated in parentheses when known. (as) indicates a steady-state permeation rate.

Source: U.S. Coast Guard Research and Development Center  
Testing Laboratory: Texas Research International

**APPENDIX C**

**CHEMICAL MIXTURE PERMEATION TEST RESULTS  
(TEXAS RESEARCH INTERNATIONAL)**

TABLE C-1. CHEMICAL MIXTURE PERMEATION TEST RESULTS

| Mix. # | Mixture             |                    | Material            | Component #1 |          | Component #2 |              | Component #3 |          | Component #1 |              | Component #2 |          | Component #3 |              |
|--------|---------------------|--------------------|---------------------|--------------|----------|--------------|--------------|--------------|----------|--------------|--------------|--------------|----------|--------------|--------------|
|        | Component #1        | Component #2       |                     | MDL (ppm)    | BT (min) | Component #1 | Component #2 | MDL (ppm)    | BT (min) | Component #1 | Component #2 | MDL (ppm)    | BT (min) | Component #1 | Component #2 |
| 1      | Acetone             | Vinyl Acetate      |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 2      | Acetonitrile        | Chlorobenzene      |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 3      | Acetonitrile        | 1,2-Dichloroethane |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 4      | Acetonitrile        | Nitrobenzene       |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 5      | Acetonitrile        | Chlorobenzene      | Nitrobenzene        |              |          |              |              |              |          |              |              |              |          |              |              |
| 6      | Acrylonitrile       | Trichloroethylene  |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 7      | Carbon Disulfide    | Dichloromethane    | (75%)               |              |          |              |              |              |          |              |              |              |          |              |              |
| 8      | Carbon Disulfide    | Dichloromethane    | (50%)               |              |          |              |              |              |          |              |              |              |          |              |              |
| 9      | Carbon Disulfide    | Dichloromethane    | (25%)               |              |          |              |              |              |          |              |              |              |          |              |              |
| 10     | Carbon Disulfide    | Dimethylformamide  |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 11     | Chlorobenzene       | Dichloromethane    |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 12     | Dichloromethane     | Nitrobenzene       |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 13     | Dichloromethane     | Trichloroethylene  | (75%)               |              |          |              |              |              |          |              |              |              |          |              |              |
| 14     | Dichloromethane     | Trichloroethylene  | (50%)               |              |          |              |              |              |          |              |              |              |          |              |              |
| 15     | Dichloromethane     | Trichloroethylene  | (25%)               |              |          |              |              |              |          |              |              |              |          |              |              |
| 16     | Acetone             | Chlorobenzene      |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 17     | Acetone             | 1,2-Dichloroethane |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 18     | Acetone             | Epichlorohydrin    |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 19     | Acetone             | Nitrobenzene       |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 20     | Acetone             | Toluene            |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 21     | Acetone             | Toluene            | Methyl Ethyl Ketone |              |          |              |              |              |          |              |              |              |          |              |              |
| 22     | Acetone             | Toluene            | Nitrobenzene        |              |          |              |              |              |          |              |              |              |          |              |              |
| 23     | Benzene             | Dimethyl Sulfide   |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 24     | Benzene             | Dimethyl Sulfide   | 1,2-Dichloroethane  |              |          |              |              |              |          |              |              |              |          |              |              |
| 25     | Chloroform          | Dimethylformamide  |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 26     | Chloroform          | Dimethyl Sulfide   |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 27     | Chloroform          | Nitromethane       |                     |              |          |              |              |              |          |              |              |              |          |              |              |
| 28     | Methyl Ethyl Ketone | 2-Nitropropane     | Toluene             |              |          |              |              |              |          |              |              |              |          |              |              |
| 29     | Nitrobenzene        | Toluene            |                     |              |          |              |              |              |          |              |              |              |          |              |              |

\* Reported MDL values did not indicate whether they were for specific mixture components or generic values for the mixture.

\*\* Reported MDLs are generic mixture values. The breakthrough times report the time at which some component was detected but the specific component was not identified.

Source: U.S. Coast Guard Research and Development Center

Testing Laboratory: Texas Research International

**APPENDIX D**

**CHEMICAL MIXTURE PERMEATION TEST RESULTS  
(ARTHUR D. LITTLE)**

**TABLE D-1. DATA REPORT FOR CARBON DISULFIDE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Carbon Disulfide   | N/A                | N/A                |
| CAS Number:      | 75-15-0            | N/A                | N/A                |
| Concentration:   | Neat               | N/A                | N/A                |
| Chemical Source: | Fisher             |                    |                    |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 23-24                                       |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 7.7                | N/A                | N/A                |
| Test System Sensitivity Factor:         | 2.3                | N/A                | N/A                |
| Comments/Other Conditions:              | none               | N/A                | N/A                |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 3                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min:) |                    |                    |                    |
| Test Specimen #1         | 41                 | N/A                | N/A                |
| Test Specimen #2         | 49                 | N/A                | N/A                |
| Test Specimen #3         | <u>49</u>          | <u>N/A</u>         | <u>N/A</u>         |
| Mean                     | 46                 | N/A                | N/A                |

TABLE D-1 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |             |            |            |
|------------------|-------------|------------|------------|
| Test Specimen #1 | 0.63        | N/A        | N/A        |
| Test Specimen #2 | 0.58        | N/A        | N/A        |
| Test Specimen #3 | <u>0.54</u> | <u>N/A</u> | <u>N/A</u> |
| Mean             | 0.58        | N/A        | N/A        |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested:

7-31-89

Temperature ( $^{\circ}\text{C}$ ):

24

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 4.1               | 1.58               | N/A                | N/A                |
| 2                 | 12.2              | 1.58               | N/A                | N/A                |
| 3                 | 44.7              | 7.51               | N/A                | N/A                |
| 4                 | 101.5             | 54.12              | N/A                | N/A                |
| 5                 | 125.9             | 88.09              | N/A                | N/A                |
| 6                 | 166.5             | 152.47             | N/A                | N/A                |
| 7                 | 190.8             | 189.21             | N/A                | N/A                |
| 8                 | 223.3             | 237.00             | N/A                | N/A                |
| 9                 | 247.7             | 271.37             | N/A                | N/A                |
| 10                | 288.3             | 341.28             | N/A                | N/A                |

Test Specimen 2:

Date Tested:

8-2-89

Temperature ( $^{\circ}\text{C}$ ):

23

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 4.1               | 0.76               | N/A                | N/A                |
| 2                 | 12.2              | 2.29               | N/A                | N/A                |
| 3                 | 44.7              | 12.95              | N/A                | N/A                |
| 4                 | 101.5             | 80.77              | N/A                | N/A                |
| 5                 | 125.9             | 123.83             | N/A                | N/A                |
| 6                 | 166.5             | 203.07             | N/A                | N/A                |
| 7                 | 190.8             | 252.98             | N/A                | N/A                |
| 8                 | 223.3             | 323.09             | N/A                | N/A                |
| 9                 | 247.7             | 376.05             | N/A                | N/A                |
| 10                | 288.3             | 462.15             | N/A                | N/A                |

TABLE D-1 (Continued)

Test Specimen 3:

Date Tested:

8-3-89

Temperature (°C):

23

Concentration (µg/L)

