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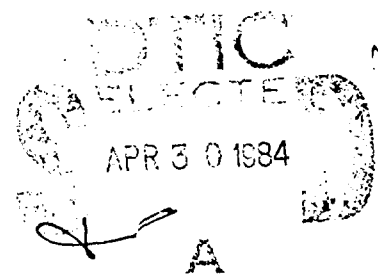
REVISION AND EXPERIMENTAL VERIFICATION OF THE
HAZARD ASSESSMENT COMPUTER SYSTEM MODELS FOR
SPREADING, MOVEMENT, DISSOLUTION, AND DISSIPATION OF
INSOLUBLE CHEMICALS SPILLED ONTO WATER — —

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FINAL REPORT

JUNE 1983

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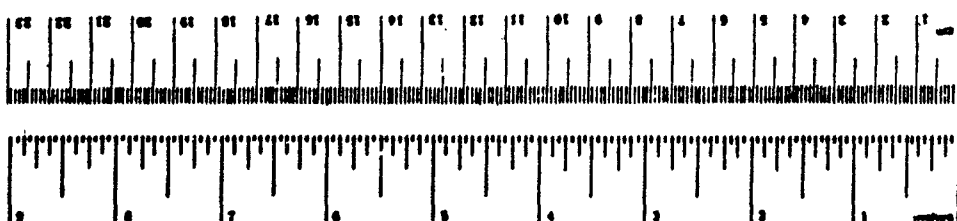
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16. Abstract Computerized models are developed to predict the spreading, movement, evaporation, and dissolution of floating slicks formed by accidental spills of insoluble chemicals. Separate models are developed for continuous and instantaneous spills. The waterway can be a river, channel, lake, or coastal water. The models emphasize the dynamics of the thick slick (i.e., the gravity-viscous spreading phase) since the thick slick contains nearly all the spilled chemical and represents the most prolonged hazard. Predictions of the spreading models are compared to results of instantaneous and continuous spill tests conducted in a large laboratory basin and a laboratory channel. The evaporation and dissolution predictions are compared to wind tunnel and wind-wave tunnel tests. Agreement of the models and the tests is generally good.			
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METRIC CONVERSION FACTORS

Approximate Conversions to Metric Measures

Symbol	When You Know	Multiply by	To Find	Symbol
LENGTH				
in	inches	2.5	centimeters	cm
ft	feet	30	centimeters	cm
yd	yards	0.9	meters	m
mi	miles	1.6	kilometers	km
AREA				
sq in	square inches	6.5	square centimeters	cm ²
sq ft	square feet	0.09	square meters	m ²
sq yd	square yards	0.8	square meters	m ²
sq mi	square miles	2.6	square kilometers	km ²
acre	acres	0.4	hectares	ha
MASS (weight)				
oz	ounces	28	grams	g
lb	pounds	0.45	kilograms	kg
	short tons (2000 lb)	0.9	tonnes	t
VOLUME				
teaspoon	teaspoons	5	milliliters	ml
fluid ounce	fluid ounces	30	milliliters	ml
cup	cups	0.24	liters	l
quart	quarts	0.95	liters	l
gallon	gallons	3.8	liters	l
cu in	cubic inches	0.016	cubic centimeters	cc
cu ft	cubic feet	0.028	cubic meters	m ³
cu yd	cubic yards	0.76	cubic meters	m ³
TEMPERATURE (degrees)				
°F	Fahrenheit temperature	5/9 (after subtracting 32)	Celsius temperature	°C

Symbol	When You Know	Multiply by	To Find	Symbol
LENGTH				
mm	millimeters	0.04	inches	in
cm	centimeters	0.4	inches	in
m	meters	1.1	yards	yd
km	kilometers	0.6	miles	mi
AREA				
sq cm	square centimeters	0.16	square inches	in ²
sq m	square meters	1.2	square yards	yd ²
sq km	square kilometers or 100 hectares (10,000 m ²)	0.4	square miles	mi ²
ha	hectares (10,000 m ²)	2.5	acres	ac
MASS (weight)				
g	grams	0.035	ounces	oz
kg	kilograms	2.2	pounds	lb
t	tonnes (1000 kg)	1.1	short tons	sh
VOLUME				
ml	milliliters	0.03	fluid ounces	fl oz
l	liters	1.06	quarts	qt
l	liters	0.26	gallons	gal
cc	cubic centimeters	36	cubic feet	cu ft
m ³	cubic meters	1.3	cubic yards	cu yd
TEMPERATURE (degrees)				
°C	Celsius temperature	9/5 (then add 32)	Fahrenheit temperature	°F



* 1 in = 2.54 cm exactly. For more exact conversions and more detailed tables, see 1966 NIST Publ. 278, Units of Weight and Measure, NIST-278, 50 Catalog No. C13.10.206.

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LIST OF PRINCIPAL SYMBOLS

Common Symbols

t	time
ρ	water density
ρ_0	chemical density
ν_w	water kinematic viscosity

Spreading Models

$A, \bar{A}$	area of thick and thin slick
$A_i, \bar{A}_i$	initial areas of thick and thin slick
C_{1m}, C_{2m}	constants in channel spreading models; $m = 0$ for instantaneous spill; $m = 1$ for continuous spill; $m = 2$ for continuous spill in a current.
g	acceleration of gravity
$h, \bar{h}$	thickness of thick and thin slick
$h_i, \bar{h}_i$	initial thickness of thick and thin slick
K_{1m}, K_{2m}	constants in open water spreading models; $m = 0$ for instantaneous spill; $m = 1$ for continuous spill; $m = 2$ for continuous spill in a current.
$\dot{m}$	discharge rate of continuous spill
$\dot{m}_{loss}$	rate of mass lost from thick slick
R	radius of thick slick
T	tidal period
U_c	current
U_0, U_1	steady and oscillating amplitude of tidal current
U_T	surface transport velocity; $\bar{U}_c + 0.035 \bar{V}_w$
V_0	volume of instantaneous spill
V_w	wind speed
w	river or channel width

LIST OF PRINCIPAL SYMBOLS (CONTD)

W	width of triangular slick
x	location of downstream (leading) edge of triangular slick
α	tidal phase
Δ	$1 - \rho/\rho_0$
θ	wind direction angle
μ_w	viscosity of water
$\sigma_{aw}, \sigma_{ow}, \sigma_{oa}$	interfacial tensions: air-water; chemical-water; chemical-air.
σ	net spreading coefficient

Evaporation and Dissolution Models

c_*	friction concentration, $-J_0/\rho u_*$
c_+	$(C - C_s)/c_*$
C	mean local concentration
C_s	surface concentration (saturation value)
C_f	friction coefficient, $2 \tau_0/\rho_a V_w^2$
C_∞	freestream concentration ($= 0$)
d	river or channel depth
D	molecular diffusivity; subscript a = air; subscript w = water.
Da	Dalton number, $J_0/\rho_a V_w (C_s - C_\infty)$
Da_*	inner-scale Dalton number, $J_0/\rho u_* (C_s - C_\infty)$
h_m	mean wave height
h_{m+}	$h_m u_*/v_a$
h_s	bottom roughness
J_0	mass flux from slick surface

LIST OF PRINCIPAL SYMBOLS (CONTD)

Re_L	Reynolds number based on slick length
Re_x	Reynolds number based on downstream position x
Sc	Schmidt number, ν_a/D_a or ν_w/D_w
Sc_t	turbulent Schmidt number, equals 0.85 [28]
u_*	friction velocity, $\sqrt{\tau_0/\rho}$
u_+	$(U - U_s)/u_*$
U	mean local velocity
U_s	wind-induced surface velocity
z	height above surface
z_0	roughness parameter
z_+	$z u_*/\nu_w$ or $z u_*/\nu_a$
z_{0+}	$z_0 u_*/\nu_w$ or $z_0 u_*/\nu_a$
δ	boundary layer thickness
δ_+	inner-scale boundary layer thickness, $\delta u_*/\nu_a$ or $\delta u_*/\nu_w$
δ_{c+}	inner-scale concentration boundary layer thickness
κ	von Karman's constant
ν	kinematic viscosity; subscript a = air; subscript w = water.
ρ_a	air density
τ_0	surface shear stress

I. EXECUTIVE SUMMARY

This final report covers all four tasks of a project to revise and verify experimentally the spreading, movement, dissolution, and dissipation models for lighter-than-water insoluble chemicals of the Hazard Assessment Computer System. The report documents (1) the analysis, development, and verification of the final form of the models, (2) experimental procedures and representative test data, and (3) listings and flow charts for the computerized models.

I.1 Background

Analytical and computer models have been developed previously for the U. S. Coast Guard for use in predicting the spreading, evaporation, and dissolution of a lighter-than-water insoluble chemical spilled into a waterway. A later independent study found that the models contain a number of serious deficiencies:

1. Only instantaneous spills are treated in detail, and the continuous spill model neglects many important effects.
2. Effects of currents and winds on the spreading processes are neglected.
3. Spreading of the slick is not coupled to the loss of mass by evaporation and dissolution.
4. The evaporation and dissolution models are based upon questionable mass-transfer assumptions.
5. Movement of the slick by winds, currents, and waves is not included.
6. None of the empirical constants in the models have been verified experimentally.

For these reasons, the Coast Guard has sponsored the present program to correct the indicated deficiencies and to validate the revised models experimentally.

I.2 Program Tasks

I.2.1 Literature Review and Reformulation/Revision of Models

The literature review on spreading, evaporation, and dissolution of floating chemicals performed for this task concluded that major revisions to the models were needed to treat continuous spills and spills in a current. More realistic evaporation and dissolution models were also indicated. Since the methods used in the existing models did not generally represent the best available state-of-the-art techniques and, further, the models could give unreliable predictions for many types of spills and chemicals of interest, only the existing model for an instantaneous spill in calm water could be retained, and it had to be modified to account for mass loss by evaporation and dissolution. New or modified models were indicated for all other cases of interest.

In summary, the following new or modified models were developed:

1. Instantaneous spill in a current;
2. Continuous spill in calm water;
3. Continuous spill in a current;
4. Rate of mass transfer by evaporation;
5. Rate of mass transfer by dissolution; and
6. Movement of slick.

In addition, all the spill models now include the effects of a loss of mass. The models are also in a form suitable to treat spills in channels, rivers, lakes, and coastal waters. The waterway current can be constant, or it can be made to vary in time or spatial position, or both. The wind can be specified as constant or as a function of time. In short, the revised models can be used for nearly every practical combination of chemical properties, waterway type, chemical spill discharge rate and duration, and spill volume.

The models have been programmed for computerized solution, and program listings and flow charts are given in this report.

I.2.2 Experimental Design

In order to provide data to verify the models, an extensive test program was designed. The program was organized into two separate types of tests: (1) the spreading of large-scale spills in water with and without a current, and (2) the determination of evaporation and dissolution mass-transfer rates for non-spreading, floating spills. A sensitivity analysis of the models was conducted to aid in the test design. This analysis revealed those parameters that have the most influence on the spreading, evaporation, and dissolution predictions and therefore should require control and accurate measurement. The test plan was approved by the Coast Guard.

I.2.3 Data Collection and Analysis

Tests of the spreading dynamics of spills were conducted in two facilities:

1. A specially-constructed outdoor basin, approximately 18 meters square by 0.3 meter deep, in which large quantities of chemical could be spilled instantaneously or continuously in water without a current, and
2. A modified indoor channel, about 14 meters long and 2.5 meters wide, in which the spreading of continuous spills in various currents could be conducted.

Over one hundred spreading tests were conducted in these facilities. The primary data measured were the size and shape of the slick as a function of time.

Tests to determine mass transfer rates due to evaporation and dissolution of floating chemicals were conducted in two different facilities:

1. A specially-constructed environmental wind tunnel, in which winds up to 5 meters/second could be blown over chemicals floating in a pan about 0.4 meter wide by 1.2 meters long, and
2. A wind-wave tunnel at Flow Research, Inc. (Kent, Washington), in which floating chemicals could be subjected to the simultaneous influence of wind and waves.

About fifty evaporation and dissolution tests were conducted. Detailed concentration measurements as a function of wind speed and wave characteristics constituted the primary data measured in these tests.

1.2.4 Revision and Demonstration of the Models

In this task, the models of spreading, evaporation, and dissolution of instantaneous and continuous spills were compared to the data from a few typical tests, and the "best" values of each empirical constant appearing in the models were selected. The results of the remaining tests were then used as independent data for model verification. Generally good comparisons were obtained between the test data and the models.

It is concluded that the revised models are satisfactory for use in the Hazard Assessment Computer System. Some further experimental and analytical work is recommended to increase the applicability of the models:

- o dissolution of slick into the water caused by wave action;
- o slick formation for a continuous spill when the net transport velocity is very small;
- o anomalous behavior of some chemicals for some spill conditions;
- o long-term movement and breakup of the slick in open water.

II. INTRODUCTION

As part of the Hazard Assessment Computer System of the Chemical Hazards Response Information System, models have been developed previously to predict the spreading, evaporation, and dissolution of lighter-than-water insoluble chemicals spilled in waterways from accidental punctures of ship tanks ([1], Models 3, 8, and 10; [2], Models II and IV). Since the models are used both for contingency planning and for the evaluation of accidents in progress, they were formulated in a general enough way to treat spreading, evaporation, and dissolution processes without requiring a complete description of water velocity profiles, bottom roughnesses, waterway cross-sections, puncture shapes, and other data that are unlikely to be available in practice. As a result, the models are more idealized than a corresponding model developed specifically for a given spill and waterway would need to be. Critical reviews [3,4] have shown that, even so, the models are overly limited in scope and contain errors in their basic physical representations. Therefore, the Coast Guard has sponsored the present program to correct the indicated deficiencies and to validate the revised models experimentally.

The previous reviews [3,4] and the review conducted as part of the present work have concluded that the current HACCS models are deficient in the following ways.

Spreading Processes

1. Only instantaneous spills are treated in detail.
2. The continuous spill model neglects many important effects and predicts absurd results for a chemical whose density is nearly the same as water.
3. The effects of currents and winds in altering the dynamics of the spreading and the shape of the slick are neglected.
4. The model describing the spreading of low-viscosity chemicals is based upon unrealistic assumptions.
5. Spreading of the slick is not coupled to the loss of mass by evaporation and dissolution.

6. The empirical constants in the models have not been verified experimentally.

Evaporation Processes

1. The evaporation mass transfer coefficients used in the models apply strictly only to smooth flat plates.
2. The latent heat of evaporation is assumed to be supplied by the underlying water and the chemical itself, neglecting the much larger heat transfer from solar radiation and from the air to the slick. Evaporative cooling of the chemical and the water is substantially overpredicted in most cases as a result.

Dissolution Processes

1. The dissolution mass transfer coefficient, which is derived from empirical data on the absorption of gas into water, is not relevant for the dissolution of insoluble chemicals. (It is recognized, however, that the prediction of dissolution of an "insoluble" chemical in a waterway with wind, current, and waves is a formidable task and that a simplified model is necessary.)

Slick Movement

1. Movement of the chemical slick by winds, currents, and waves is not included in the models.

Because of these deficiencies, the use of the available models is limited to instantaneous spills in channels or in unbounded, open expanses of water, without currents, winds, or waves. Even for the small range of cases where the models can be used, the predictions are not always reliable because of the use of empirical constants that have not been experimentally verified.

The present program was designed to reformulate the models in the light of the above criticisms and to validate the models experimentally. The program efforts were arranged into four tasks.

Task 1 - Literature Review and Reformulation/Revision of Models

For this task, the spreading-evaporation-dissolution-movement models for lighter-than-water insoluble chemicals were reformulated to remove the limitations and to correct the deficiencies listed above.

Task 2 - Experimental Design

For this task, a set of experiments was designed to validate the reformulated models. Emphasis was placed on the spreading dynamics of instantaneous and continuous spills and on the evaporation and dissolution processes of floating chemical slicks.

Task 3 - Data Collection and Analysis

For this task, the experimental program designed in Task 2 was executed. The spreading of both instantaneous and continuous spills was investigated in calm water and in a flowing channel, using large-scale facilities at Southwest Research Institute. Mass transfer coefficients for evaporation and dissolution of floating, insoluble chemicals were determined from wind tunnel tests at Southwest Research Institute and from wind-wave tunnel tests at Flow Research, Inc. at Kent, Washington.

Task 4 - Revision and Demonstration of Mathematical Models

For this task, the reformulated models were compared to the experimental results and revised as indicated by the comparisons. Each model was also computerized and documented.