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 4.1               | 0.40               | N/A                | N/A                |
| 2                 | 12.2              | 0.79               | N/A                | N/A                |
| 3                 | 44.7              | 6.72               | N/A                | N/A                |
| 4                 | 101.5             | 58.86              | N/A                | N/A                |
| 5                 | 125.9             | 90.85              | N/A                | N/A                |
| 6                 | 166.5             | 157.21             | N/A                | N/A                |
| 7                 | 190.8             | 200.27             | N/A                | N/A                |
| 8                 | 223.3             | 259.12             | N/A                | N/A                |
| 9                 | 247.7             | 306.92             | N/A                | N/A                |
| 10                | 288.3             | 386.31             | N/A                | N/A                |

Other Observations:

None

Source of Data:

Arthur D. Little, Inc.  
Acorn Park  
Cambridge, MA 02140  
(617) 864-5770

**TABLE D-2. DATA REPORT FOR VINYL ACETATE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Vinyl Acetate      | N/A                | N/A                |
| CAS Number:      | 108-05-04          | N/A                | N/A                |
| Concentration:   | Neat               | N/A                | N/A                |
| Chemical Source: | Fisher             | N/A                | N/A                |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 23-26                                       |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 0.22               | N/A                | N/A                |
| Test System Sensitivity Factor:         | 0.07               | N/A                | N/A                |
| Comments/Other Conditions:              | none               | N/A                | N/A                |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           |                                |
| Number of Replicates:  | 3                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min:) |                    |                    |                    |
| Test Specimen #1         | 44                 | N/A                | N/A                |
| Test Specimen #2         | 22                 | N/A                | N/A                |
| Test Specimen #3         | <u>44</u>          | <u>N/A</u>         | <u>N/A</u>         |
| Mean                     | 37                 | N/A                | N/A                |

TABLE D-2 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

Test Specimen #1

0.06

N/A

N/A

Test Specimen #2

0.06

N/A

N/A

Test Specimen #3

0.06N/AN/A

Mean

0.06

N/A

N/A

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested:

5-30-89

Temperature ( $^{\circ}\text{C}$ ):

26

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 1.9               | 0.14               | N/A                | N/A                |
| 2                 | 50.0              | 0.37               | N/A                | N/A                |
| 3                 | 101.8             | 1.70               | N/A                | N/A                |
| 4                 | 149.9             | 5.02               | N/A                | N/A                |
| 5                 | 201.6             | 11.13              | N/A                | N/A                |
| 6                 | 253.4             | 19.34              | N/A                | N/A                |
| 7                 | 301.5             | 28.40              | N/A                | N/A                |
| 8                 | 353.3             | 38.81              | N/A                | N/A                |
| 9                 | 401.4             | 48.43              | N/A                | N/A                |
| 10                | 453.2             | 58.23              | N/A                | N/A                |

Test Specimen 2:

Date Tested:

6-1-89

Temperature ( $^{\circ}\text{C}$ ):

23

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 3.6               | 0.02               | N/A                | N/A                |
| 2                 | 54.4              | 0.29               | N/A                | N/A                |
| 3                 | 105.1             | 0.88               | N/A                | N/A                |
| 4                 | 155.9             | 2.88               | N/A                | N/A                |
| 5                 | 206.6             | 7.15               | N/A                | N/A                |
| 6                 | 250.1             | 12.66              | N/A                | N/A                |
| 7                 | 300.9             | 21.14              | N/A                | N/A                |
| 8                 | 351.6             | 31.13              | N/A                | N/A                |
| 9                 | 402.4             | 41.65              | N/A                | N/A                |
| 10                | 453.1             | 52.07              | N/A                | N/A                |

TABLE D-2 (Continued)

Test Specimen 3:

Date Tested:

6-5-89

Temperature (°C):

24

| <u>Data Point</u> | <u>Time (min)</u> | <u>Concentration (µg/L)</u> |                    |                    |
|-------------------|-------------------|-----------------------------|--------------------|--------------------|
|                   |                   | <u>Component 1</u>          | <u>Component 2</u> | <u>Component 3</u> |
| 1                 | 3.6               | 0.08                        | N/A                | N/A                |
| 2                 | 54.5              | 0.27                        | N/A                | N/A                |
| 3                 | 105.1             | 0.96                        | N/A                | N/A                |
| 4                 | 155.9             | 2.88                        | N/A                | N/A                |
| 5                 | 206.6             | 6.98                        | N/A                | N/A                |
| 6                 | 250.1             | 12.31                       | N/A                | N/A                |
| 7                 | 300.9             | 20.50                       | N/A                | N/A                |
| 8                 | 351.6             | 30.07                       | N/A                | N/A                |
| 9                 | 402.4             | 40.00                       | N/A                | N/A                |
| 10                | 453.1             | 50.06                       | N/A                | N/A                |

Other Observations:

None

Source of Data:

Arthur D. Little, Inc.  
Acom Park  
Cambridge, MA 02140  
(617) 864-5770

**TABLE D-3. DATA REPORT FOR ETHANOL PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Ethanol            | N/A                | N/A                |
| CAS Number:      | 64-17-5            | N/A                | N/A                |
| Concentration:   | Neat               | N/A                | N/A                |
| Chemical Source: | Fisher             | N/A                | N/A                |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 23-24                                       |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 3.0                | N/A                | N/A                |
| Test System Sensitivity Factor:         | 0.9                | N/A                | N/A                |
| Comments/Other Conditions:              | none               | N/A                | N/A                |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 2                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min:) |                    |                    |                    |
| Test Specimen #1         | 303                | N/A                | N/A                |
| Test Specimen #2         | 250                | N/A                | N/A                |
| Test Specimen #3         | <u>NT</u>          | <u>N/A</u>         | <u>N/A</u>         |
| Mean                     | 277                | N/A                | N/A                |

TABLE D-3 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |        |     |     |
|------------------|--------|-----|-----|
| Test Specimen #1 | 0.0038 | N/A | N/A |
| Test Specimen #2 | 0.0033 | N/A | N/A |
| Test Specimen #3 | NT     | N/A | N/A |
| Mean             | 0.0036 | N/A | N/A |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested:

8-1-89

Temperature ( $^{\circ}\text{C}$ ):

23

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 8.9               | 3.37               | N/A                | N/A                |
| 2                 | 44.6              | 3.17               | N/A                | N/A                |
| 3                 | 116.0             | 3.25               | N/A                | N/A                |
| 4                 | 151.7             | 3.25               | N/A                | N/A                |
| 5                 | 205.3             | 3.17               | N/A                | N/A                |
| 6                 | 258.8             | 3.58               | N/A                | N/A                |
| 7                 | 312.4             | 4.24               | N/A                | N/A                |
| 8                 | 348.1             | 4.77               | N/A                | N/A                |
| 9                 | 401.6             | 5.39               | N/A                | N/A                |
| 10                | 455.2             | 6.17               | N/A                | N/A                |

Test Specimen 2:

Date Tested:

8-2-89

Temperature ( $^{\circ}\text{C}$ ):

24

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 8.9               | -0.08              | N/A                | N/A                |
| 2                 | 44.6              | 0.00               | N/A                | N/A                |
| 3                 | 116.0             | -0.13              | N/A                | N/A                |
| 4                 | 151.7             | 0.13               | N/A                | N/A                |
| 5                 | 205.3             | 0.55               | N/A                | N/A                |
| 6                 | 258.8             | 0.93               | N/A                | N/A                |
| 7                 | 312.4             | 1.40               | N/A                | N/A                |
| 8                 | 348.1             | 1.95               | N/A                | N/A                |
| 9                 | 401.6             | 2.37               | N/A                | N/A                |
| 10                | 455.2             | 3.18               | N/A                | N/A                |

TABLE D-3 (Continued)

|                     |                                                                              |
|---------------------|------------------------------------------------------------------------------|
| Other Observations: | None                                                                         |
| Source of Data:     | Arthur D. Little, Inc.<br>Acom Park<br>Cambridge, MA 02140<br>(617) 864-5770 |

**TABLE D-4. DATA REPORT FOR CARBON DISULFIDE (90%) AND  
VINYL ACETATE (10%) MIXTURE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Carbon Disulfide   | Vinyl Acetate      | N/A                |
| CAS Number:      | 75-15-0            | 108-05-4           | N/A                |
| Concentration:   | 90%                | 10%                | N/A                |
| Chemical Source: | Fisher             | Fisher             | N/A                |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 23-24                                       |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 4.2                | 0.5                | N/A                |
| Test System Sensitivity Factor:         | 1.2                | 0.2                | N/A                |
| Comments/Other Conditions:              | none               | none               | N/A                |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 3                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min:) |                    |                    |                    |
| Test Specimen #1         | 30                 | 107                | N/A                |
| Test Specimen #2         | 48                 | 144                | N/A                |
| Test Specimen #3         | 521                | 122                | N/A                |
| Mean                     | 43                 | 124                | N/A                |

TABLE D-4 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |             |              |            |
|------------------|-------------|--------------|------------|
| Test Specimen #1 | 0.50        | 0.021        | N/A        |
| Test Specimen #2 | 0.50        | 0.017        | N/A        |
| Test Specimen #3 | <u>0.55</u> | <u>0.018</u> | <u>N/A</u> |
| Mean             | 0.51        | 0.019        | N/A        |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested:

6-28-89

Temperature ( $^{\circ}\text{C}$ ):

24

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 2.71               | 0.12               | N/A                |
| 2                 | 61.1              | 18.23              | 0.19               | N/A                |
| 3                 | 90.7              | 52.35              | 0.41               | N/A                |
| 4                 | 120.3             | 97.34              | 0.74               | N/A                |
| 5                 | 149.9             | 148.14             | 1.23               | N/A                |
| 6                 | 179.5             | 200.49             | 1.90               | N/A                |
| 7                 | 212.8             | 260.99             | 3.01               | N/A                |
| 8                 | 242.4             | 314.12             | 4.14               | N/A                |
| 9                 | 272.0             | 367.25             | 5.48               | N/A                |
| 10                | 301.6             | 418.05             | 7.00               | N/A                |

Test Specimen 2:

Date Tested:

6-28-89

Temperature ( $^{\circ}\text{C}$ ):

24

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 1.72               | 0.20               | N/A                |
| 2                 | 61.1              | 11.98              | 0.28               | N/A                |
| 3                 | 90.7              | 34.64              | 0.36               | N/A                |
| 4                 | 120.3             | 67.99              | 0.50               | N/A                |
| 5                 | 149.9             | 107.75             | 0.74               | N/A                |
| 6                 | 179.5             | 152.22             | 1.11               | N/A                |
| 7                 | 212.8             | 204.82             | 1.68               | N/A                |
| 8                 | 242.4             | 253.58             | 2.36               | N/A                |
| 9                 | 272.0             | 304.06             | 3.24               | N/A                |
| 10                | 301.6             | 354.13             | 4.35               | N/A                |

TABLE D-4 (Continued)

Test Specimen 3:

Date Tested:

6-30-89

Temperature (°C):

23

| <u>Data Point</u> | <u>Time (min)</u> | <u>Concentration (µg/L)</u> |                    |                    |
|-------------------|-------------------|-----------------------------|--------------------|--------------------|
|                   |                   | <u>Component 1</u>          | <u>Component 2</u> | <u>Component 3</u> |
| 1                 | 31.5              | 2.57                        | 0.09               | N/A                |
| 2                 | 61.1              | 12.83                       | 0.11               | N/A                |
| 3                 | 90.7              | 36.34                       | 0.13               | N/A                |
| 4                 | 120.3             | 71.39                       | 0.23               | N/A                |
| 5                 | 149.9             | 112.01                      | 0.48               | N/A                |
| 6                 | 179.5             | 157.34                      | 0.89               | N/A                |
| 7                 | 212.8             | 212.93                      | 1.48               | N/A                |
| 8                 | 242.4             | 264.26                      | 2.24               | N/A                |
| 9                 | 272.0             | 318.60                      | 3.23               | N/A                |
| 10                | 301.6             | 373.37                      | 4.40               | N/A                |

Other Observations:

None

Source of Data:

Arthur D. Little, Inc.  
Acom Park  
Cambridge, MA 02140  
(617) 864-5770

**TABLE D-5. DATA REPORT FOR CARBON DISULFIDE (50%) AND  
VINYL ACETATE (50%) MIXTURE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Carbon Disulfide   | Vinyl Acetate      | N/A                |
| CAS Number:      | 75-15-0            | 108-05-4           | N/A                |
| Concentration:   | 50%                | 50%                | N/A                |
| Chemical Source: | Fisher             | Fisher             | N/A                |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 20-24                                       |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 5.7                | 0.6                | N/A                |
| Test System Sensitivity Factor:         | 1.7                | 0.2                | N/A                |
| Comments/Other Conditions:              | none               | none               | N/A                |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 3                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min): |                    |                    |                    |
| Test Specimen #1         | 59                 | 89                 | N/A                |
| Test Specimen #2         | 59                 | 78                 | N/A                |
| Test Specimen #3         | <u>52</u>          | <u>93</u>          | <u>N/A</u>         |
| Mean                     | 57                 | 87                 | N/A                |

TABLE D-5 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |             |              |            |
|------------------|-------------|--------------|------------|
| Test Specimen #1 | 0.41        | 0.041        | N/A        |
| Test Specimen #2 | 0.40        | 0.035        | N/A        |
| Test Specimen #3 | <u>0.56</u> | <u>0.047</u> | <u>N/A</u> |
| Mean             | 0.46        | 0.041        | N/A        |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested:

5-31-89

Temperature ( $^{\circ}\text{C}$ ):

20

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | -0.35              | 0.25               | N/A                |
| 2                 | 61.1              | 6.31               | 0.40               | N/A                |
| 3                 | 90.7              | 20.32              | 0.62               | N/A                |
| 4                 | 120.3             | 42.40              | 1.03               | N/A                |
| 5                 | 149.9             | 68.68              | 1.73               | N/A                |
| 6                 | 179.5             | 98.11              | 2.58               | N/A                |
| 7                 | 209.1             | 131.05             | 3.83               | N/A                |
| 8                 | 242.4             | 169.94             | 5.64               | N/A                |
| 9                 | 272.0             | 205.68             | 7.73               | N/A                |
| 10                | 301.6             | 243.88             | 10.22              | N/A                |