This report is generally organized in agreement with the four tasks; the major exception is that the model revisions indicated by the test results are incorporated in the descriptions of the models at the time they are first given. All the data from the tests are presented in the companion Test Data Volume of this Final Report.

III. REFORMULATION OF MODELS

III.1 Background and Common Assumptions

The models developed in this report are based upon a number of assumptions that have been made primarily to eliminate the need for detailed descriptions of the waterway and the spill, rather than to simplify the basic physical phenomena. To avoid repetition, the assumptions common to all the models are listed together here.

Waterway Assumptions

- W.1 If the waterway is a river or channel, the width is constant. The surface current can be a function of time but, at any time, it is the same at all points along the surface. If the waterway is a lake or coastal water, the current can vary over the surface in a discrete fashion as well as with time.
- W.2 Blockage and interference effects due to the presence of the cargo ship in the waterway are neglected.

Spill Assumptions

- SP.1 A continuous spill is characterized by a constant mass flow rate, a specified spilling duration, and the relevant physico-chemical properties.
- SP.2 An instantaneous spill is characterized by the total mass of chemical released and the relevant physico-chemical properties.

Spreading Assumptions

- S.1 Details of the spill source, such as the puncture size, the discharge velocity, and the location of the puncture with respect to the waterline, are neglected.



- S.2 The variation of physico-chemical properties, such as the spreading coefficient, as the chemical dissolves into the water is neglected.

Evaporation and Dissolution Assumptions

- E.1 Mass transfer on both sides of the air-water-chemical interface is described by a convective process based upon boundary layer theory.
- E.2 Sufficient heating of the slick from the surrounding environment (solar radiation and heat transfer from the air and the water) is assumed such that the temperature change of the slick from evaporative cooling can be neglected.

The consequences of these assumptions are not severely limiting. The waterway assumptions imply only that localized effects cannot be predicted. The spill assumptions are all physically reasonable. The spreading assumptions imply that the dynamics of the spreading cannot be predicted in detail at points very close to the source, but this is acceptable since floating spills typically spread over large areas and the potential lack of an accurate spreading-rate prediction near the source is therefore not of crucial importance. Assumption E.2, concerning the smallness of evaporative cooling, has been made to eliminate the need for a complicated heat transfer model. (For very volatile or cryogenic chemicals, which are not of interest here, the assumption may be invalid.) Dissolution, as computed on the basis of boundary layer theory (assumption E.1), may account for only a small part of the mass transfer into the water when droplets of the chemical are dispersed directly into the water by the action of the waves. In addition, other kinds of diffusion processes may be important for those chemicals that have an affinity for water at the molecular level, even though they are insoluble. Thus, of all the models developed here, the dissolution model is the most idealized. However, there are no models available at this time that can describe more realistically the actual dissolution processes that occur for a floating slick of insoluble chemical in the presence of winds, waves, and currents.

The analytical models used to predict the spreading, evaporation, dissolution, and movement of continuous and instantaneous spills are presented in Sections III.2 through III.5. Table III.1 summarizes the presentations and can serve as a guide for reference.

III.2 Spreading Models

III.2.1 General Discussion

The venting rate model of the Hazard Assessment Computer System has been revised and validated [5,6], and it may be used to estimate both the total amount of cargo released into the waterway and the duration of the discharge. (Discharges of moderate duration, say about 10 minutes, can be analyzed as a continuous release, but in the computerized version of the models, recommendations, based on physical considerations, are made in the output as to whether such a spill should be analyzed more appropriately as instantaneous.) Knowing the amount of chemical discharged and the discharge duration, spreading models are needed to predict the size and shape of the floating slick and how the size and shape change with time. Models are developed below that can be applied to rivers, channels, lakes, and coastal waters to make the required predictions. In general, only calm water with or without a current will be treated; waves may alter somewhat the rate of spreading predicted for calm water, but these effects are beyond the present state-of-the-art. The spreading models also provide a convenient center about which to make mass balances of the spilled material.

In the past, two different methods have been used to formulate spreading models [7,8]. In one, the forces tending to promote and to retard the spreading are determined from physical laws, and the spreading models are deduced from the balance of the forces. In the other, the spreading is merely hypothesized to be similar to turbulent diffusion, and the spreading law is formulated using the principles of Fickian diffusion. The first method is chosen here for several reasons:

1. The dynamical basis of the diffusion models is obscure [8]. Spreading by turbulent diffusion is physically justifiable

TABLE III.1 GUIDE TO ANALYTICAL MODEL DEVELOPMENT

WATERWAY	CURRENT AND WIND	SPILL TYPE	DESCRIPTION	REPORT PAGES
Channel or River	Zero or Non-zero	Instantaneous	One-dimensional spreading model	19-21
Channel or River	Zero	Continuous	One-dimensional spreading model	21-23
Open Water	Zero or Non-zero	Instantaneous	Radial spreading model	13-19
Open Water	Zero	Continuous	Radial spreading model	21-23
Channel or River	Non-zero	Continuous	One-dimensional spreading with effects of current included	24
Open Water	Non-zero	Continuous	Elongated triangular spreading model	23-24
Channel or River	Non-zero wind	Instantaneous or Continuous	Evaporation rate model	29-32
Open Water	Non-zero wind	Instantaneous or Continuous	Evaporation rate model	29-32
Channel or River	Non-zero wind	Instantaneous or Continuous	Dissolution rate model	36-39
Open Water	Non-zero wind	Instantaneous or Continuous	Dissolution rate model	36-39
Channel or River	Non-zero	Instantaneous or Continuous	Slick movement model	40-41
Open Water	Non-zero	Instantaneous or Continuous	Slick movement model	41-43

only for "passive" substances that dissolve in water and become indistinguishable from it (except for "marked particles").

2. Methods for predicting diffusion coefficients for the surface spreading of insoluble, floating chemicals are not available. Most work in the past has been after-the-fact curve fitting to the observed spreading rates of large-scale spills in open water [7,9,10].

A third approach combines both types of models [11,12], but this does not avoid the problem of finding diffusion coefficients. The models developed in this report are based upon the first approach mentioned above. Such models are capable of being interpreted physically and lead to expressions containing a minimum of empirical constants; in addition, the empirical constants can be determined readily by laboratory-scale experiments.

III.2.2 General Description

The revisions that have been made to the previous spreading models [1,2] consist of:

- o adding realistic models of continuous spills;
- o including the effects of current and wind on the shape and the spreading of continuous and instantaneous spills; and
- o including the effects of a loss of mass from the spill (evaporation and dissolution).

In addition, the models have been put in a form that permits a ready solution when a loss of mass occurs. The empirical constants in the models have been determined by experimentation, in some cases for the first time, and in all cases by the use of larger spills than had previously been used.

III.2.3 Instantaneous Spills

The development of predictive methods for instantaneous spills is exemplified by Fay's work [13], which has since been expanded and modified

by others [14,15]. Earlier Blokker [16] had considered some parts of the same problem. The final forms of the models used in the present report are similar to the modifications suggested by Mackay [17].

Figure III.1 shows several stages in the idealized spreading of a floating, insoluble chemical in an open body of calm water without a current. The spill is assumed to occur instantaneously. During the time period when the slick is relatively thick, gravity (i.e., buoyancy) causes the chemical to spread laterally. As can be seen from Figure III.1a, there is unbalanced force, F_g , directed radially outward around the non-submerged part of the periphery of the slick; the magnitude of the force is roughly:

$$F_g = 2\pi R \left[\frac{1}{2} \rho_0 g h^2 (1 - \rho_0/\rho) \right] \quad (\text{III.1})$$

Here, g is the acceleration of gravity and the other quantities are defined in the figure. Because of the unbalanced force, the spilled chemical rapidly attains a radial velocity that can be estimated roughly as R/t , where t is the elapsed time since the spill occurred. The average acceleration of the spilled liquid is thus $R/2t^2$. Fay [13] hypothesized that, in this early phase, the gravitational spreading force is balanced almost entirely by the inertial force associated with the acceleration of the slick. Thus:

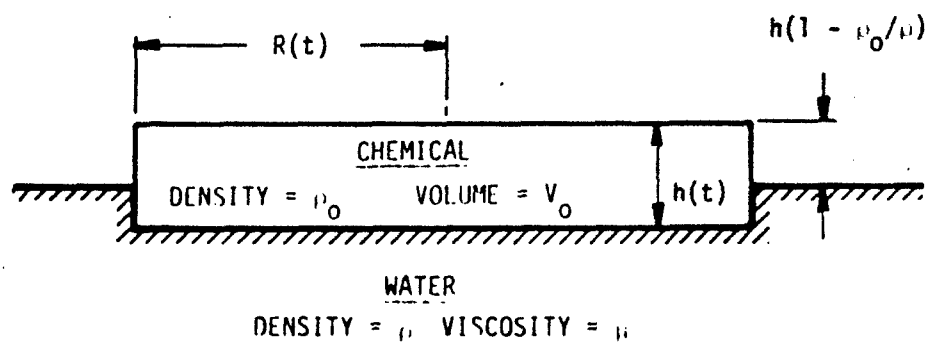
$$2\pi R \left[\frac{1}{2} \rho_0 g h^2 (1 - \rho_0/\rho) \right] \approx \rho_0 (\pi R^2 h) (R/2t^2) \quad (\text{III.2})$$

Solving for R as a function of time gives:

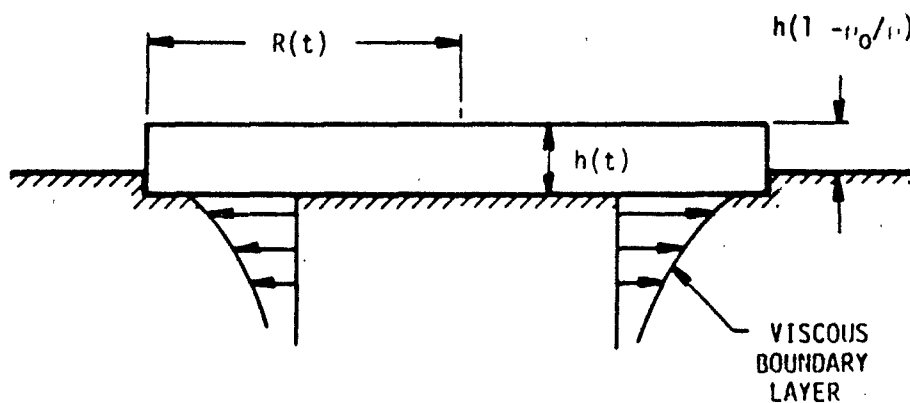
$$R = K_{10} (V_0 g \Delta)^{1/3} t^{2/3} \quad (\text{III.3})$$

Here, K_{10} is a constant of proportionality, $V_0 = \pi R^2 h$ is the volume of the spill, and $\Delta = 1 - \rho_0/\rho$.

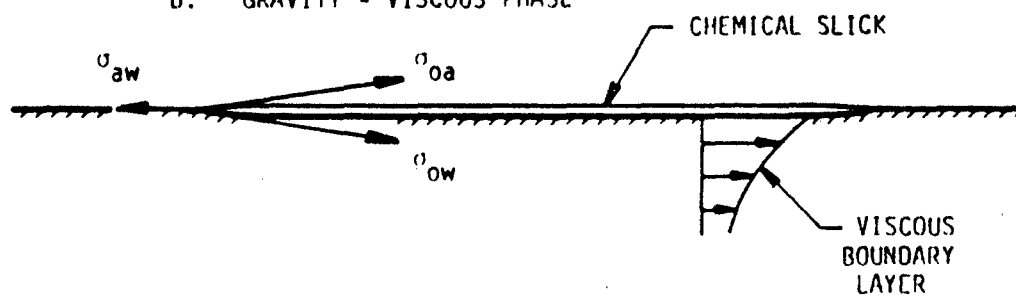
At some later time, the acceleration of the spill will have decreased significantly because the viscous drag of the water on the slick will have become predominant; see Figure III.1b. The viscous drag can be estimated as follows. The thickness δ of an unsteady, viscous boundary layer is



a. GRAVITY - INERTIAL PHASE



b. GRAVITY - VISCIOUS PHASE



c. SURFACE TENSION - VISCIOUS PHASE

Figure III.1 Phases in the Idealized Spreading of a Floating, Insoluble Chemical

roughly $(\mu_w t / \rho_w)^{1/2}$, and the viscous shear at the water-chemical interface is about $\mu_w V / \delta$. The velocity V will again be approximated as R/t . During this period, the balance of gravitational and viscous drag forces is thus:

$$2\pi R \left[\frac{1}{2} \rho_0 g h^2 (1 - \rho_0 / \rho) \right] \leq \pi R^2 \left[\mu_w (R/t) / (\mu_w t / \rho)^{1/2} \right] \quad (III.4)$$

Solving for R as a function of time gives:

$$R = K_{20} V_0^{2/3} g^{1/3} \rho_w^{1/3} t^{1/3} \quad (III.5)$$

where $\nu_w = \mu_w / \rho$ is the kinematic viscosity of the water. A factor of $(\rho_0 / \rho)^{1/6}$ in Equation (III.5) has been neglected on the basis that it is close to unity. In fact, in all the spreading models, ρ_0 and ρ will be assumed to be interchangeable except when their ratio is subtracted from one (i.e., except in Δ). Equation (III.5) is strictly valid only when the thickness h of the slick is less than the thickness δ of the boundary layer. When this is the case, the slick appears to move as a "slug". The flow in the slick is undoubtedly of the slug type when the viscosity μ_0 of the spilled material is much greater than μ_w , but Buckmaster [18] has shown that a slug flow is the type of flow that occurs even when $\mu_0 < \mu_w$, so long as $\mu_0 / \mu_w > 0.1$ or so. Since $\mu_0 / \mu_w > 0.1$ includes all chemicals of interest to the Coast Guard, a separate "low viscosity" spreading model such as given in [1] is not developed here.

At some point, the slick becomes so thin that gravity forces are negligible. Then, the relatively small interfacial tension at the periphery will be the dominant spreading force. From Figure III.1c, the net spreading force is now roughly $2\pi R (\sigma_{aw} - \sigma_{oa} - \sigma_{ow}) = 2\pi R \sigma$, where σ is the "spreading coefficient". Here, σ is assumed to be positive, although negative values are also possible; the case when $\sigma < 0$ will be discussed later. The balance of forces is:

$$2\pi R \sigma \leq \pi R^2 \left[\mu_w (R/t) / (\mu_w t / \rho)^{1/2} \right] \quad (III.6)$$

Solving for R as a function of time gives:

$$R = K_{30} (\sigma^2 / \rho \nu_w)^{1/3} t^{2/3} \quad (III.7)$$

Note that in this phase of the spreading, the rate of spreading is independent of the spilled volume. But since the time at which Equation (III.7) becomes applicable depends on the spilled volume, the magnitude of R is actually an implicit function of V_0 . It is also worth noting that Equations (III.1) - (III.7) apply even when the volume V_0 itself changes with time, as it would for a continuous spill or when evaporation and dissolution occur.

The approximate elapsed time when one phase of spreading ends and another begins is assumed to be the time when the preceding and the succeeding phases predict the same slick radius [13,14,15]. Thus, the end of the gravity-inertial phase, and the beginning of the gravity-viscous phase, can be found by equating (III.3) and (III.5) to give:

$$t_1 = (K_{20}/K_{10})^{1/2} [V_0 / \nu_w g \Delta]^{1/3} \quad (III.8)$$

Likewise, the beginning of the surface tension-viscous phase occurs at

$$t_2 = (K_{20}/K_{30})^{1/2} [V_0 / \rho \nu_w g \Delta / \sigma^3]^{1/3} \quad (III.9)$$

In the surface tension-viscous spreading regime, the slick is extremely thin, on the order of 10^{-5} to 10^{-4} meters, according to the experiments to be described later. The evaporation and dissolution from such thin slicks is negligible; that is, a thin slick would rapidly disappear if the evaporation and dissolution were not negligible. Most of the hazards are presented by the earlier phases of spreading (the so-called "thick slick"). Thus, in the instantaneous models developed here, the "thin" or surface tension-gravity slick will be neglected. Further, the end of the first phase (the gravity-inertial phase) of the spreading occurs soon after the spill occurs, in comparison to the total time duration over which the thick slick spreads. In addition, the spreading during the first phase is somewhat dependent on the size of the puncture in the ship tank, whether the puncture is submerged or not, and other details of the source of the spill that cannot be included in the model. For those reasons, the gravity-inertial phase of the spreading is only included in the model as an initial

condition on the gravity-viscous phase. Since the gravity-viscous phase constitutes the great bulk of the thick slick spreading time, neglecting the details of the gravity-inertial phase is not a serious limitation to the model.