Test Specimen 2:

Date Tested:

6-9-89

Temperature ( $^{\circ}\text{C}$ ):

24

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 0.00               | 0.21               | N/A                |
| 2                 | 61.1              | 9.19               | 0.37               | N/A                |
| 3                 | 90.7              | 27.57              | 0.65               | N/A                |
| 4                 | 120.3             | 52.20              | 1.05               | N/A                |
| 5                 | 149.9             | 80.87              | 1.64               | N/A                |
| 6                 | 179.5             | 113.22             | 2.51               | N/A                |
| 7                 | 209.1             | 144.83             | 3.67               | N/A                |
| 8                 | 242.4             | 186.01             | 5.50               | N/A                |
| 9                 | 272.0             | 225.71             | 7.57               | N/A                |
| 10                | 301.6             | 266.88             | 10.04              | N/A                |

TABLE D-5 (Continued)

Test Specimen 3:

Date Tested:

6-27-89

Temperature (°C):

24

Concentration (µg/L)

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 1.94               | 0.51               | N/A                |
| 2                 | 61.1              | 12.02              | 0.65               | N/A                |
| 3                 | 90.7              | 34.13              | 0.89               | N/A                |
| 4                 | 120.3             | 67.09              | 1.47               | N/A                |
| 5                 | 149.9             | 107.81             | 2.49               | N/A                |
| 6                 | 179.5             | 154.34             | 4.01               | N/A                |
| 7                 | 209.1             | 206.31             | 6.34               | N/A                |
| 8                 | 242.4             | 268.36             | 9.73               | N/A                |
| 9                 | 272.0             | 324.59             | 13.57              | N/A                |
| 10                | 301.6             | 383.15             | 18.00              | N/A                |

Other Observations:

None

Source of Data:

Arthur D. Little, Inc.  
Acorn Park  
Cambridge, MA 02140  
(617) 864-5770

**TABLE D-6. DATA REPORT FOR CARBON DISULFIDE (10%) AND  
VINYL ACETATE (90%) MIXTURE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Carbon Disulfide   | Vinyl Acetate      | N/A                |
| CAS Number:      | 75-15-0            | 108-05-4           | N/A                |
| Concentration:   | 10%                | 90%                | N/A                |
| Chemical Source: | Fisher             | Fisher             | N/A                |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 23-26                                       |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 14.7               | 0.5                | N/A                |
| Test System Sensitivity Factor:         | 4.4                | 0.2                | N/A                |
| Comments/Other Conditions:              | none               | none               | N/A                |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 3                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min:) |                    |                    |                    |
| Test Specimen #1         | 89                 | 89                 | N/A                |
| Test Specimen #2         | 52                 | 26                 | N/A                |
| Test Specimen #3         | <u>85</u>          | <u>67</u>          | <u>N/A</u>         |
| Mean                     | 75                 | 61                 | N/A                |

TABLE D-6 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |             |              |            |
|------------------|-------------|--------------|------------|
| Test Specimen #1 | 0.36        | 0.066        | N/A        |
| Test Specimen #2 | 0.28        | 0.065        | N/A        |
| Test Specimen #3 | <u>0.25</u> | <u>0.046</u> | <u>N/A</u> |
| Mean             | 0.30        | 0.059        | N/A        |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested:

6-21-89

Temperature ( $^{\circ}\text{C}$ ):

23

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 1.27               | 0.06               | N/A                |
| 2                 | 61.1              | 6.78               | 0.10               | N/A                |
| 3                 | 90.7              | 15.26              | 0.32               | N/A                |
| 4                 | 120.3             | 28.42              | 0.87               | N/A                |
| 5                 | 149.9             | 45.42              | 1.91               | N/A                |
| 6                 | 183.1             | 65.87              | 3.77               | N/A                |
| 7                 | 212.7             | 86.79              | 5.14               | N/A                |
| 8                 | 242.3             | 109.44             | 9.13               | N/A                |
| 9                 | 271.9             | 131.28             | 12.57              | N/A                |
| 10                | 301.5             | 151.04             | 16.37              | N/A                |

Test Specimen 2:

Date Tested:

6-21-89

Temperature ( $^{\circ}\text{C}$ ):

26

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 3.84               | 0.38               | N/A                |
| 2                 | 61.1              | 14.45              | 0.79               | N/A                |
| 3                 | 90.7              | 32.71              | 1.73               | N/A                |
| 4                 | 120.3             | 55.28              | 3.52               | N/A                |
| 5                 | 149.9             | 81.74              | 6.49               | N/A                |
| 6                 | 183.1             | 112.55             | 11.01              | N/A                |
| 7                 | 212.7             | 141.71             | 16.11              | N/A                |
| 8                 | 242.3             | 170.08             | 21.89              | N/A                |
| 9                 | 271.9             | 198.91             | 28.18              | N/A                |
| 10                | 301.5             | 227.33             | 34.67              | N/A                |

TABLE D-6 (Continued)

Test Specimen 3:

Date Tested:

6-22-89

Temperature (°C):

24

| <u>Data Point</u> | <u>Time (min)</u> | <u>Concentration (µg/L)</u> |                    |                    |
|-------------------|-------------------|-----------------------------|--------------------|--------------------|
|                   |                   | <u>Component 1</u>          | <u>Component 2</u> | <u>Component 3</u> |
| 1                 | 31.5              | 3.83                        | 0.33               | N/A                |
| 2                 | 61.1              | 8.51                        | 0.61               | N/A                |
| 3                 | 90.7              | 22.51                       | 1.16               | N/A                |
| 4                 | 120.3             | 41.21                       | 2.19               | N/A                |
| 5                 | 149.9             | 62.07                       | 3.86               | N/A                |
| 6                 | 183.1             | 88.94                       | 6.69               | N/A                |
| 7                 | 212.7             | 114.60                      | 10.15              | N/A                |
| 8                 | 242.3             | 139.45                      | 14.19              | N/A                |
| 9                 | 271.9             | 165.18                      | 18.78              | N/A                |
| 10                | 301.5             | 189.67                      | 23.53              | N/A                |

Other Observations:

None

Source of Data:

Arthur D. Little, Inc.  
Acom Park  
Cambridge, MA 02140  
(617) 864-5770

**TABLE D-7. DATA REPORT FOR CARBON DISULFIDE (50%) AND  
ETHANOL (50%) MIXTURE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Carbon Disulfide   | Ethanol            | N/A                |
| CAS Number:      | 75-15-0            | 64-17-5            | N/A                |
| Concentration:   | 50%                | 50%                | N/A                |
| Chemical Source: | Fisher             | Fisher             | N/A                |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C)                          | 26                                          |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 7.3                | 5.0                | N/A                |
| Test System Sensitivity Factor:         | 2.1                | 1.5                | N/A                |
| Comments/Other Conditions:              | none               | none               | N/A                |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 2                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min:) |                    |                    |                    |
| Test Specimen #1         | 37                 | 426                | N/A                |
| Test Specimen #2         | 37                 | 272                | N/A                |
| Test Specimen #3         | NT                 | NT                 | N/A                |
| Mean                     | 37                 | 349                | N/A                |