When mass is lost from the spill by evaporation and dissolution, the preceding formulation of the model is inconvenient, since V_0 is then a function of time. For that reason, the model of gravity-viscous spreading is rewritten as suggested by Mackay [17]. From Equation (III.5), the surface area of the slick is:

$$A = \pi K_{20}^2 [V_0 g \Delta / \sqrt{\rho_w}]^{1/3} t^{2/3} \quad (\text{III.10})$$

The rate of change of the area with respect to time is thus:

$$\begin{aligned} \frac{dA}{dt} &= \frac{2}{3} \pi K_{20}^2 [V_0 g \Delta / \sqrt{\rho_w}]^{1/3} t^{-1/3} \\ &+ \frac{2}{3} \pi K_{20}^2 [g \Delta V_0 / \sqrt{\rho_w}]^{1/3} t^{2/3} (dV_0/dt) \end{aligned} \quad (\text{III.11})$$

Eliminating the time variable between Equations (III.10) and (III.11) and using the definition that $\dot{m}_{\text{loss}} = -\rho_0 dV_0/dt$ gives:

$$\begin{aligned} \frac{dA}{dt} &= \frac{2}{3} (\pi K_{20}^2)^{2/3} [g \Delta / \sqrt{\rho_w}]^{2/3} h^{1/3} A^{1/3} \\ &- \frac{2}{3} (\dot{m}_{\text{loss}} / \rho_0 h) \end{aligned} \quad (\text{III.12})$$

This equation must be augmented by the initial condition that $A = A_i$, where A_i is the area of the thick slick at the end of the gravity-inertial phase:

$$A_i = \pi K_{20}^2 (K_{20}/K_{10}) [V_0 g \Delta / \sqrt{\rho_w}]^{1/3} \quad (\text{III.13a})$$

The time at which A_i occurs is given by Equation (III.4):

$$t_i = (K_{20}/K_{10})^3 [V_0 g \Delta / \sqrt{\rho_w}]^{1/3} \quad (\text{III.13b})$$

Equation (III.13a) is obtained by combining Equations (III.8) with either (III.3) or (III.5). A relation predicting the value of $h(t)$ is also needed; since $\rho_0 Ah$ is equal to the total mass in the spill, it is evident that:

$$\frac{dh}{dt} = -[\dot{m}_{loss} + \rho_0 h (dA/dt)]/\rho_0 A \quad (III.14)$$

with the initial condition that $h_i = V_0/A$ at time t_i . Note that the loss of mass is neglected during the short period when the slick is spreading in the gravity-inertial phase.

Models for a spill in a channel of width w , where the spreading occurs one-dimensionally rather than radially, can be developed analogously. Table III.2 summarizes these one-dimensional and radial instantaneous-spill models. The numerical values for the empirical constants, C_{10} , C_{20} , K_{10} , and K_{20} shown in the table will be discussed in Section V.1.

In the computerized models, the radial-spreading model is also used to compute the initial phases of spreading of a spill in a channel. The one-dimensional spreading model is used to continue the computations after the slick has spread completely across the width of the channel (that is, after the effects of the channel boundaries become evident). The radial and one-dimensional models can also be applied to spills occurring when there is a current or a wind. The current and wind merely translate the entire slick as a body without affecting the spreading. Motion of the slick is discussed later in Section III.5.

When the surface tension spreading coefficient σ is negative, the models developed above for the surface tension-viscous phase of spreading are no longer applicable. In fact, a surface tension spreading phase does not exist when $\sigma < 0$, and the spreading ceases when the gravity force is balanced by the interfacial tension. At that time, the slick breaks up into many smaller slicks, or "lenses" [19]. The main effect on the spreading of the thick slick, which is the part of the slick of primary interest here, is that the spreading may cease at a somewhat larger thickness than when $\sigma > 0$. The ultimate thickness can be estimated [19] as

TABLE III.2 SPREADING MODELS FOR INSTANTANEOUS SPILLS
WITH OR WITHOUT A UNIFORM CURRENT OR WIND

Spill Location	Spreading Model	Initial Conditions
Channel	$\frac{dA}{dt} = \frac{3}{2} \frac{1}{h} (C_{20})^{\frac{1}{3}} \left[\frac{w^4 (g\Delta)^2}{v_w} \right]^{\frac{1}{3}} h^{\frac{1}{3}} A^{-\frac{1}{3}}$ $-\frac{1}{2} (\dot{m}_{loss}/\rho_0 h)$ $\frac{dh}{dt} = - \left[\dot{m}_{loss} + \rho_0 h \left(\frac{dA}{dt} \right) \right] / \rho_0 A$	$t_i = \left(\frac{C_{20}}{C_{10}} \right)^{\frac{2}{3}} \left[\frac{(V_0/w)^4}{(g\Delta)^2 v_w^3} \right]^{\frac{1}{3}}$ $A_i = 2 C_{20} \left(\frac{C_{20}}{C_{10}} \right)^{\frac{1}{3}} \left[\frac{V_0^5 w^2 (g\Delta)}{v_w^2} \right]^{\frac{1}{3}}$ $h_i = V_0/A_i$
Open Water	$\frac{dA}{dt} = \frac{1}{2} (-\pi K_{20})^2 \left[\frac{(g\Delta)^2}{v_w} \right]^{\frac{1}{3}} h^{\frac{1}{3}} A^{-\frac{1}{3}}$ $-\frac{2}{3} (\dot{m}_{loss}/\rho_0 h)$ $\frac{dh}{dt} = - \left[\dot{m}_{loss} + \rho_0 h \left(\frac{dA}{dt} \right) \right] / \rho_0 A$	$t_i = \left(\frac{K_{20}}{K_{10}} \right)^{\frac{2}{3}} \left[\frac{V_0}{g \Delta v_w} \right]^{\frac{1}{3}}$ $A_i = \pi K_{20}^2 \left(\frac{K_{20}}{K_{10}} \right)^{\frac{1}{3}} \left[\frac{V_0^5 g \Delta}{v_w^2} \right]^{\frac{1}{3}}$ $h_i = V_0/A_i$

$$h_{\text{minimum}} = (-2\sigma/\rho_0 g \Delta)^{1/2} \quad (\text{III.15})$$

For example, if $\sigma = -1 \times 10^{-3}$ newtons/meter, $\rho_0 = 900 \text{ kg/m}^3$, and $\Delta = 0.1$, the predicted h_{minimum} is about 1.5×10^{-3} meters. It is recommended that, when $\sigma < 0$, Equation (III.15) should be used to compute a minimum value of slick thickness; this value can then be used as an input to the computerized model to account for the diminished spreading of the thick slick.

III.2.4 Continuous Spills

The models described in Section III.2.3 for instantaneous spills are readily modified to cover continuous spills when there are no currents or winds. The spilled volume V_0 is merely replaced by the volume discharged up to time t , i.e., by $\dot{m}t/\rho_0$. (Recall that the derivation of the models did not require that V_0 be constant.) For example, Equation (III.5) becomes

$$R = K_{21} \left[\left(\frac{\dot{m}}{\rho_0} \right)^2 \frac{g\Delta}{\sqrt{\nu_w}} \right]^{1/2} t^{3/2} \quad (\text{III.16})$$

(The constant of proportionality K_{21} is allowed for generality to be different from K_{20} , the constant in Equation (III.5)). When the models are expressed in terms of areas, the resemblance to the instantaneous models is even more clear. Table III.3 summarizes these models. Once again, the model for an open-water spill is used in the computerized version to predict the spreading of a spill in a channel until the time when the spill completely fills the width of the channel. (The numerical values of C_{11} , C_{21} , K_{11} , and K_{21} are discussed in Section V.1)

One major difference between a continuous and an instantaneous spill is that for a continuous spill the surface tension-viscous phase occurs simultaneously with the gravity-viscous phase rather than following it in time. Thus, the part of the slick that is spreading in the gravity-viscous phase (i.e., the thick slick) must supply the mass needed by that part of the slick spreading in the surface tension-viscous phase (i.e., the thin slick). Although the apparent loss of mass from the thick slick is small, the models do account for it. The method used is that suggested by Mackay [17]. The thin

TABLE III.3 SPREADING MODELS FOR CONTINUOUS SPILLS WHEN THERE IS NO CURRENT OR WIND ($A, h \sim$ thick slick; $\bar{A}, \bar{h} \sim$ thin slick)

Spill Location	Spreading Model	Initial Conditions
Channel	$\frac{dA}{dt} = \frac{3}{2} \frac{(C_{21})^{3/2}}{v_w} \left[\frac{w^2 (g\Delta)^2}{v_w} \right]^{1/2} h^{1/2} v_w^{1/2} A^{1/2} + \frac{1}{2} (\dot{m} - \dot{m}_{loss}) / \rho_0 h$ $\frac{dh}{dt} = \left[\dot{m} - \dot{m}_{loss} - \rho_0 \bar{h} \left(\frac{d\bar{A}}{dt} \right) - \rho_0 h \left(\frac{dA}{dt} \right) \right] / \rho_0 A$ $\frac{d\bar{A}}{dt} = 2.76 \left[\left(\frac{\sigma w^2}{\rho} \right)^2 / v_w \right]^{1/2} v_w^{1/2} / \bar{A}^{1/2}$ $\frac{d\bar{h}}{dt} = 0$	$t_i = \left(\frac{C_{21}}{C_{11}} \right)^6 \left[\frac{(\dot{m}/\rho_0 w)^4}{(g\Delta)^2 v_w^3} \right]^{1/2}$ $A_i = 2 C_{21} \left(\frac{C_{21}}{C_{11}} \right)^7 \left[\frac{(\dot{m}/\rho_0 w)^4 w^3}{(g\Delta)^2 v_w^3} \right]^{1/2}$ $h_i = \dot{m} t_i / \rho_0 A_i$ $\bar{A}_i = 8 A_i$ $\bar{h}_i \approx 10^{-4} - 10^{-5} \text{ meters}$
Open Water	$\frac{dA}{dt} = \frac{1}{2} (\pi K_{21}^2)^2 \left[\frac{(g\Delta)^2}{v_w} \right]^{1/2} h^{1/2} v_w^{1/2} A^{1/2} + \frac{2}{3} \left[\dot{m} - \dot{m}_{loss} - \rho_0 \bar{h} \left(\frac{d\bar{A}}{dt} \right) \right] / \rho_0 h$ $\frac{dh}{dt} = \left[\dot{m} - \dot{m}_{loss} - \rho_0 \bar{h} \left(\frac{d\bar{A}}{dt} \right) - \rho_0 h \left(\frac{dA}{dt} \right) \right] / \rho_0 A$ $\frac{d\bar{A}}{dt} = 6.02 \left[\frac{(\sigma/\rho)^2}{v_w} \right]^{1/2} v_w^{1/2} / \bar{A}^{1/2}$ $\frac{d\bar{h}}{dt} = 0$	$t_i = \left(\frac{K_{21}}{K_{11}} \right)^6 \left[\frac{(\dot{m}/\rho_0)}{g\Delta v_w} \right]^{1/2}$ $A_i = \pi K_{21}^2 \left(\frac{K_{21}}{K_{11}} \right)^7 \left[\frac{(\dot{m}/\rho_0)}{g\Delta v_w^3} \right]^{5/4}$ $h_i = \dot{m} t_i / \rho_0 A_i$ $\bar{A}_i = 8 A_i$ $\bar{h}_i \approx 10^{-4} - 10^{-5} \text{ meters}$

slick is assumed to have a constant thickness $\bar{h}$. Further, the initial area of the thin slick is assumed to be some multiple (Mackay suggests eight) of the initial area of the thick slick. The rate of change of the thin slick area, $\bar{A}$, is also shown in Table III.3. Since the experiments to be described later did not attempt to establish the empirical constants of the surface tension-viscous phase, the constants suggested in the literature [7,8,13,14] are used in the models. It is emphasized that the spreading of the thin slick is used only to compute a relatively small, apparent loss of mass from the thick slick so, these approximations used in developing thin slick models are not a limiting factor in the accuracy of the models.

When there is a current or wind that transports the slick, the shape of a continuous spill is distorted and the previous models are not applicable. The upstream edge of the slick remains fixed to the source but the rest of the spill is transported downstream. Thus, the slick is no longer symmetric (one-dimensional or circular) about the source. Waldman, et al. [7] has, however, developed a model of a continuous spill in a current that is adapted here for a loss of mass. For a spill in open water, as an example, the downstream edge is assumed to be swept away from the source at a speed equal to the current U_T . (U_T will also be made to include the effects of wind, as discussed later.) The upstream edge remains attached to the source. The sides of the slick are assumed to spread laterally in accordance with one-dimensional gravity-viscous spreading. The resulting slick has a triangular shape, with the vertex at the source and the base at the downstream edge. To develop the model, it is imagined that a stream of instantaneous spills, each of volume $\dot{m} \delta t / 2\rho_0$ is transported downstream with a speed U_T , and the slick from each such spill spreads along a channel of width $U_T \delta t$ perpendicular to the direction of the current. (The factor of one-half accounts for the fact that only half the spill spreads in each direction.) The width $W(x)$ of the resulting slick at any downstream location x can therefore be derived from transforming the one-dimensional instantaneous-spill spreading model as follows:

$$W(x) = 2 K_{21} \left[\frac{g \Delta (\dot{m} \delta t / 2\rho_0)^2}{(U_T \delta t)^2 \sqrt{\nu_w}} \right]^{1/3} t^{2/3} \\ = \frac{2 K_{21}}{U_T} \left[\frac{g \Delta (\dot{m} / 2\rho_0)^2 \sqrt{U_T}}{\sqrt{\nu_w}} \right]^{1/3} x^{2/3}; \quad x = U_T t \quad (\text{III.17})$$

The initial conditions for the gravity-viscous phase can be derived similarly. Waldman's type of model will not accurately represent the shape of the slick or the area when the transport velocity U_T is small compared to the gravitationally-induced spreading velocity. When U_T is small, the slick will not take the shape of a triangle with the vertex at the source, but instead will be an ellipse that surrounds the source and extends somewhat farther downstream of the source than upstream. This kind of spreading may arise when there is a wind but no current, since only a small part of the total wind contributes to U_T . The computerized models do not include such cases explicitly. It is suggested that they be treated by first setting U_T to zero identically to compute the size of the slick as a function of time, and then repeating the calculations with the true value of U_T to compute both the downstream position of the slick and an estimate of the mass evaporated from the slick.

For a continuous spill in a channel, the model assumes that the spreading is in the downstream direction. The upstream edge of the slick remains attached to the source and the downstream edge is swept away by a combination of spreading and transport. Thus, $U_T w$ must be added to the dA/dt expression derived previously for a continuous spill in a channel without a current.

Table III.4 summarizes the models of continuous spills in a current. In the computerized versions of the continuous spill models, an appropriate instantaneous spill model is used to continue the spreading predictions after the discharge has stopped. For example, for a spill in open water, the instantaneous spill model for open water is used with an initial area, thickness, and mass equal to the final values of the slick from the continuous spill. There may be a mismatch in the shape of the slick at the time the switch is made, since the instantaneous spill assumes a circular shape while a continuous spill in a current predicts a triangular shape, but a more complicated transition model is not believed to be warranted. After some time has elapsed, the predicted shape of the instantaneous spill is, in any event, more in accordance with expectations. (The numerical values of C_{12} , C_{22} , K_{12} , and K_{22} are discussed in Section V.1.)

TABLE III.4 SPREADING MODELS FOR CONTINUOUS SPILLS IN A CURRENT
(A, h ~ thick slick; $\bar{A}, \bar{h}$ ~ thin slick)

Spill Location	Spreading Model	Initial Conditions
Channel	$\frac{dA}{dt} = \frac{3}{2} (C_{22})^{3/2} \left[\frac{w^2 (g\Delta)^2}{v_w} \right]^{1/2} h^{1/2} A^{-1/2} + \frac{1}{2} \left[\dot{m} - \dot{m}_{loss} - \rho_0 \bar{h} \left(\frac{d\bar{A}}{dt} \right) \right] / \rho_0 h + U_T w$ $\frac{dh}{dt} = \left[\dot{m} - \dot{m}_{loss} - \rho_0 \bar{h} \left(\frac{d\bar{A}}{dt} \right) - \rho_0 h \left(\frac{dA}{dt} \right) \right] / \rho_0 A$ $z_{upstream} = 0$ $z_{downstream} = A/w$ $\frac{d\bar{A}}{dt} = 2.76 \left[\left(\frac{ow^2}{\rho} \right)^2 / v_w \right]^{1/2} / \bar{A}^{1/2} + U_T w$ $\frac{d\bar{h}}{dt} = 0$	$t_i = \left(\frac{C_{22}}{C_{12}} \right)^{3/2} \left[\frac{(\dot{m}/\rho_0 w)^4}{(g\Delta)^2 v_w^3} \right]^{1/2}$ $A_i = 2 C_{22} \left(\frac{C_{22}}{C_{12}} \right)^{3/2} \left[\frac{(\dot{m}/\rho_0 w)^3 w^3}{g\Delta v_w^3} \right]^{1/2}$ $h_i = \dot{m} t_i / \rho_0 A_i$ $\bar{A}_i = 8 A_i$ $\bar{h}_i \approx 10^{-4} - 10^{-5} \text{ meters}$
Open Water	$\frac{dA}{dt} = \frac{11}{8} (K_{22})^{3/2} \left[\frac{(g\Delta)^2 U_T^4 (\dot{m}/2\rho_0)^4}{v_w} \right]^{1/2} A^{1/2}$ $\dot{m} = \dot{m} - \dot{m}_{loss} - \rho_0 \bar{h} \left(\frac{d\bar{A}}{dt} \right)$ $\frac{dh}{dt} = \left[\dot{m} - \rho_0 h \left(\frac{dA}{dt} \right) \right] / \rho_0 A$ $z_{upstream} = 0$ $z_{downstream} = U_T t$ $\frac{d\bar{A}}{dt} = 2.06 \left[\frac{(\rho U_T^2 / \rho)^2}{v_w} \right]^{1/2} / \bar{A}^{1/2}$ $\frac{d\bar{h}}{dt} = 0$	$t_i = \left(\frac{K_{22}}{K_{12}} \right)^{3/2} \left[\frac{(\dot{m}/2\rho_0)^4}{(g\Delta)^2 v_w^3 U_T^4} \right]^{1/2}$ $A_i = K_{22} \left(\frac{K_{22}}{K_{12}} \right)^{3/2} \left[\frac{(\dot{m}/2\rho_0)^3}{(g\Delta) U_T^2 v_w^3} \right]^{1/2}$ $h_i = \dot{m} t_i / \rho_0 A_i$ $\bar{A}_i = 8 A_i$ $\bar{h}_i \approx 10^{-4} - 10^{-5} \text{ meters}$

III.2.5 Maximum Size of Slick

All the models must take into account the possibility that the slicks attain a maximum possible size. For oil, it has been observed that spreading eventually stops for a variety of reasons [7,8]. Experiments with pure chemicals, as described later, show that although the thin slick may never cease to spread (when $\sigma > 0$), the thick slick apparently stops spreading when the average thickness is of the order of 10^{-4} meters. When the thickness is less than 10^{-4} meters, the thick slick becomes indistinguishable from the thin slick. Since the interest in the Hazard Assessment Computer System is primarily in the thick slick, the spreading is assumed to stop when the thickness of the thick slick is less than 10^{-4} meters. (In the computerized version, the user has the option of changing the minimum allowable thickness for the thick slick.)

III.3 Evaporation Models

III.3.1 Discussion

In general, the mass and heat transfer processes associated with chemical spills in the environment will be turbulent. For chemical spills which float on water, the convective mass transfer associated with evaporation will be by a turbulent boundary layer. The primary source of information applicable to the present problem for spills on water is the literature on air-sea interactions. The air-sea interaction research involves all of the relevant mechanisms associated with chemical spills on open water. An excellent review of the subject has been written by Coantic [20], and a recent collection of papers on the subject is contained in Favre and Hasselmann [21].

According to Resch and Selva [22], the fluxes for momentum and mass transfer are given by

$$\tau_0 = \rho_a V_w^2 (C_f/2) \quad (III.18)$$

$$J_0 = \rho_a V_w (C_s - C_{\infty}) Da \quad (III.19)$$

where τ_0 is the shear stress, ρ_a the air density, V_w the freestream wind velocity, C_f the friction coefficient, J_0 the mass flux, C_s the mass fraction of chemical vapor at the surface which is assumed to be at saturation, C_∞ its freestream value which is assumed to be zero, and Da the Dalton number. From these equations the surface shear stress and mass flux can be predicted if C_f and Da are known from theory. The other quantities can be measured either directly or indirectly. From Schlichting [23] and classical turbulent boundary-layer theory, the friction coefficient for a smooth flat plate is

$$C_f/2 = 0.037 Re_L^{-1/5} \quad (III.20)$$

where $Re_L = V_w L/\nu_a$ is the Reynolds number based upon the length, L , of the plate. By Reynolds analogy from Eckert and Drake [24], the Dalton number is

$$Da = 0.037 Re_L^{-1/5} Sc^{-2/3} \quad (III.21)$$

where $Sc = \nu_a/D$ is the Schmidt number and D the molecular diffusivity of the chemical in air. This Dalton number relation was used in [1] for the calculation of mass transfer in the present HACS program.

The present flat plate boundary layer model in HACS is not applicable to flows over water for the following reasons:

- (a) According to Wu [25], the ocean is aerodynamically smooth only for wind speeds of less than 3 m/s.
- (b) A water surface is not rigid.
- (c) Reynolds analogy is not valid for rough surfaces. Roughness will increase momentum transfer, but heat and mass transfer may diminish with roughness.
- (d) A length scale L is difficult to define in an atmospheric boundary layer.

The previous theoretical development for turbulent boundary layers is based upon outer-scale variables where the outer scales are V_w , L , and the

boundary layer thickness δ_a . The boundary layer thickness is related to the longitudinal length scale by

$$\delta_a/x = 0.37 \text{ Re}_x^{-1/5} \quad (\text{III.22})$$

The revised model for HACS is based on inner-scale variables. Near the water surface the velocity and concentration profiles are universal and independent of the outer scales. The fluxes away from the surface where molecular effects are small are given by

$$\tau/\rho_a = - \langle uw \rangle \quad (\text{III.23})$$

$$J/\rho_a = \langle cw \rangle \quad (\text{III.24})$$

where the cross-correlation $\langle uw \rangle$ is also known as the Reynolds Stress. In the layer outside the viscous sublayer the fluxes are constant and the profiles are logarithmic. As a consequence of the constant flux hypothesis, the profiles are

$$u_+ = (U - U_s)/u_* = A \ln (z_+/z_{0+}) \quad (\text{III.25})$$

$$c_+ = (C - C_s)/c_* = A \text{ Sc}_t \ln (z_+/z_{0c+}) \quad (\text{III.26})$$

where $A = \kappa^{-1}$ is the reciprocal Von Karman constant, z_0 the integration constant or roughness parameter, Sc_t the turbulent Schmidt number, $z_+ = zu_*/\nu$, u_* and c_* are the friction velocity and concentration, and U_s and C_s are the surface values of velocity and concentration. The profiles in Equations (III.25) and (III.26) are dependent only on the surface roughness and not on any external length scale.

III.3.2 General Description

The evaporation model for the HACS revision is based on inner-scale variables in contrast to outer-scale variables of the previous HACS model. The new model has the following features and advantages:

- (a) No external length scale such as a spill dimension is required for the calculation of Dalton number, Da .
- (b) Roughness effects, i.e., wave height, are included. The flow is defined to be rough at wind speeds above 5 m/s.
- (c) Only standard meteorological and oceanographic data (that is, air temperature, barometric pressure, wind velocity, sea surface temperature, and wave height) are required as input data.
- (d) Wind velocity data are based upon a standard height of 10 meters.

Additionally, all the necessary physical property data for air, water, and some representative chemicals have been included in the computerized model to make the mass transfer calculations. Chemical diffusivities are required for the Schmidt number in the mass transfer calculations, but this information is not included in the present CHRIS Hazardous Chemical Data files. A detailed description of the mathematical models for the chemical properties is contained in Appendix A with tables of the properties at standard conditions.

III.3.3 Evaporation Rate

A reciprocal Dalton number is calculated for mass transfer from a theory by Kader and Yaglom [26,27] and Yaglom and Kader [28] which is given by

$$Da_{\star} = A Sc_t \ln \delta_{+} + B (Sc, h_m) + \beta_1 \quad (III.27)$$

where δ_{+} is the boundary layer thickness in inner-scale variables, B is a universal function based upon Schmidt number and the mean protrusion (wave) height h_m , and β_1 is a constant dependent on flow geometry. For a boundary layer β_1 is 2.35. The Dalton number $Da_{\star}$ is non-dimensionalized with $u_{\star}$ rather than V_w . The inner and outer scale Dalton numbers are related by

$$Da = Da_{\star} (u_{\star}/V_w) \quad (III.28)$$

Thus, the mass transfer calculation is accomplished in Equation (III.19) by replacement of $V_w Da$ by $u_{\star} Da_{\star}$. The B function for a smooth surface

from Kader and Yaglom [27] is

$$\beta = 12.5 Sc^{2/3} + A Sc_t \ln Sc - 5.3 \quad (\text{III.29a})$$

and for a rough surface from Yaglom and Kader [28] is

$$\beta = 0.55 \sqrt{h_{m+}} (Sc^{2/3} - 0.2) - A Sc_t \ln h_{m+} + 11.2 Sc_t \quad (\text{III.29b})$$

Also, from [28] the turbulent Schmidt number, Sc_t , is 0.85.

A sample calculation of Dalton number for the evaporation of water from a smooth surface is presented in Figure III.2 where the Schmidt number for water vapor is 0.593. The theory of Kader and Yaglom [27] is compared to that of Street [29] which is a related theory. A review of these and other mass transfer theories is presented in [30]. Also, for comparison, the results of wind tunnel experiments [22,31] are also included in Figure III.2. The results in [22] are probably from smooth flow since their wind speed was 3.5 m/s; however, some results in [31] are for rough flow. Since no wave height measurements were reported for either set of experiments, no comparison is possible with rough flow theory. The following conclusions can be drawn from Figure III.2:

- (a) The scatter in data for evaporation experiments is large.
- (b) The agreement between theory and experiment is poor.
- (c) The theories of either Yaglom and Kader [28] or Street [29] are adequate for the present application.

The only information required in addition to the meteorological and oceanographic data for the calculation of mass transfer is the friction velocity. The friction velocity is computed from the wind-stress coefficient as follows:

$$u_* = V_w (C_f/2)^{1/2} \quad (\text{III.30})$$

where V_w is the wind velocity measured at 10 meters above the water and $C_f/2$ is the wind-stress coefficient. Numerous models of wind-stress

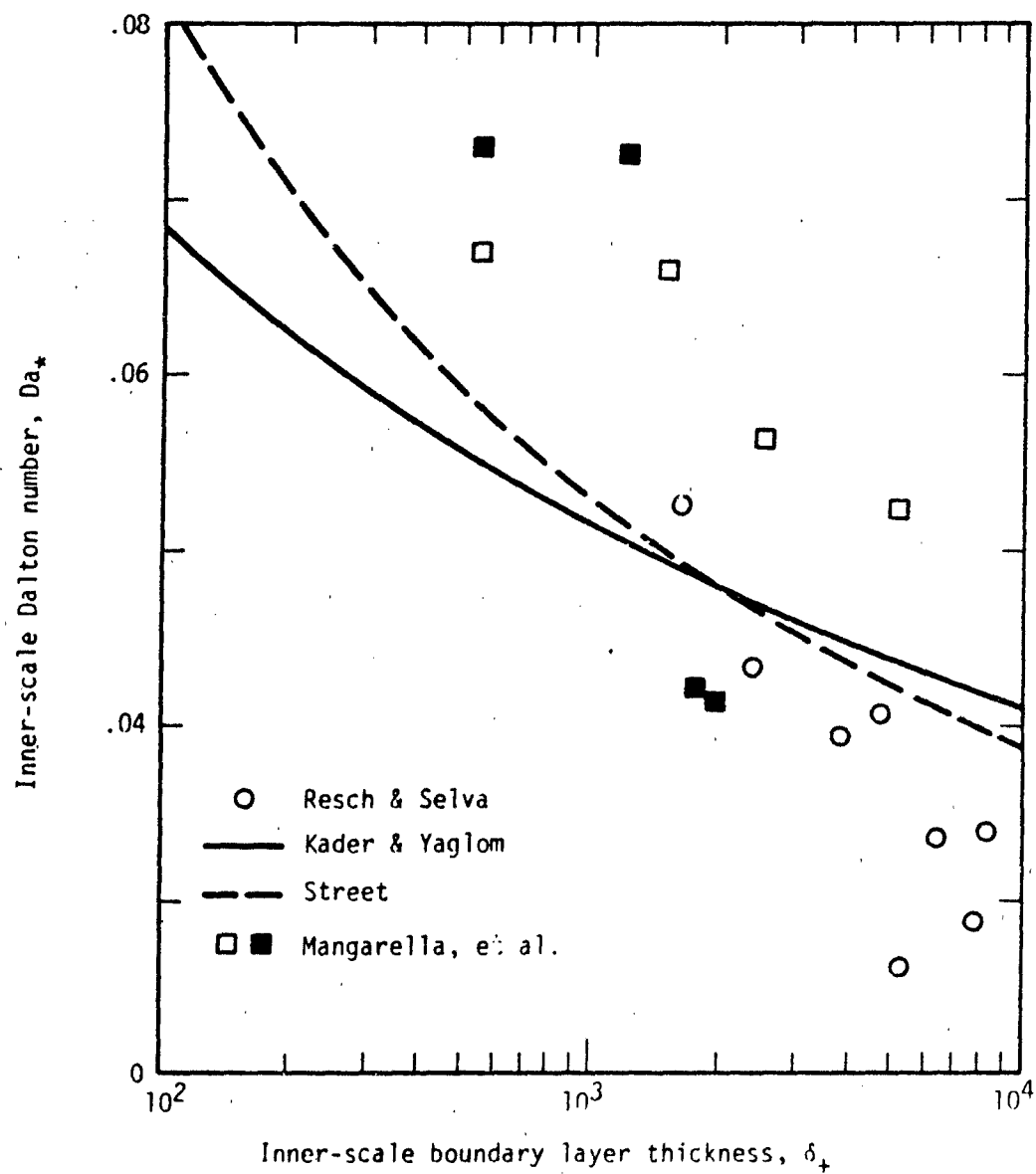


Figure III.2. Comparison of Theoretical and Experimental Dalton Numbers for Smooth Flow Over Water ($Sc = 0.593$). Open Symbols are for Wind Waves and Closed Symbols are for wind and mechanical waves

coefficient are available in the oceanographic literature. Some representative relations are summarized in Table III.5.¹ The equations selected for this program are from Wu [25]

$$C_f/2 = (0.8 + 0.065 V_w) \times 10^{-3} \quad (\text{III.31a})$$

for $1 < V_w < 20$ m/s and

$$C_f/2 = (1.25/V_w^{1/5}) \times 10^{-3} \quad (\text{III.31b})$$

for $V_w \leq 1$ m/s. In the computer program, the 1 m/s boundary between the two values of wind-stress coefficient is set at 3.064 m/s. At this wind velocity the two wind-stress coefficients have the same value. In addition, Wu [25] states that the flow is aerodynamically smooth for $V_w < 3$ m/s. The selection of Wu's model was arbitrary. However, the Wu model is simple, and it is similar to those of other investigators.

In the event that wave height information is not available, the wave height can be modeled with the following relation from Van Dorn [34]

$$h_m = 0.01384 V_w \quad (\text{III.32})$$

where V_w is in meters/second and the mean wave height, h_m , is in meters. This equation is valid only for a fully developed sea; thus, it is an upper bound for wind generated waves. With Equations (III.31a) and (III.32) the wave height can be calculated from the wind speed as an inner-variable scale. The result is plotted in Figure III.3.

¹ A plot of some of these relations is presented in [32,33]

TABLE III.5 WIND-STRESS COEFFICIENTS OF VARIOUS AUTHORS

Author	Year	$10^3(C_f/2)$	Velocity Range (m/s)
Amorocho & DeVries	1981	$1.21 \left\{ 1 + \exp \left[(2.5 - V_w)/1.56 \right] \right\}^{-1} + 1.04$	0-40
Garratt	1977	$0.75 + 0.067 V_w$	4-21
Large & Pond	1981	1.2	4-11
		$0.49 + 0.065 V_w$	11-25
Smith	1980	$0.61 + 0.063 V_w$	6-22
Smith & Banke	1975	$0.63 + 0.066 V_w$	3-21
Wu	1980	$0.08 + 0.065 V_w$	1-20
Wu	1969	$1.25/V_w^{1/2}$	0-1

NOTE: V_w is the wind velocity at 10 meters.