TABLE D-7 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |           |           |            |
|------------------|-----------|-----------|------------|
| Test Specimen #1 | 0.74      | No SSPR   | N/A        |
| Test Specimen #2 | 0.74      | No SSPR   | N/A        |
| Test Specimen #3 | <u>NT</u> | <u>NT</u> | <u>N/A</u> |
| Mean             | 0.74      | No SSPR   | N/A        |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested:

Temperature ( $^{\circ}\text{C}$ ):

| Data Point | Time (min) | Concentration ( $\mu\text{g}/\text{L}$ ) |             |             |
|------------|------------|------------------------------------------|-------------|-------------|
|            |            | Component 1                              | Component 2 | Component 3 |
| 1          | 31.5       | 5.98                                     | 0.74        | N/A         |
| 2          | 61.1       | 32.06                                    | 0.80        | N/A         |
| 3          | 90.7       | 77.79                                    | 0.87        | N/A         |
| 4          | 120.3      | 136.34                                   | 1.02        | N/A         |
| 5          | 149.9      | 203.87                                   | 1.42        | N/A         |
| 6          | 179.4      | 276.10                                   | 1.86        | N/A         |
| 7          | 209.0      | 350.90                                   | 2.51        | N/A         |
| 8          | 242.3      | 437.66                                   | 3.24        | N/A         |
| 9          | 271.9      | 516.73                                   | 4.02        | N/A         |
| 10         | 301.5      | 593.23                                   | 4.77        | N/A         |

Test Specimen 2:

Date Tested:

Temperature ( $^{\circ}\text{C}$ ):

7-31-89

26

| Data Point | Time (min) | Concentration ( $\mu\text{g}/\text{L}$ ) |             |             |
|------------|------------|------------------------------------------|-------------|-------------|
|            |            | Component 1                              | Component 2 | Component 3 |
| 1          | 9.3        | 1.21                                     | -0.17       | N/A         |
| 2          | 31.5       | 3.64                                     | -0.31       | N/A         |
| 3          | 46.3       | 10.11                                    | -0.54       | N/A         |
| 4          | 57.4       | 19.42                                    | -0.65       | N/A         |
| 5          | 74.4       | 43.28                                    | -0.66       | N/A         |
| 6          | 125.0      | 123.37                                   | -0.76       | N/A         |
| 7          | 175.6      | 230.97                                   | -0.31       | N/A         |
| 8          | 226.2      | 347.06                                   | 0.05        | N/A         |
| 9          | 276.8      | 472.86                                   | 1.25        | N/A         |
| 10         | 327.4      | 598.26                                   | 2.27        | N/A         |

**TABLE D-7 (Continued)**

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|                            |                               |
|----------------------------|-------------------------------|
| <b>Other Observations:</b> | <b>None</b>                   |
| <b>Source of Data:</b>     | <b>Arthur D. Little, Inc.</b> |
|                            | <b>Acom Park</b>              |
|                            | <b>Cambridge, MA 02140</b>    |
|                            | <b>(617) 864-5770</b>         |

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**TABLE D-8. DATA REPORT FOR VINYL ACETATE (50%) AND  
ETHANOL (50%) MIXTURE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Vinyl Acetate      | Ethanol            | N/A                |
| CAS Number:      | 108-05-4           | 64-17-5            | N/A                |
| Concentration:   | 50%                | 50%                | N/A                |
| Chemical Source: | Fisher             | Fisher             | N/A                |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 23                                          |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 0.3                | ND                 | N/A                |
| Test System Sensitivity Factor:         | 0.1                | --                 | N/A                |
| Comments/Other Conditions:              | none               | none               | N/A                |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 2                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min): |                    |                    |                    |
| Test Specimen #1         | 137                | ND                 | N/A                |
| Test Specimen #2         | 4                  | ND                 | N/A                |
| Test Specimen #3         | <u>NT</u>          | <u>NT</u>          | <u>N/A</u>         |
| Mean                     | 71                 | ND                 | N/A                |

TABLE D-8 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |       |         |     |
|------------------|-------|---------|-----|
| Test Specimen #1 | 0.024 | No SSPR | N/A |
| Test Specimen #2 | 0.027 | No SSPR | N/A |
| Test Specimen #3 | NT    | NT      | N/A |
| Mean             | 0.026 | No SSPR | N/A |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested: 7-6-89

Temperature ( $^{\circ}\text{C}$ ): 23

| Data Point | Time (min) | Concentration ( $\mu\text{g}/\text{L}$ ) |             |             |
|------------|------------|------------------------------------------|-------------|-------------|
|            |            | Component 1                              | Component 2 | Component 3 |
| 1          | 31.5       | -0.13                                    | -0.15       | N/A         |
| 2          | 61.1       | -0.16                                    | -0.32       | N/A         |
| 3          | 90.7       | -0.13                                    | -0.50       | N/A         |
| 4          | 120.3      | 0.11                                     | -0.41       | N/A         |
| 5          | 149.9      | 0.48                                     | -0.48       | N/A         |
| 6          | 179.4      | 1.07                                     | -0.55       | N/A         |
| 7          | 212.7      | 2.00                                     | -0.51       | N/A         |
| 8          | 242.3      | 3.23                                     | -0.36       | N/A         |
| 9          | 271.9      | 4.65                                     | -0.33       | N/A         |
| 10         | 301.5      | 6.44                                     | -0.36       | N/A         |

Test Specimen 2:

Date Tested: 7-6-89

Temperature ( $^{\circ}\text{C}$ ): 23

| Data Point | Time (min) | Concentration ( $\mu\text{g}/\text{L}$ ) |             |             |
|------------|------------|------------------------------------------|-------------|-------------|
|            |            | Component 1                              | Component 2 | Component 3 |
| 1          | 31.5       | 1.80                                     | -0.12       | N/A         |
| 2          | 61.1       | 2.80                                     | -0.22       | N/A         |
| 3          | 90.7       | 3.66                                     | -0.38       | N/A         |
| 4          | 120.3      | 4.57                                     | -0.28       | N/A         |
| 5          | 149.9      | 5.69                                     | -0.40       | N/A         |
| 6          | 179.4      | 7.11                                     | -0.28       | N/A         |
| 7          | 212.7      | 9.23                                     | -0.10       | N/A         |
| 8          | 242.3      | 11.48                                    | -0.00       | N/A         |
| 9          | 271.9      | 14.17                                    | 0.24        | N/A         |
| 10         | 301.5      | 17.12                                    | 0.43        | N/A         |

TABLE D-8 (Continued)

|                     |                                                                              |
|---------------------|------------------------------------------------------------------------------|
| Other Observations: | None                                                                         |
| Source of Data:     | Arthur D. Little, Inc.<br>Acom Park<br>Cambridge, MA 02140<br>(617) 864-5770 |

**TABLE D-9. DATA REPORT FOR CARBON DISULFIDE (45%), VINYL ACETATE (45%),  
AND ETHANOL (10%) MIXTURE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Carbon Disulfide   | Vinyl Acetate      | Ethanol            |
| CAS Number:      | 75-15-0            | 108-05-4           | 64-17-5            |
| Concentration:   | 45%                | 45%                | 10%                |
| Chemical Source: | Fisher             | Fisher             | Fisher             |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 24                                          |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 7.0                | 0.3                | 2.5                |
| Test System Sensitivity Factor:         | 2.1                | 0.1                | 0.7                |
| Comments/Other Conditions:              | none               | none               | none               |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 2                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min): |                    |                    |                    |
| Test Specimen #1         | 41                 | 67                 | 352                |
| Test Specimen #2         | 41                 | 74                 | 433                |
| Test Specimen #3         | NT                 | NT                 | NT                 |
| Mean                     | 41                 | 71                 | 393                |