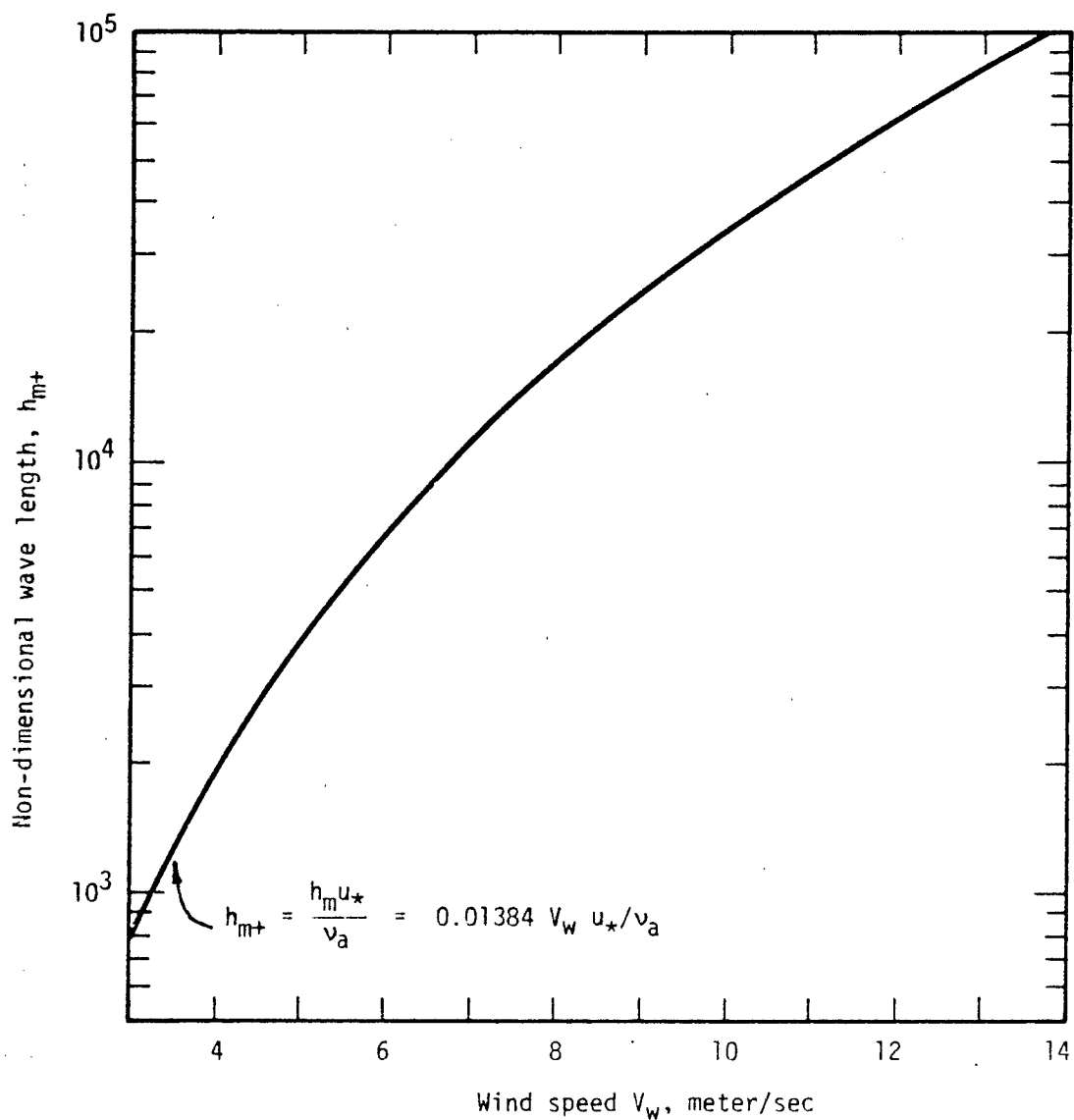


Figure III.3. Mean Wave Height in Law-of-the-Wall Coordinate for a Fully Developed Sea as a Function of Wind Speed

III.4 Dissolution Models

III.4.1 Discussion

The dissolution model in the present HACS model is one which is valid only in rivers and streams. The dissolution model included in HACS [2] was developed by Fortescue and Pearson [35] for the dissolution of gases in flowing water. A more recent model has been included in the revision.

For dissolution in open bodies of water such as lakes and coastal waters, the mass transfer model described in the previous section has been applied to dissolution. The mass transfer process on the two sides of the gas-liquid interface has been assumed to be the same. A boundary layer is formed in the liquid by the transfer of momentum to the water by the wind. Since the shear stress across the interface is assumed to be continuous, the friction velocities in air and water are related as follows:

$$u_{*w} = u_{*a} (\rho_a/\rho)^{1/2} \quad (\text{III.33})$$

With this assumption, dissolution of the chemical spill into the water can be computed with the same equations as its evaporation into the air.

III.4.2 General Description

The dominant effect in dissolution is the Schmidt number for the chemicals in water, which is on the order of a thousand. According to Shaw and Hanratty [36], the Dalton number for sufficiently large Reynolds number and Schmidt number will reduce to

$$\text{Da}_* = K \text{Sc}^{-n} \quad (\text{III.34})$$

where $2/3 \leq n \leq 3/4$ and K is a constant determined from experiment. As the previous section states, information for Schmidt number is not included in CHRIS. The description in Section III.3.2 for evaporation is also valid for dissolution. The length dimension for δ_+ in Equation (III.27) must be large compared to δ_c and was assumed to be one meter.

III.4.3 Mass Transfer From Slick Into Water

The mass transfer calculations for dissolution in lakes, coastal waters, and the open ocean are accomplished with the same equations as for evaporation. From the wind velocity, the friction velocity in air is computed from Equations (III.30) and (III.31a,b) and the friction velocity in water from Equation (III.33). The Dalton number Da_* is calculated from Equations (III.27) and (III.29a,b) where the physical properties such as Schmidt number, density, and viscosity are for water. Then, the mass transfer in physical units is computed from Equations (III.28) and (III.19) where the density is now the water density, C_s now the water solubility of the chemical in mass fraction of water, and the freestream concentration, C_∞ is zero.

The Dalton number for dissolution in a river or stream is calculated from a formula recommended by Ueda, et al. [37] as follows:

$$Da_* = 0.0626 Sc^{-2/3} \quad (III.35)$$

In this formulation, the Dalton number Da_* is based upon the friction velocity for the bottom. No correlation for the friction coefficient for rivers exists which is similar to that for wind stress in Table III.5. In the absence of such a correlation, the following was applied from Schlichting [23] for a completely rough regime.

$$(C_f/2)^{-1/2} = U_c/u_* = 5.66 \log (2d/h_s) + 4.92 \quad (III.36)$$

where h_s is Nikuradse's sand roughness, d is the depth of the river, and U_c is the mean current. Also, Fischer, et al. [38] claim a reasonable assumption is $u_* = 0.1 U_c$.

Shear stress velocity can easily be computed from Equation (III.36) for a river; however, an estimate must be made for the bottom roughness. Experimental results for various channels compiled from Fischer, et al. [38,39] are summarized in Table III.6 and plotted in Figure III.4. The data in Figure III.4 are compared with the smooth channel theory of

TABLE III.6 SKIN FRICTION COEFFICIENT FOR OPEN CHANNEL EXPERIMENTS*

Author	Year	Channel	Mean Depth d (cm)	Mean Velocity U_C (cm/s)	Shear Velocity u_* (cm/s)	$10^3 C_f/2$	10^{-6}Re_d
1. Yotsukura, et al.	1970	Missouri River Blair, Nebraska	270	175	7.4	1.788	18.82
2. Holley & Abraham	1973a	Lab. model of Ijssel River	90	13	0.78	3.6	0.47
3. Holley & Abraham	1973b	Ijssel River	400	96	7.5	6.104	15.30
4. Mackay	1970	McKenzie River Fort Simpson	670	177	15.2	7.375	47.25
5. Yotsukura & Sayre	1976	Missouri River Cooper Nuclear Station, Nebraska	400	540	8.0	0.220	86.06
6. Glover	1964	Columbia River	305	135	8.8	4.249	16.40
7. Fischer	1967	Irrigation Canal	68.3 66.7	63 66	6.3 6.1	10.0 8.542	1.714 1.754

* Compiled from Fischer, et al. [34] and Fischer [39]

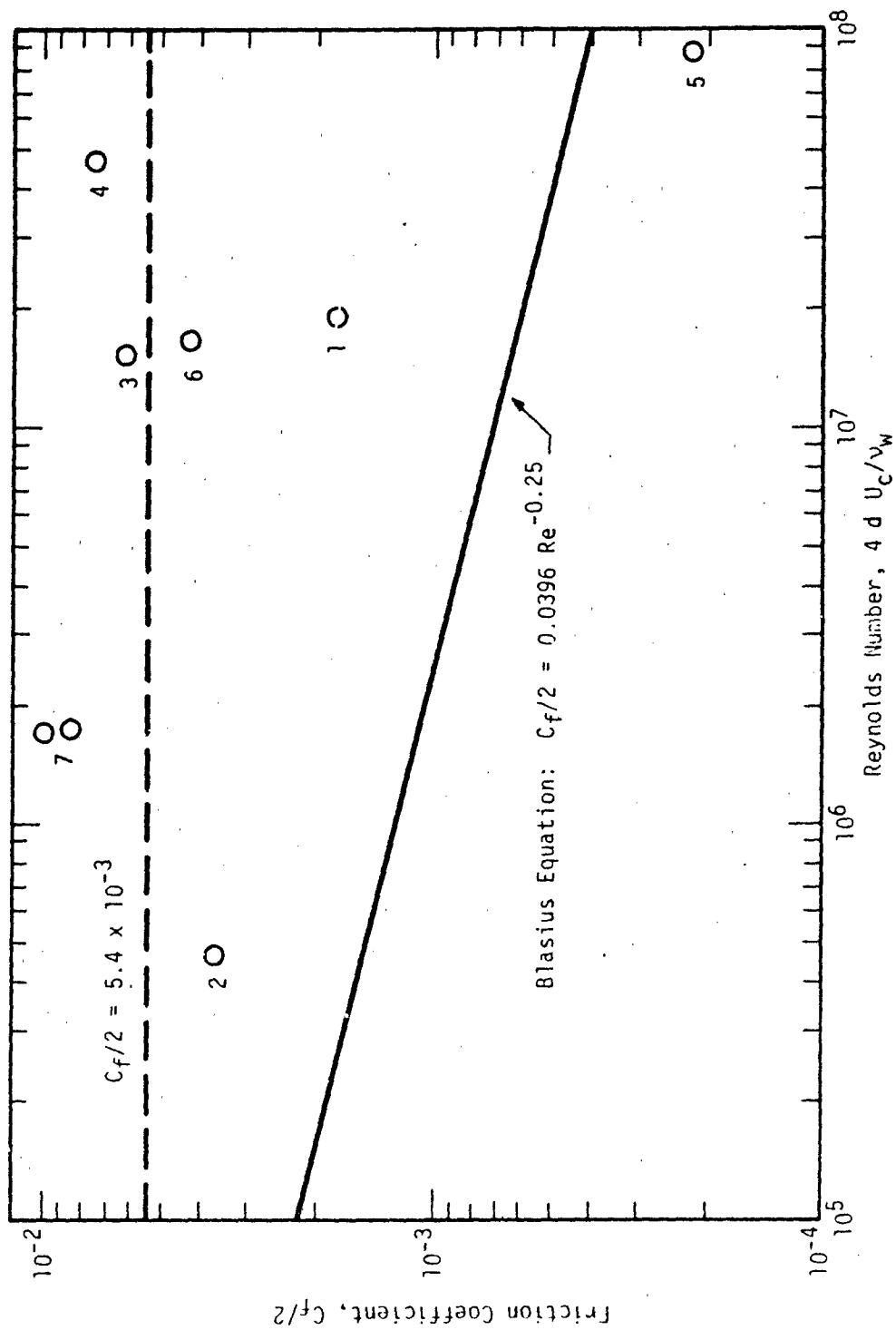


Figure III.4. Friction Coefficient for Open Channel Flows. Numbers Correspond to Experimental Data in Table, and Solid Line is Blasius Equation.

Blasius for turbulent flow. All data, with the exception of Yotsukura and Sayre [40] are consistent with a rough wall hypothesis. The average value of the shear stress coefficient, $C_f/2$, for the experimental data is 5.4×10^{-3} which corresponds to a relative roughness of $2d/h_s = 34.4$ from Equation (III.36). Thus, roughness height can be estimated from

$$h_s = 0.0581 d \quad (\text{III.37})$$

where the mean depth, d of the river must be given.

III.5 Movement Models

III.5.1 Discussion

Wind, waves, and currents affect both the shape of a continuous spill, as was discussed in Section III.2.4, and the drift or overall movement of either an instantaneous or a continuous spill. Nearly all the transport predictions in the literature conform to the basic premises of the "Navy" model [41] which states that the vector displacement $\Delta \vec{R}$ of an element of the slick is

$$\Delta \vec{R} = \vec{U}_c \Delta t + K_w \vec{V}_w \Delta t + \vec{U}_w \Delta t \quad (\text{III.38})$$

Here Δt is the computational time period; $\vec{U}_c$ is any current that is not produced by the wind; $\vec{V}_w$ is the wind 10 meters above the water and K_w is a factor that relates the wind to the current produced by it; and $\vec{U}_w$ is a drift-current produced by any waves not directly due to the wind. The value of the wind factor K_w is subject to some dispute, but values of 0.03 to 0.04 are commonly accepted [7]. In the computerized models here, a value of $K_w = 0.035$ is used. The effect of waves in producing a net transport current $\vec{U}_w$ is usually small and is neglected [7, 8, 42]. For the computerized models developed here, the currents and wind values are supplied as input data, as described below. Sets of typical data for selected bodies of water of unusual importance can also be developed in advance, which is the method used in the Norwegian "OILSIM" model [11].

III.5.2 Rivers and Channels

For rivers and channels, either a constant current or a tidally-varying current can be used in the computerized models. Tidal currents are assumed to be of the form

$$U_c = U_0 + U_1 \sin \left[\frac{2\pi}{T} (t + \alpha) \right] \quad (\text{III.39})$$

where U_0 and U_1 are the constant and the time-varying components of the current, T is the tidal period, and α is a parameter chosen such that the appropriate phase of the tide will coincide with time $t = 0$ of the spill initiation. The wind is assumed either to be constant or a specified function of time. A time-varying wind is simulated by giving the wind speed at up to ten different instants of time.

Instantaneous Spills. - The slick formed from an instantaneous spill is transported in accordance with the motion of its centroid. That motion is computed directly from Equation (III.38); however, only the component of the wind aligned with the channel is used in the wind term, $0.035 \bar{V}_w \Delta t$.

Continuous Spills. - Equation (III.38) is used to evaluate the transport velocity U_T needed in the spreading model. Since a time-varying U_T is not permitted in the continuous-spill spreading models as formulated here, a time-average $\bar{U}_T$ is computed whenever $\bar{U}_c$ or $\bar{V}_w$ is a function of time; the average is taken over the shorter of the spill duration or the tidal cycle to give

$$U_T = U_c + 0.035 V_w \cos \theta \quad (\text{III.40})$$

where θ is the angle the wind makes with the current direction.

The slick formed by a continuous spill must remain attached to the source. If the current is tidal, and the reverse flow is significant, the slick is allowed to move with the reversed flow after the spreading has been accounted for. The condition used to determine the significance of the

movement is whether the average value of U_T is greater or less than three-tenths of the maximum value of U_T . When $\bar{U}_T > 0.3 (U_T)_{\text{maximum}}$, the back-and-forth motion of the slick is small compared to the overall downstream motion of the leading edge, and the reversed motion of the slick is neglected. When $\bar{U}_T < 0.3 (U_T)_{\text{maximum}}$, on the other hand, a definite reverse motion of the slick is noticeable, and the slick may move upstream of the source temporarily. In the computerized version, the motion of the leading and trailing edges of the slick for this latter case are approximated as:

$$\Delta z_{le} = \Delta A / 2w + U_T \Delta t \quad (\text{III.41a})$$

$$\Delta z_{te} = -\Delta A / 2w + U_T \Delta t \quad (\text{III.41b})$$

Here ΔA is the change in area caused by the spreading (computed from the average $\bar{U}_T$) over the time interval Δt . If Equation (III.41b) predicts that $z_{te} > 0$ (where $z_{te} = \sum \Delta z_{te}$ summed up to the time of interest), the computerized model sets $z_{te} = 0$ since the trailing edge of the slick cannot move downstream of the source. (That is, a tidal current may transport part of the slick back past the source but it cannot separate the slick from the source.)