TABLE D-9 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |      |       |         |
|------------------|------|-------|---------|
| Test Specimen #1 | 0.66 | 0.052 | No SSPR |
| Test Specimen #2 | 0.64 | 0.050 | No SSPR |
| Test Specimen #3 | NT   | NT    | NT      |
| Mean             | 0.65 | 0.051 | No SSPR |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested:

7-12-89

Temperature ( $^{\circ}\text{C}$ ):

24

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 4.32               | 0.09               | 0.20               |
| 2                 | 61.1              | 24.62              | 0.19               | 0.25               |
| 3                 | 90.7              | 63.50              | 0.66               | 0.27               |
| 4                 | 120.3             | 114.48             | 1.59               | 0.15               |
| 5                 | 149.9             | 174.53             | 3.23               | 0.47               |
| 6                 | 179.4             | 239.76             | 5.68               | 0.38               |
| 7                 | 212.7             | 317.52             | 9.36               | 0.60               |
| 8                 | 242.3             | 388.37             | 13.38              | 0.72               |
| 9                 | 271.9             | 457.92             | 17.86              | 1.07               |
| 10                | 301.5             | 527.04             | 22.93              | 1.41               |

Test Specimen 2:

Date Tested:

7-13-89

Temperature ( $^{\circ}\text{C}$ ):

24

Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 2.16               | -0.01              | -0.13              |
| 2                 | 61.1              | 23.76              | 0.13               | -0.09              |
| 3                 | 90.7              | 62.64              | 0.58               | -0.12              |
| 4                 | 120.3             | 111.46             | 1.53               | -0.15              |
| 5                 | 149.9             | 169.34             | 3.06               | -0.12              |
| 6                 | 179.4             | 230.26             | 5.27               | 0.06               |
| 7                 | 212.7             | 301.10             | 8.44               | 0.15               |
| 8                 | 242.3             | 366.34             | 11.95              | 0.19               |
| 9                 | 271.9             | 432.43             | 16.00              | 0.58               |
| 10                | 301.5             | 505.87             | 21.00              | 0.88               |

TABLE D-9 (Continued)

Other Observations:

None

Source of Data:

Arthur D. Little, Inc.  
Acorn Park  
Cambridge, MA 02140  
(617) 864-5770

**TABLE D-10. DATA REPORT FOR CARBON DISULFIDE (25%), VINYL ACETATE (25%),  
AND ETHANOL (50%) MIXTURE PERMEATION TESTS**

**DESCRIPTION OF PRODUCT EVALUATED**

|                         |                              |
|-------------------------|------------------------------|
| Condition Before Test:  | Flat sheet material          |
| Manufacturer:           | Chemical Fabrics Corporation |
| Product Identification: | Challenge 5200               |
| Nominal Thickness (mm): | 0.27                         |
| Material Type:          | Teflon                       |
| Description:            | Teflon-Glass Fiber-Teflon    |

**CHALLENGE CHEMICAL**

|                  | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|------------------|--------------------|--------------------|--------------------|
| Chemical Name:   | Carbon Disulfide   | Vinyl Acetate      | Ethanol            |
| CAS Number:      | 75-15-0            | 108-05-4           | 64-17-5            |
| Concentration:   | 25%                | 25%                | 50%                |
| Chemical Source: | Fisher             | Fisher             | Fisher             |

**TEST METHOD**

|                                           |                                             |
|-------------------------------------------|---------------------------------------------|
| Standard Test Method Used:                | ASTM F739                                   |
| Deviations From Standard Test Method:     | None                                        |
| Testing Laboratory:                       | Arthur D. Little, Inc., Cambridge, MA 02140 |
| Analytical Method:                        | IR                                          |
| Temperature (°C):                         | 23                                          |
| Specimen Area Exposed (cm <sup>2</sup> ): | 20.27                                       |
| Collection System:                        | Closed-Loop (Recirculating)                 |
| Collection Medium:                        | Air                                         |
| Collection Medium Volume (L):             | 6                                           |
| Collection Medium Flowrate (L/min):       | 10                                          |

|                                         | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-----------------------------------------|--------------------|--------------------|--------------------|
| Ave. Breakthrough Concentration (µg/L): | 6.8                | 0.3                | ND                 |
| Test System Sensitivity Factor:         | 2                  | 0.1                | --                 |
| Comments/Other Conditions:              | none               | none               | none               |

**TEST RESULTS**

|                        |                                |
|------------------------|--------------------------------|
| Date Tested:           | See below                      |
| Number of Replicates:  | 2                              |
| Location Sampled From: | Random sample from sheet stock |

|                          | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|--------------------------|--------------------|--------------------|--------------------|
| Breakthrough Time (min:) |                    |                    |                    |
| Test Specimen #1         | 44                 | 81                 | 444                |
| Test Specimen #2         | 52                 | 111                | ND                 |
| Test Specimen #3         | NT                 | NT                 | NT                 |
| Mean                     | 48                 | 96                 | >444               |

TABLE D-10 (Continued)

Steady-State Perm. Rate ( $\mu\text{g}/\text{cm}^2/\text{min}$ ):

|                  |           |           |           |
|------------------|-----------|-----------|-----------|
| Test Specimen #1 | 0.50      | 0.034     | No SSPR   |
| Test Specimen #2 | 0.54      | 0.036     | No SSPR   |
| Test Specimen #3 | <u>NT</u> | <u>NT</u> | <u>NT</u> |
| Mean             | 0.51      | 0.035     | No SSPR   |

## SELECTED DATA POINTS

Test Specimen 1:

Date Tested: 6-28-89

Temperature ( $^{\circ}\text{C}$ ): 23Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 2.61               | 0.11               | 0.15               |
| 2                 | 61.1              | 15.21              | 0.17               | 0.21               |
| 3                 | 90.7              | 43.03              | 0.40               | 0.07               |
| 4                 | 120.3             | 79.97              | 0.87               | 0.34               |
| 5                 | 149.9             | 122.56             | 1.62               | 0.40               |
| 6                 | 179.4             | 169.49             | 2.78               | 0.46               |
| 7                 | 212.7             | 225.99             | 4.56               | 0.71               |
| 8                 | 242.3             | 278.14             | 6.66               | 0.94               |
| 9                 | 301.5             | 378.97             | 11.65              | 1.53               |
| 10                | 331.1             | 428.95             | 14.62              | 1.99               |

Test Specimen 2:

Date Tested: 6-28-89

Temperature ( $^{\circ}\text{C}$ ): 23Concentration ( $\mu\text{g}/\text{L}$ )

| <u>Data Point</u> | <u>Time (min)</u> | <u>Component 1</u> | <u>Component 2</u> | <u>Component 3</u> |
|-------------------|-------------------|--------------------|--------------------|--------------------|
| 1                 | 31.5              | 1.74               | -0.08              | -0.15              |
| 2                 | 61.1              | 12.60              | -0.12              | -0.16              |
| 3                 | 90.7              | 39.11              | 0.07               | -0.20              |
| 4                 | 120.3             | 73.45              | 0.45               | -0.08              |
| 5                 | 149.9             | 112.13             | 1.08               | -0.17              |
| 6                 | 179.4             | 156.02             | 2.05               | -0.07              |
| 7                 | 212.7             | 209.91             | 3.61               | 0.17               |
| 8                 | 242.3             | 259.89             | 5.44               | 0.32               |
| 9                 | 301.5             | 365.50             | 10.26              | 0.98               |
| 10                | 331.1             | 421.13             | 13.26              | 1.31               |

TABLE D-10 (Continued)

|                     |                                                                               |
|---------------------|-------------------------------------------------------------------------------|
| Other Observations: | None                                                                          |
| Source of Data:     | Arthur D. Little, Inc.<br>Acorn Park<br>Cambridge, MA 02140<br>(617) 864-5770 |

## APPENDIX E

### FICK'S LAW DATA ANALYSIS PROCEDURES

The available permeation-time curves were analyzed to assess whether the behavior could be accurately described by a solution-diffusion mechanism using Fick's laws of diffusion. As reported in Section 4, mathematical relationships based on Fick's law describe the permeation rate,  $J$ , and the cumulative amount permeated,  $M$ , at any time following initiation of chemical contact. These relationships require two fundamental parameters: the diffusion coefficient,  $D$ , and the solubility,  $S$ , of the permeant in the material of interest:

$$J = (DS/l) \left[ 1 + 2 \sum_{n=1}^{\infty} (-1)^n \exp(-\pi^2 n^2 \psi) \right] \quad \text{Eq. (E-1)}$$

and

$$M = (Sl) \left[ \psi - 1/6 - 2 \sum_{n=1}^{\infty} [(-1)^n / (\pi n)^2] \exp(-(\pi n)^2 \psi) \right] \quad \text{Eq. (E-2)}$$

|           |   |                                                        |
|-----------|---|--------------------------------------------------------|
| where $J$ | = | permeation rate, $\mu\text{g}/\text{cm}^2\text{-min}$  |
| $M$       | = | cumulative amount permeated, $\mu\text{g}/\text{cm}^2$ |
| $\psi$    | = | $Dt/l^2$ , dimensionless                               |
| $D$       | = | diffusion coefficient, $\text{cm}^2/\text{min}$        |
| $S$       | = | equilibrium solubility, $\mu\text{g}/\text{cm}^3$      |
| $l$       | = | membrane thickness, cm                                 |
| $t$       | = | time, min                                              |

These equations can be used to solve for values of  $D$  and  $S$  given a set of  $J$  versus  $t$  or  $M$  versus  $t$  data. For the permeation test results analyzed in this effort, the permeation-time curves provide sets of  $J$  versus  $t$  data that can also be converted to  $M$  versus  $t$  data by analysis of the areas under the curves at various times. Two approaches to extract  $D$  and  $S$  values were pursued depending on the type of curve available. For permeation curves in which steady-state was reached, values for  $D$  and  $S$  were solved for directly using Eq. (E-2). For permeation-time curves in which permeation rates were still increasing with time, values for  $D$  and  $S$  were determined using Eq. (E-1) and an iterative curve-fitting technique.

## STEADY-STATE PERMEATION CURVE ANALYSIS

For permeation-time curves that reached steady-state, values for  $D$  and  $S$  were calculated by applying Eq. (E-2) at long times (i.e., when steady-state is reached). At steady-state, Eq (E-2) predicts that  $M$  increases linearly with time with a slope equal to the steady-state permeation rate that is defined by  $D$ ,  $S$ , and  $l$ :

$$M = (\text{Slope})(t) + \text{Intercept} \quad \text{Eq. (E-3)}$$

where:

$$\text{Slope} = DS/l \quad \text{Eq. (E-4)}$$

The intercept of Eq. (E-3) with the y-axis (or the value at which  $t$  equals 0) is defined from Eq. (E-2) as:

$$\text{Intercept} = (-Sl)/6 \quad \text{Eq. (E-5)}$$

Thus, by analyzing the  $M$  versus  $t$  data at steady-state, one can calculate the slope and intercept of Eq. (E-3) and directly calculate a value for  $S$  given the barrier film thickness,  $l$ . Using this value for  $S$ , one can calculate a value for  $D$  using Eq. (E-4). The value of  $D$  can be separately confirmed by calculating the lag time,  $t_L$ , or the time at which  $M$  calculated by Eq (E-3) equals 0:

$$t_L = l^2/6D \quad \text{Eq. (E-6)}$$

Thus,

$$D = l^2/6t_L \quad \text{Eq. (E-7)}$$

Use of this direct approach is only possible when the permeation-time data have reached steady state.

## TRANSIENT CURVE ANALYSIS

For permeation-time curves that have not reached steady-state, values for  $D$  and  $S$  must be calculated from the data in the transient portion of the curve. In this region, however, Eq. (E-1) and (E-2) can not be simplified to solve for  $D$  and  $S$  directly. In this case, though, we can analyze subsequent sets of  $(J, t)$  data points so as to eliminate  $S$  from the equation and solve for  $D$  through an iterative curve fitting technique. Once  $D$  is determined, a value for  $S$  can be calculated that also best fits the data.

In this analysis technique, we use the ratio of two permeation rates ( $J_1/J_2$ ) by dividing Eq. (E-1) by itself at two separate time intervals,  $t_1$  and  $t_2$ :

$$\frac{J_2}{J_1} = \frac{(DS/l)[1+2 \sum_{n=1}^{\infty} (-1)^n \exp(-\pi^2 n^2 \psi_2)]}{(DS/l)[1+2 \sum_{n=1}^{\infty} (-1)^n \exp(-\pi^2 n^2 \psi_1)]} \quad \text{Eq. (E-8)}$$

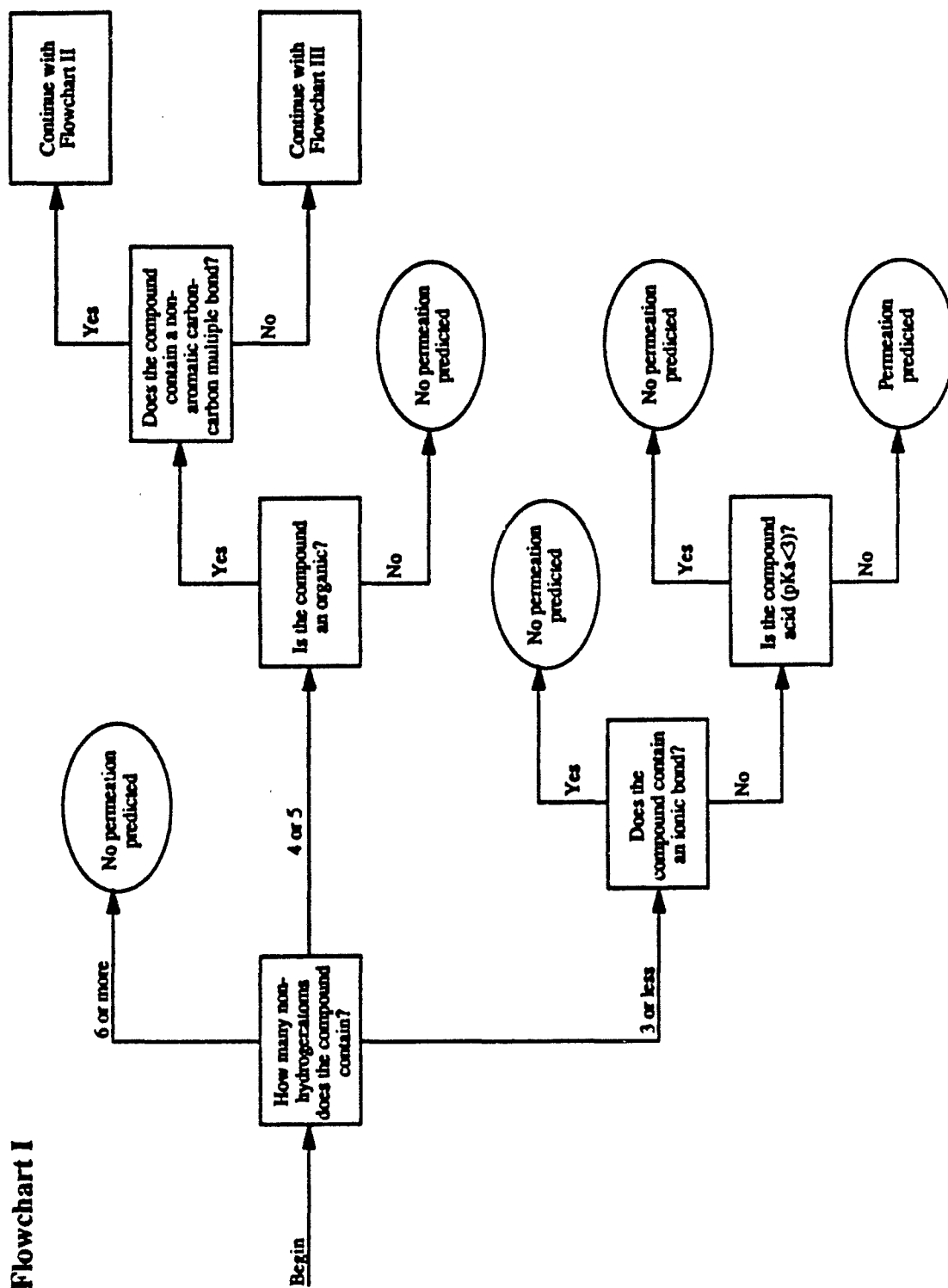
Thus, the leading term in each equation drops out and S is eliminated:

$$\frac{J_2}{J_1} = \frac{[1+2 \sum_{n=1}^{\infty} (-1)^n \exp(-\pi^2 n^2 \psi_2)]}{[1+2 \sum_{n=1}^{\infty} (-1)^n \exp(-\pi^2 n^2 \psi_1)]} \quad \text{Eq. (E-9)}$$

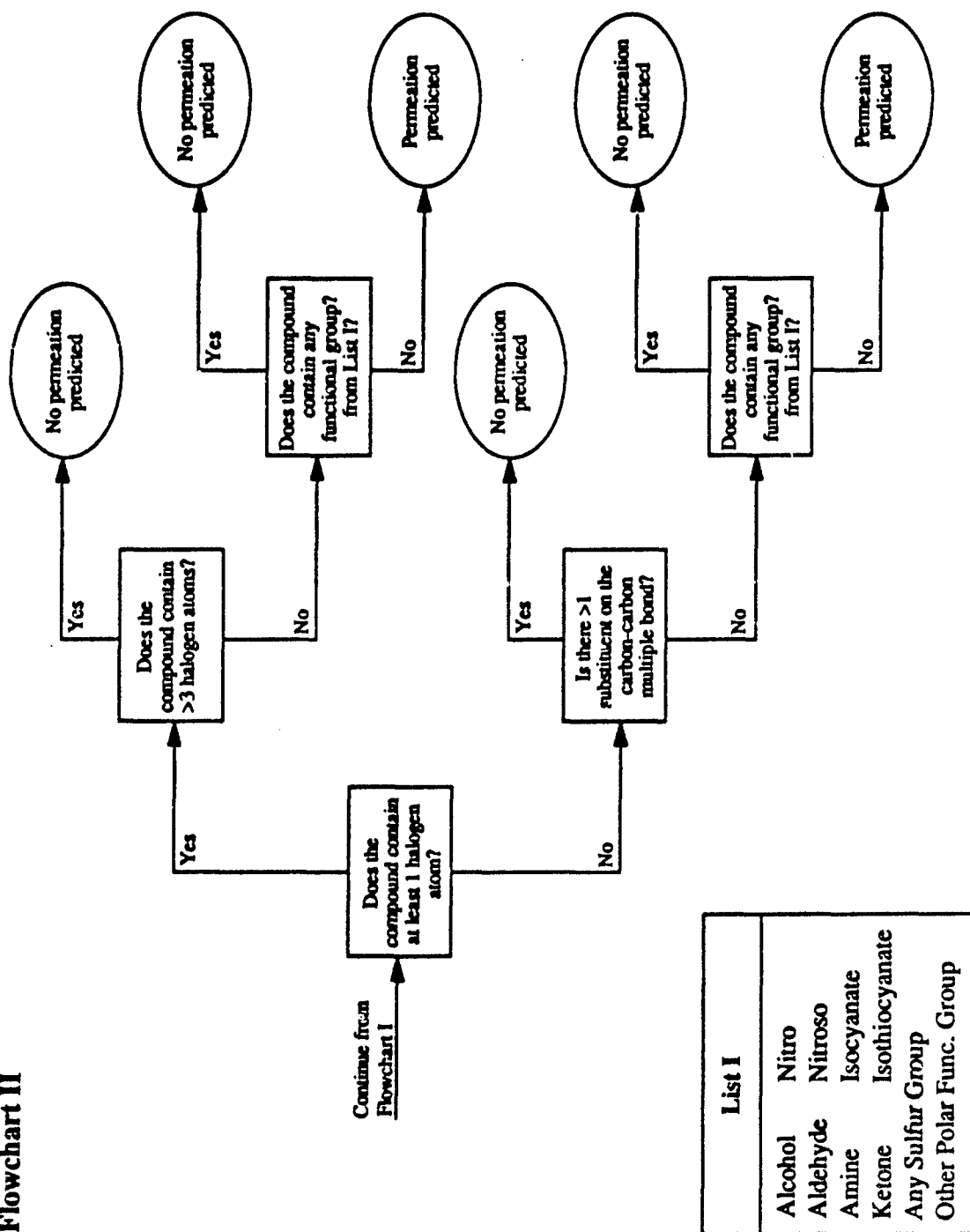
Since  $J_1$ ,  $J_2$ ,  $t_1$ , and  $t_2$  are known, a value for D can be calculated. An average or best fit value of D is determined by analyzing various pairs of (J,t) data points from the transition region of the permeation-time curve. Then, using Eq. (E-1) a value for S can be fit using the values for D and l.

**APPENDIX F**  
**EMPIRICAL MODEL DECISION TREE**

# Flowchart I



# Flowchart II



# Flowchart III