After a continuous discharge has ceased, the subsequent motion of the slick is treated similarly to that from an instantaneous spill.

III.5.3 Open Water

In the computerized models, two kinds of "open water" can be specified: lakes and coasts. A lake can be further idealized as essentially circular or rectangular, or the boundary coordinates of the lake can be specified at up to ten locations to allow a more realistic description. Likewise, a coast can be specified as straight or by giving up to ten pairs of coordinates to describe a more realistic shape. The wind can be specified either as constant or as a function of time in a way similar to that described for rivers and channels. The current can be given as a constant for the entire

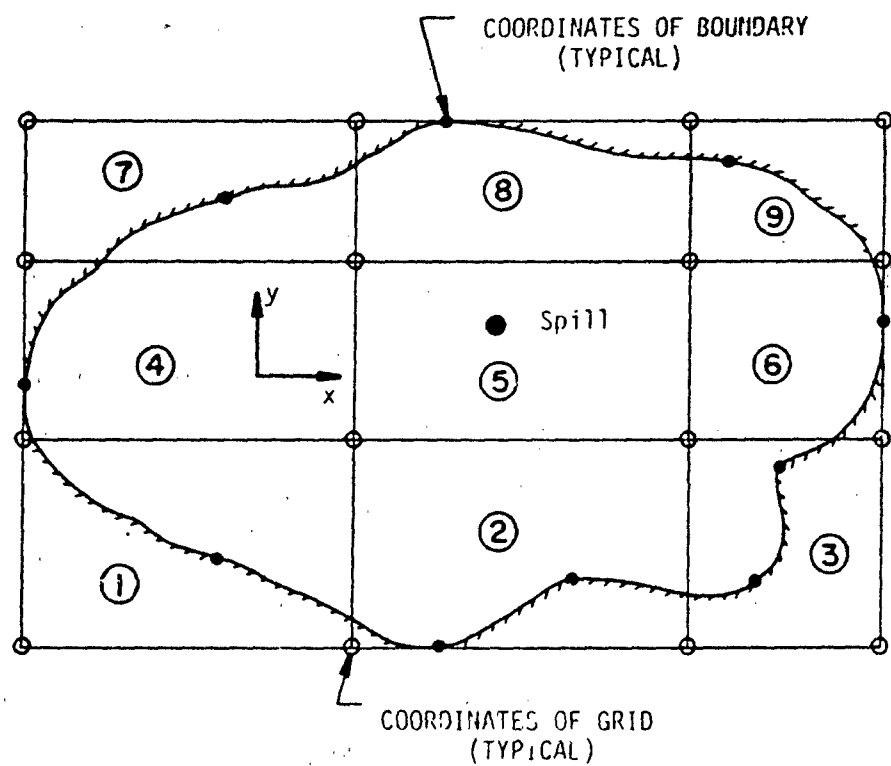
body of water, or as a function of time (by giving values at up to ten instants of time), or as a function of position (as described below), or as a function of both time and position.

To describe a current as a function of position in the computerized models, a grid is superimposed on the water-body description, as shown in Figure III.5. The x and y components of the currents must be specified for each of the nine rectangular "boxes" (for lakes) or "slices" (for coasts). (The numbering system used in the computerized models is shown in the figure.) If the current is also a function of time, the x and y components must be given for each of the boxes or slices at up to ten instants of time.

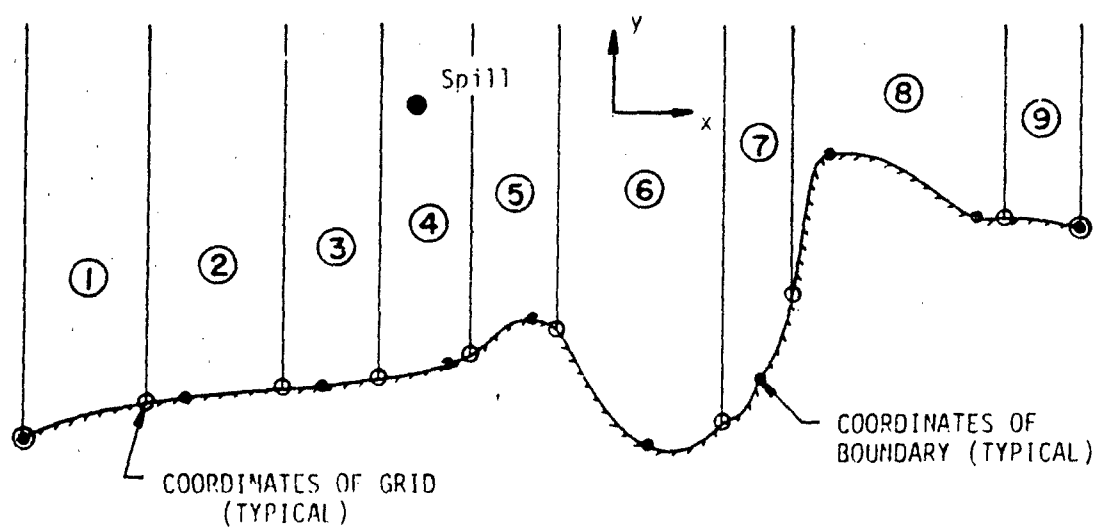
Instantaneous Spills. - The movement of the slick formed from an instantaneous spill is computed as a function of time from Equation (III.38) until the edge of the thick slick arrives at a boundary of the open water.

Continuous Spills. - For a continuous spill, the time-average value of U_T for the box or slice containing the spill source is used in the spreading models to compute the spreading rate. The positions of the leading and trailing edges of the slick are computed, however, from the currents appropriate to their positions whenever the current is a function of position. The method used is similar to that described previously for tidal currents in a river or channel. This can lead to some discrepancies between the area of the slick, the width of the slick, and the positions of the leading and trailing edges, but the computation described is the best that is possible unless a much more complicated spreading model is used.

The dynamics of the spreading are computed as a function of time until the leading edge of the thick slick arrives at a boundary. After a continuous discharge has ceased, the subsequent motion of the slick is treated similarly to that from an instantaneous spill.



a. CURRENT GRID FOR A LAKE



b. CURRENT GRID FOR A COAST

Figure III.5 Specification of Currents for Open Water

III.6 Effects of Spill Parameters on Model Predictions

III.6.1 Discussion

The spreading, evaporation, dissolution, and movement models contain a large number of parameters. In order to demonstrate the use of the models and the importance of various parameters, the effects of four of the more important parameters are investigated: volume of chemical released or discharge rate; chemical density; current; and wind speed. These parameters are varied about a "standard" set of parameters for a spill in a large water body. The standard chemical is chosen to have the same properties as octane, with the exception of density. Octane is nearly insoluble (its maximum solubility is 0.02 kg/m^3), so the effects of the parameter variations on dissolution are small in comparison to their effects on evaporation; this behavior is, however, typical of most of the chemicals of interest to the USCG.

III.6.2 Instantaneous Spills

An instantaneous spill is assumed to occur in a large body of water having a depth of 100 meters and a current of 0.51 m/sec . The wind speed is 3 m/sec oriented at 19.7° with respect to the current. The chemical has a standard density of 800 kg/m^3 , a vapor pressure of 13.92 millibars, and a spreading coefficient of $3.42 \times 10^{-3} \text{ Newton/meter}$. The standard volume of chemical spilled is 60 m^3 .

Figure III.6 shows the variation with time of the area and the thickness of the slick as a function of the spilled volume. In all cases, the area increases rapidly at first when the spill is relatively thick, followed by a longer period when the spreading rate is much slower. (The gravity-inertial phase lasts about two minutes, at which time the standard area is about $1 \times 10^4 \text{ m}^2$. Most of the spreading therefore occurs in the gravity-viscous phase, in accordance with the assumptions used in developing the models.) The rate of spreading throughout clearly depends on the spilled volume. In the absence of evaporation, the areas at any time should be in

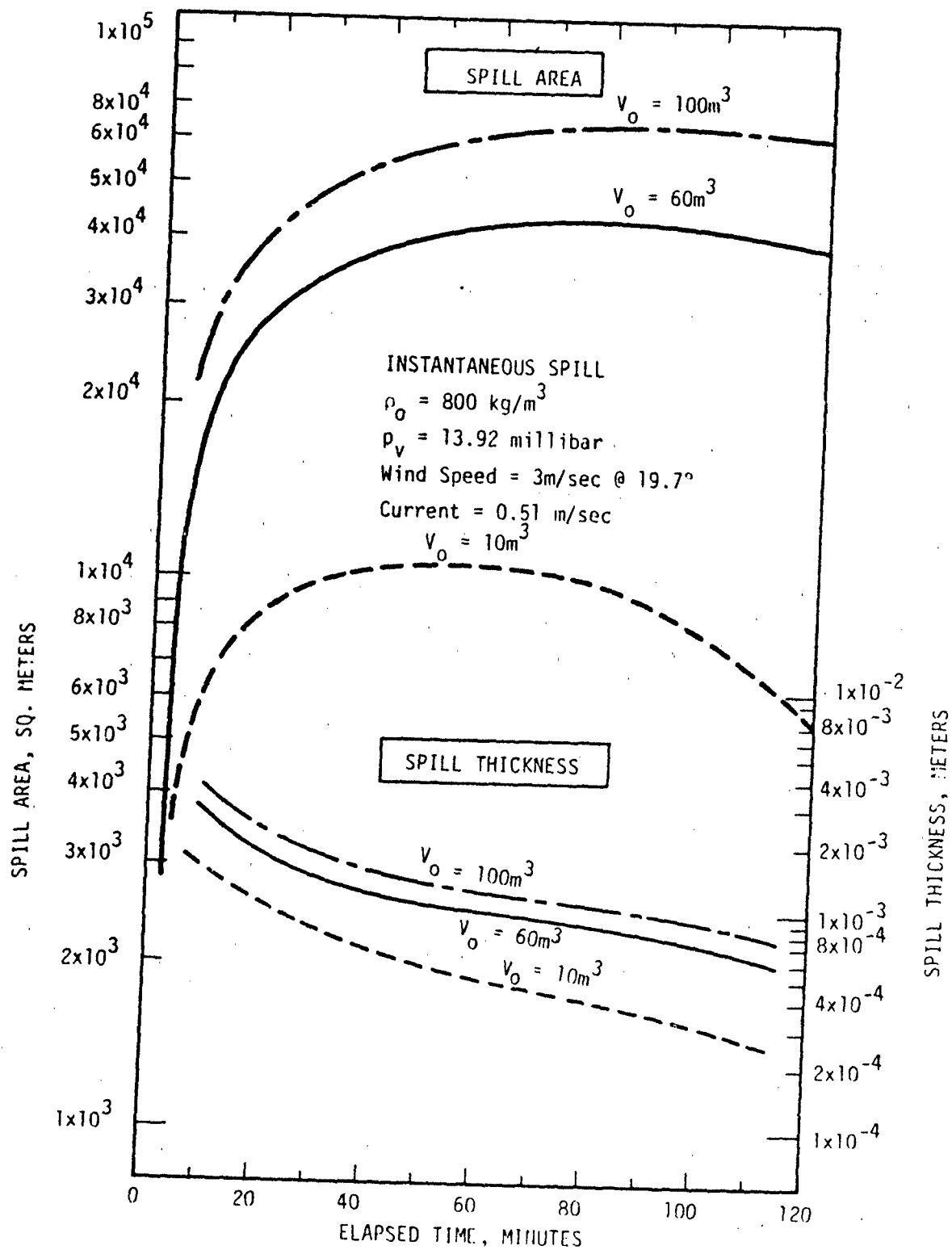


Figure III.6 Effect of Spilled Volume on Size and Thickness of Instantaneous Spills

the ratio of the spill volumes to the two-thirds power, as shown by Equation (III.10). In fact, the curves show that this ratio holds approximately during the time when the spill area increases even when evaporation occurs. The slick areas eventually decrease as a result of evaporation; more will be said about this effect below. The slick thicknesses decrease uniformly, although even after two hours the thicknesses are still well above the cut-off value of 1×10^{-4} meter.

Figure III.7 shows the effects of varying the chemical density when the spilled volume and the other parameters are held constant. Again, the variation is roughly in agreement with Equation (III.10) during the time when the areas are increasing. But, as shown by the curves for $\rho_0 = 800$ kg/m³ and $\rho_0 = 900$ kg/m³, and even more significantly for the unrealistic case of $\rho_0 = 100$ kg/m³, Equation (III.10) is not capable of predicting the correct trend when evaporation becomes dominant. The less-dense chemicals spread more rapidly initially and thus experience a higher rate of evaporation; thus, the higher evaporative losses for them cause the rate of spreading to slow earlier.

The effects of wind speed are shown in Figure III.8. Since higher wind speeds increase the rate of evaporation, the trend of these curves is similar to that shown in Figure III.7 for density variations. The curves for the extreme wind speed of 30 m/sec show the trend most clearly. (The range of wind speeds for which the models are expected to be applicable will be discussed later.)

The effects of varying the current over a factor of one-hundred (i.e., from 0.051 m/sec to 5.1 m/sec) give a trend similar to the wind speed variation, but the magnitudes of the area and thickness changes are much less and therefore are not shown here. It is concluded that the current has only an indirect effect on evaporation. Of course, the movement of the slick is directly related to the current.

Figures III.6, III.7, and III.8 all showed that the rate of spreading eventually became negative as a result of evaporative losses. Such behavior is probably physically incorrect, because as long as the slick is thicker than the cutoff value (1×10^{-4} meters), it should continue to spread in the gravity-viscous phase although at a rate slowed by evaporation. This

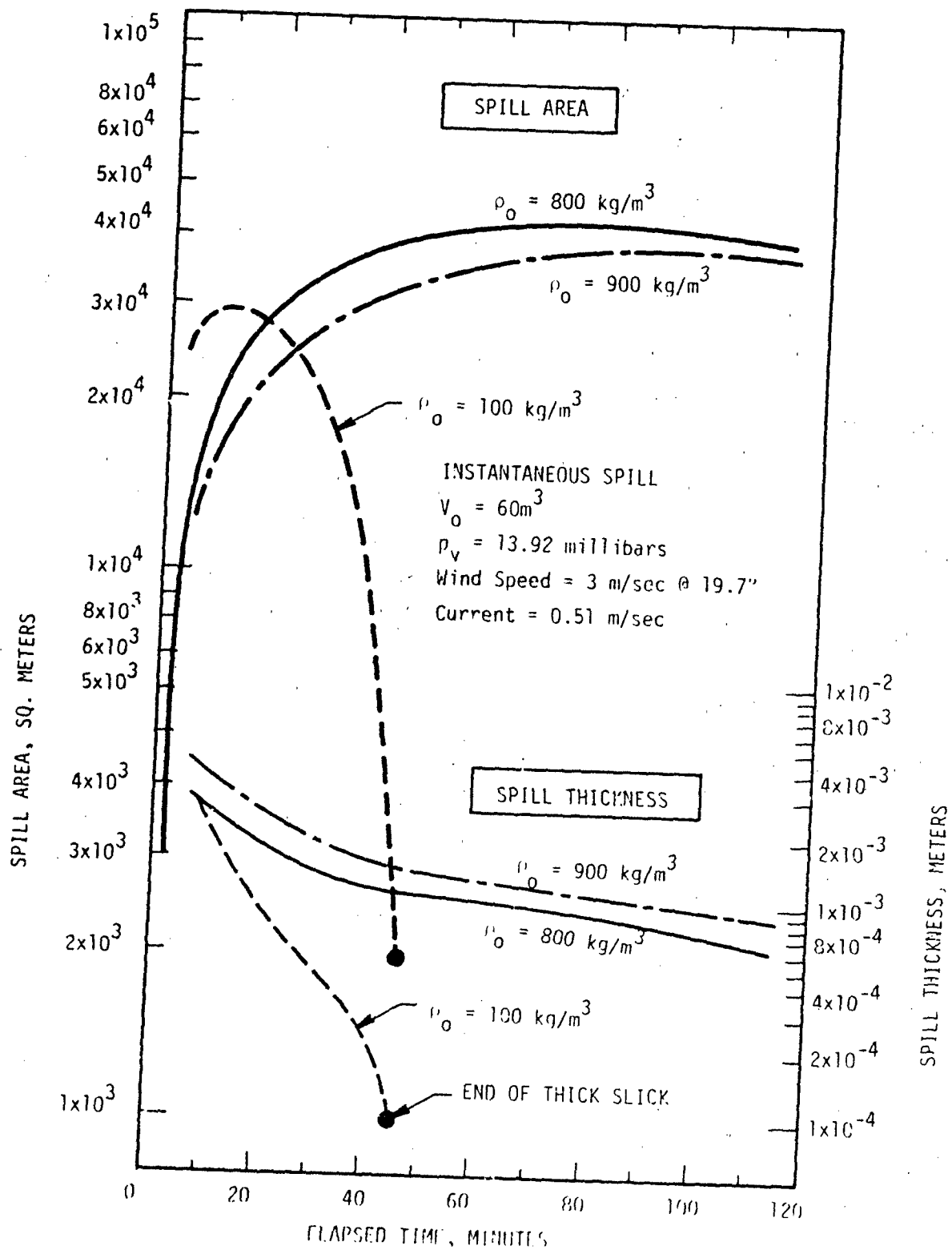


Figure III. 7 Effect of Chemical Density on Size and Thickness of Instantaneous Spills

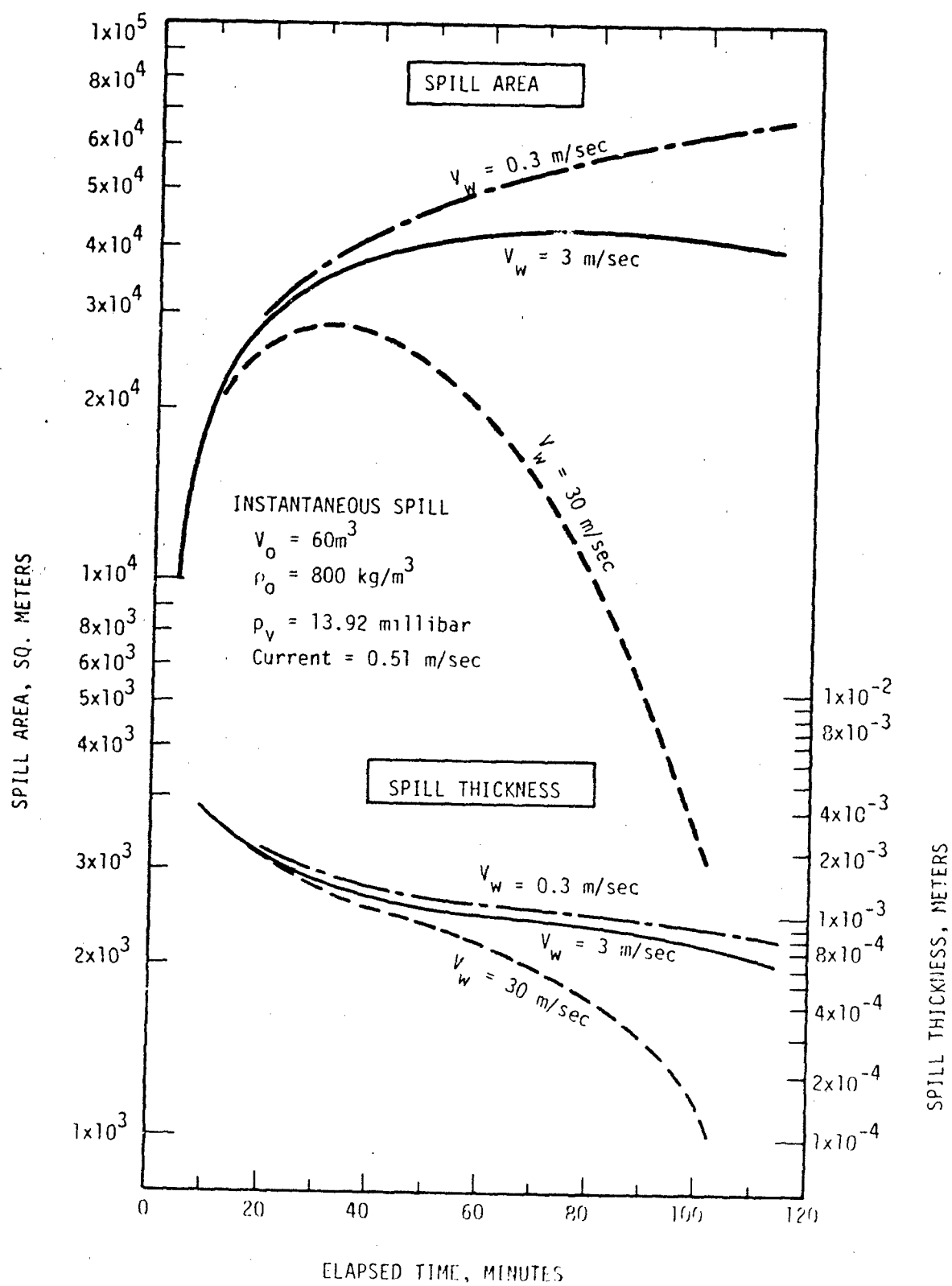


Figure III.8 Effect of Wind Speed on Size and Thickness of Instantaneous Spills

lack of physical reality in the late-time predictions is caused by the use of a "lumped" mass model rather than a differential model. For example, the dA/dt expression given in Table III.3 is based upon a constant thickness h for the entire slick. In reality, h is greater near the center and approaches the minimum value (1×10^{-4} meters) near the edges. Incorporating the variation of h in the model would tend to increase the positive terms in the expression for dA/dt and decrease the negative effect of the loss term $2 \dot{m}_{\text{loss}}/3 \rho_0 h$. More importantly, the loss term itself was derived from the assumption that evaporation and dissolution effectively act as a lumped "sink" just as the spilled mass acts as a lumped "source" at the center of the spill. In reality, the losses are distributed over the entire surface of the slick, i.e., as a distributed sink. Although the difference in the models is negligible as long as $dA/dt > 0$, the distributed model would never predict that $dA/dt < 0$. Instead, the rate of decrease of h would be accelerated late in the spreading. A differential, or distributed model would be, of course, much more complicated mathematically. Since the lumped model gives realistic results over most of the spill duration (except for extreme cases such as $\rho_0 = 100 \text{ kg/m}^3$), the effort involved in developing a differential model is not believed to be warranted.

III.6.3 Continuous Spills

The standard continuous spill has a discharge rate of $0.0333 \text{ m}^3/\text{sec}$ over a total duration of thirty minutes. The total volume of the spill is thus 60 m^3 , the same as for the standard instantaneous spill. The other parameters of the spill are the same as those of the instantaneous spills.

Figure III.9 shows the effects of changing the discharge rate. (The three rates give total spill volumes equal to 100, 60, and 10 m^3 , the same as for the instantaneous spills.) The quantities displayed in the plots are the downstream width of the triangularly-shaped slick and the slick thickness. (The spill area can be computed by multiplying half the width by the spill length, which is equal to the product of the net transport velocity U_T and the elapsed time; as discussed in Section III.5, U_T is $[(U_C + 0.035 V_W \cos \theta)^2 + (0.035 V_W \sin \theta)^2]^{1/2}$.) At the end of

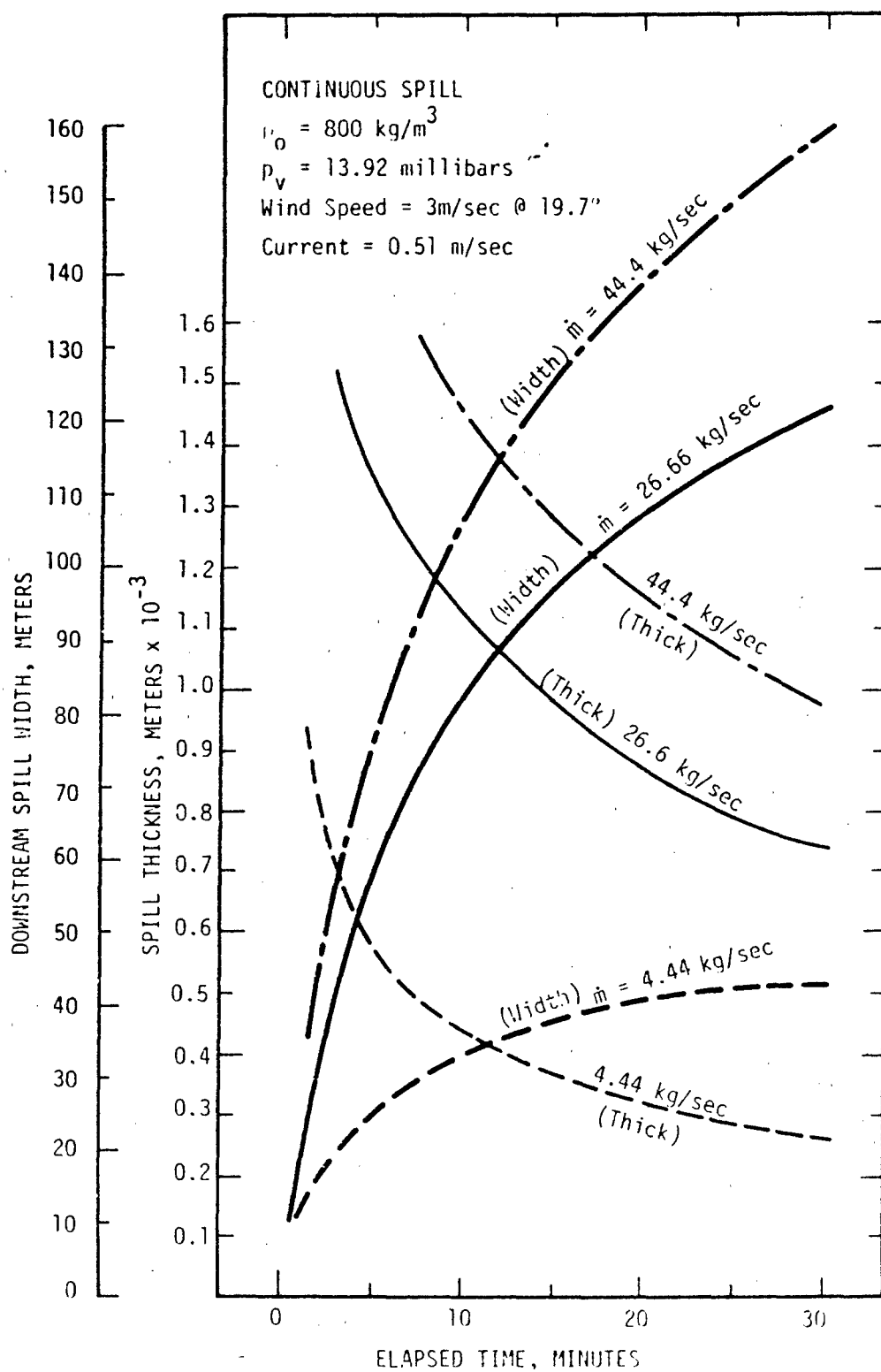


Figure III. 9 Effect of Discharge Rate on Width and Thickness of Continuous Spills

thirty minutes, the areas of the continuous spills are about twice those of the corresponding instantaneous spills, and the thicknesses about one-half. The variation with respect to discharge rate from curve-to-curve is roughly in agreement with Equation (III.16).

The variation of the spill width and thickness with chemical density is shown in Figure III.10. Two values of density around 800 kg/m^3 are shown, as well as the extreme case of $\rho_0 = 100 \text{ kg/m}^3$. It can be seen that for $\rho_0 = 100 \text{ kg/m}^3$ the width and area increase so rapidly initially that evaporative losses cause the width to decrease (but not the total area) after about ten minutes. The negative rate of change of the width is physically unrealistic, for the same reasons as discussed previously in Section III.6.2.

Figure III.11 shows the effects of current. Since the length of the slick increases when the current increases, the current has a significant effect on the width and the area of the slick formed by a continuous spill, in contrast to its negligible effect on an instantaneous spill. The decrease in the width is considerably less, however, than the increase in the length, so the net effect is that the slick area is increased when the current is increased.

Figure III.12 displays the effects of wind speed on the spill width and thickness. Most of the changes in the width and thickness are due to the changes in the evaporative losses, although there is also an effect of the wind speed on U_T and thus an indirect effect similar to that shown previously for a variation in current.

III.7 Wind and Current Limitations on Models

According to Wu [25], a water surface will form breaking waves and spray for wind speeds above about 15 m/sec . Since the slick will also begin to disintegrate, this value represents the limit on wind speeds for which the models are expected to give reliable predictions.

The models should be applicable for all normal values of current experienced in practice.

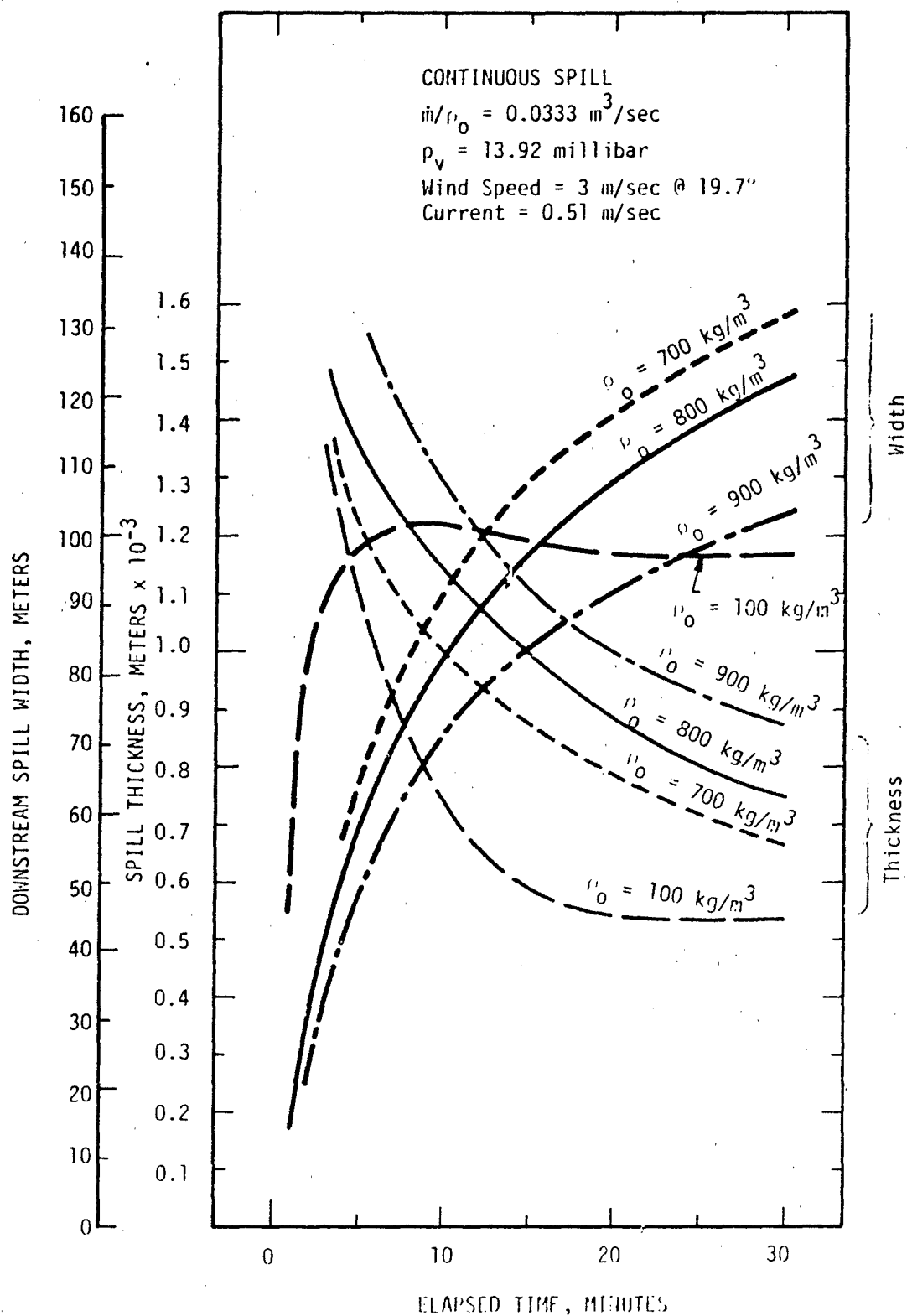


FIGURE III. 10 Effect of Chemical Density on Width and Thickness of Continuous Spills

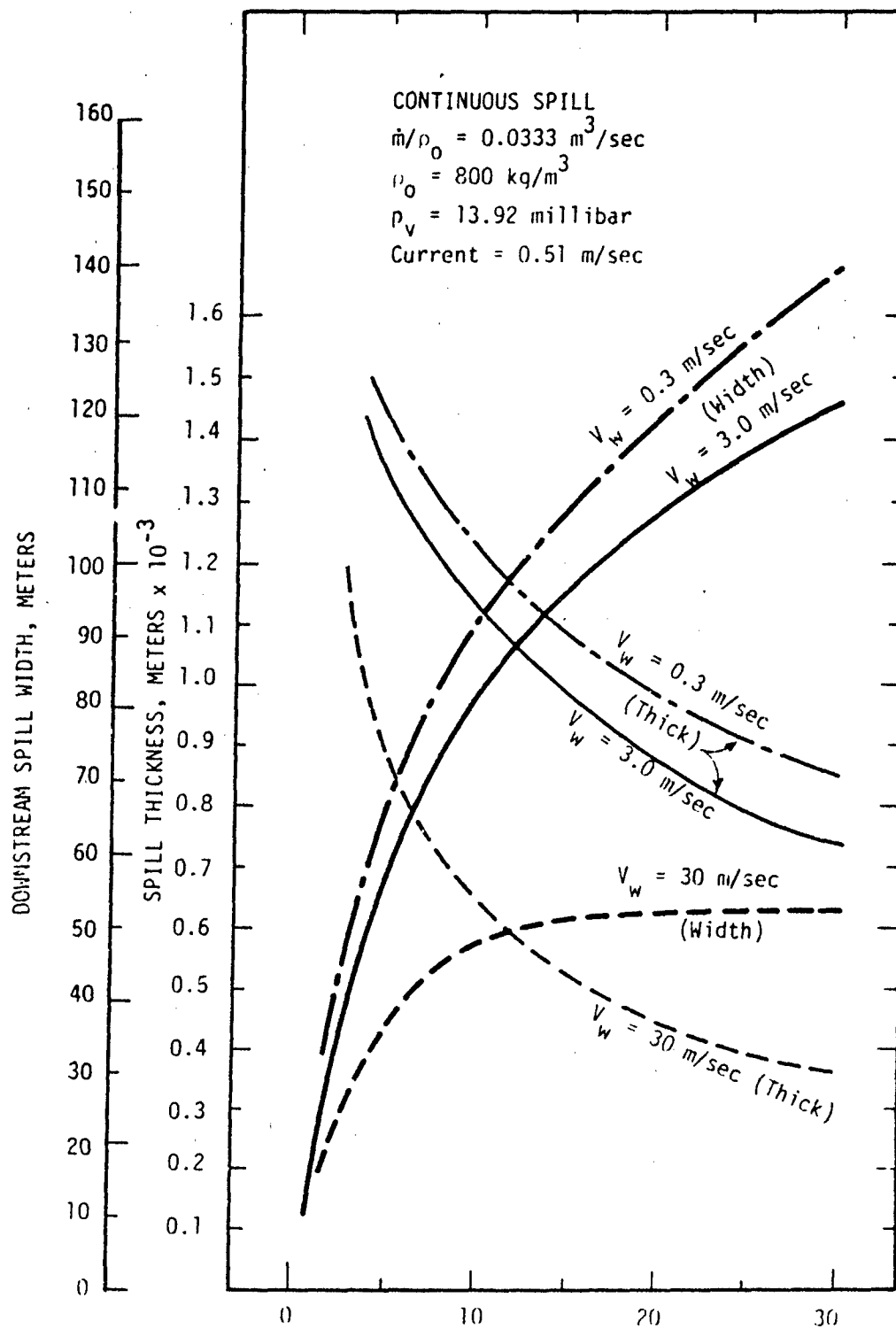


FIGURE 111.11 Effect of Wind Speed on Width and Thickness of Continuous Spills

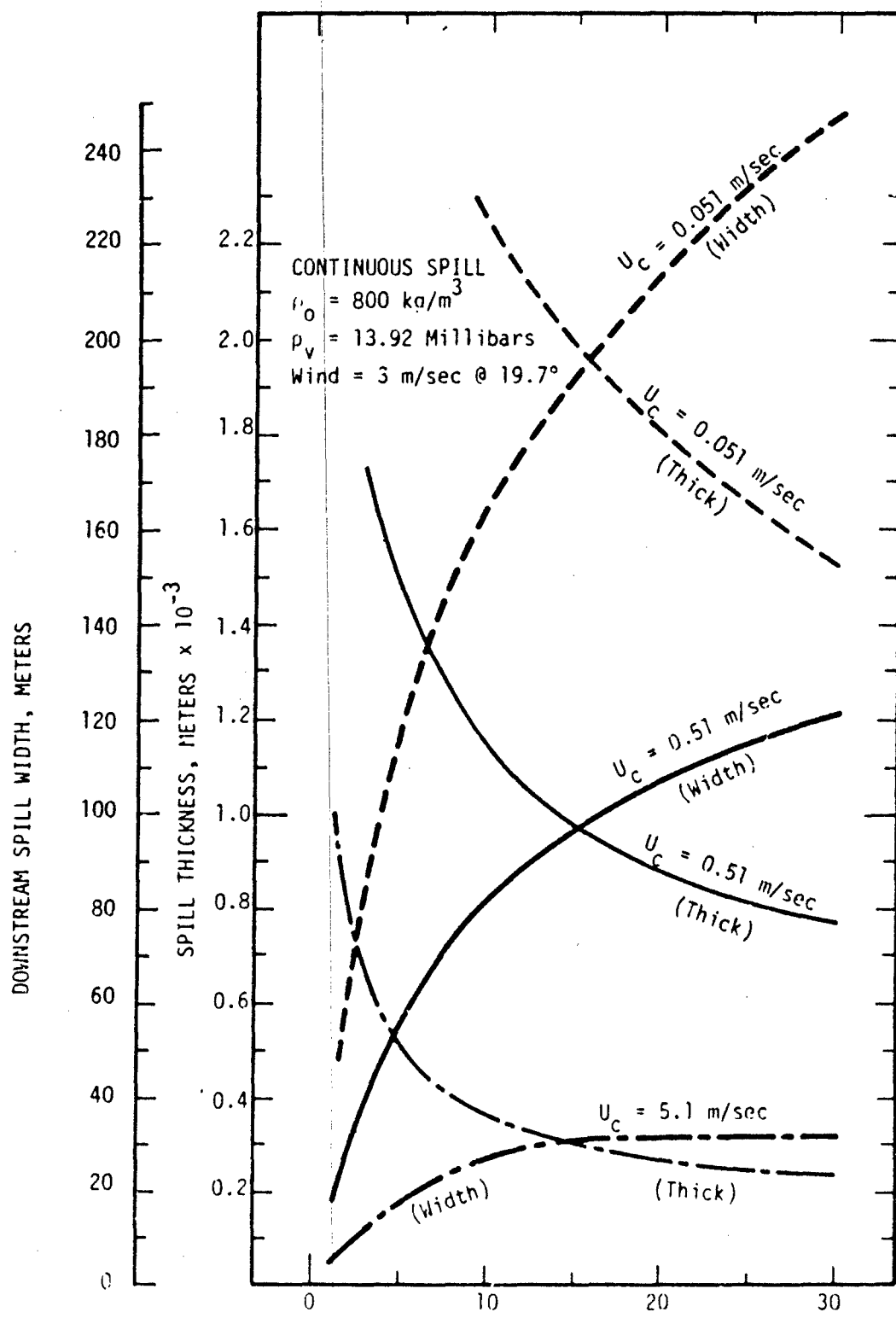


Figure III.12 Effect of Current on Width and Thickness of Continuous Spills

IV. EXPERIMENTAL DESIGN AND DATA COLLECTION

IV.1 Experimental Design

The purpose of the experimental design was to develop a test plan for experiments that would provide validation data for the revised models of both instantaneous and continuous spills. The process involved several elements:

- o test program objectives
- o model sensitivity analysis, and
- o test plan.

The work carried out in each of these elements is described in the following sections.

IV.1.1 Test Program Objectives

Objectives for the test program were formulated in two main categories:

- o spreading, and
- o evaporation and dissolution.

This breakdown of the test program was the result of the perceived impracticality of simultaneously obtaining spreading rate data and detailed mass-transfer data from large-scale spill tests. Consequently, spill tests were designed to obtain data for validating the spreading models, and separate non-spreading tests were designed to obtain data for validating the evaporation and dissolution models. A small number of spill tests were also designed to determine any effects of evaporation on spreading. No tests were conducted specifically to validate the slick motion model; that model, i.e., Equation (III.38), has been adequately verified by other tests in the past [7,8,9].

Spreading Tests. The objective of these tests was to conduct a set of spills, on as large a scale as was practical, from which spreading rates

and slick sizes could be determined. The tests were designed to systematically vary the influence of:

- o quantity spilled (instantaneous spills)
- o discharge rate (continuous spills)
- o chemical specific gravity
- o chemical spreading coefficient
- o magnitude of current (continuous spills).

The size and shape of the slick were to be determined as functions of time primarily by the use of flow visualization. To achieve these objectives, a large outdoor basin was constructed to study instantaneous and continuous spills in water without a current, and a large flow channel was modified to study continuous spills in a current. Some tests using the outdoor basin were designed to study combined evaporation and spreading. For these tests, chemicals having a range of vapor pressures were tested.

Evaporation and Dissolution Tests. The evaporation and dissolution tests were designed to vary, in a controlled environment, the influences of:

- o chemical thermophysical properties,
- o wind speed, and
- o wave height.

In order to make the detailed measurements needed to validate the mass-transfer models, it was necessary to insure that the floating chemical slick remained stationary.

Thus, to achieve the test objectives, an environmental wind tunnel was constructed in which an open pan of chemical could be exposed to various wind speeds. Tests in which the chemical could be subjected to both wind and waves were designed for a large wind-wave tunnel at Flow Research, Inc., in Kent, Washington. Mass-transfer rates were to be determined primarily through concentration sampling of the air and the water.

IV.1.2 Sensitivity Analysis

An analysis was performed on the revised spreading, evaporation, and dissolution models in order to determine the sensitivity of the predicted spreading rates and mass losses to changes in the values of the model parameters. Such an analysis is useful in determining which parameters have the greatest influence on the predicted results and therefore need to be controlled and measured during experiments. It also reveals the parameters that have little influence on the predictions and can therefore be omitted from the test specifications.

For each spreading model, the change in the slick diameter at a specified time after the spill had occurred (generally, fifteen minutes), and the time required to evaporate the entire slick, was computed for a +10% change in the value of each parameter about a selected baseline condition. The sensitivity coefficient for each parameter was then computed, using the slick area as an example, by the equation:

$$SC_X = (\Delta A/A_0)/(\Delta X/X_0)$$

Here ΔA is the computed change in area from A_0 for a ΔX change in the parameter X_0 . When SC_X is positive, A increases as X increases; the opposite holds when SC_X is negative. The magnitude of SC_X indicates the sensitivity of A to X ; if $|SC_X| = 1.0$, the percentage change in A is the same as the percentage change in X ; values of $|SC_X|$ greater or less than one indicate a greater or lesser sensitivity to a change in X .

Table IV.1 gives the results for an instantaneous spill of 90 m³ of benzene on an unbounded lake. (This sensitivity analysis had to be conducted before data from the tests were available to establish the empirical constants. Therefore, the absolute magnitudes of slick radius and evaporation time presented in the table may be in error in places, but the trends of the sensitivity coefficients, since they are computed as ratios, are generally correct.) From the table, the relative importance of the independent parameters is evident. For the slick size, for example, the chemical density and the spill volume are the dominant parameters. For evaporation, the order of relative

TABLE IV.1 SENSITIVITY ANALYSIS FOR A 90 m³ INSTANTANEOUS SPILL OF BENZENE

Run No.	Independent Variable	Units	Value	Slick Radius* (m)	Sensitivity Coefficient	Evaporation Time (min)	Sensitivity Coefficient
1	Wind Velocity (Ref.)	m/s	10.	175.13	0	23.66	0
2	Wind Velocity	m/s	9.	175.82	-0.0394	25.31	-0.697
3	Wind Velocity	m/s	11.	174.45	-0.0388	22.29	-0.579
4	Current	m/s	1.80	175.00	0.0074	23.36	0.127
5	Current	m/s	2.20	175.27	0.0080	23.96	0.127
6	Wave Height	m	1.35	174.76	0.0211	22.88	0.330
7	Wave Height	m	1.65	175.45	0.0183	24.39	0.309
8	Spill Volume	m ³	81.	167.99	0.408	23.11	0.233
9	Spill Volume	m ³	99.	181.87	0.385	24.15	0.207
10	Density	kg/m ³	991	181.40	-0.358	19.72	1.665
11	Density	kg/m ³	967.	156.78	-1.048	32.33	3.664
12	Diffusivity in Air	m ² /s	0.783 x 10 ⁻⁵	175.69	-0.032	24.98	-0.558
13	Diffusivity in Air	m ² /s	0.957 x 10 ⁻⁵	174.58	-0.031	22.53	-0.478
14	Diffusivity in Water	m ² /s	0.918 x 10 ⁻⁹	175.13	0	23.66	0
15	Diffusivity in Water	m ² /s	1.122 x 10 ⁻⁹	175.13	0	23.66	0
16	Vapor Pressure	mb	90.23	175.93	-0.0457	25.63	-0.833
17	Vapor Pressure	mb	110.29	174.30	-0.0474	22.01	-0.697
18	Spreading Coefficient	N/m	15.26 x 10 ⁻³	177.99	0.0227	23.11	-0.032
19	Spreading Coefficient	N/m	2.46 x 10 ⁻³	171.37	0.0297	24.46	-0.047
20	Solubility	%	0.1586	175.13	0	23.66	0
21	Solubility	%	0.1938	175.13	0	23.66	0

* At 15 min.

importance of parameters is density, vapor pressure, wind speed, diffusivity in air, wave height, spill volume, and current. Similar results were obtained for continuous spills. The effects previously shown in Figures III.6 to III.12 display the same trends graphically. The sensitivity analysis results were used in formulating the test plans.

IV.1.3 Test Plan

Spill Tests - As mentioned earlier, instantaneous and continuous spill tests were planned for a large outdoor basin, and continuous spill tests in a current were planned for a large channel. The final test plan is shown in Tables IV.2 through IV.6. Altogether, 102 spreading tests were planned and conducted. (Some preliminary tests that were conducted to help establish feasible limits on spill sizes, discharge rates, and chemical properties are not included in the plan.)

No tests were conducted using volatile chemicals in a current because of the hazardous vapors that would have been liberated indoors.

Evaporation and Dissolution Tests - Two series of tests for evaporation and dissolution were planned for the experimental program. The first group of tests was to be conducted in a wind tunnel at SwRI with a test section designed for these experiments. The primary objective was to measure transfer rates on a variety of chemicals over a range of wind velocities. The chemicals were selected to cover a range of physical properties important to evaporation and dissolution: Schmidt number, vapor pressure, and solubility. In addition, a range of interfacial tensions was also included since this property is likely to be important in controlling droplet dispersion in water. The chemicals were also selected to minimize health and safety hazards. A secondary objective for these experiments was to perfect experimental techniques for the second group of tests.

A second group of tests was planned for a wind-wave channel at Flow Research, Inc., at Kent, Washington. The purpose of these tests was to measure mass transfer rates for two chemicals exposed to controlled

TABLE IV.2 SUMMARY OF TEST CONDITIONS FOR SPREADING TEST SERIES I
NON-VOLATILE INSTANTANEOUS SPILLS IN BASIN

Run Number	Chemical	Specific Gravity	Spreading Coefficient (dyne/cm)	Spill Volume (liters)
I.1-1	Octane	0.703	0.3	5
I.1-2				10
I.1-3				20
I.1-4				40
I.2-1	Kerosene	0.795	-2.7	5
I.2-2				10
I.2-3				20
I.2-4				40
I.3-1	n-Hexanol	0.819	39.75	5
I.3-2				10
I.3-3				20
I.3-4				40
I.4-1	Naphtha	0.785	7.8	5
I.4-2				10
I.4-3				20
I.4-4				40
I.5-1	m-Xylene	0.864	7.0	5
I.5-2				10
I.5-3				20
I.5-4				40

TABLE IV.3 SUMMARY OF TEST CONDITIONS FOR SPREADING TEST SERIES II
NON-VOLATILE CONTINUOUS SPILLS IN BASIN

Run Number	Chemical	Specific Gravity	Spreading Coefficient (dyne/cm)	Discharge Rate (liters/sec)
II.1-1	Octane	0.703	0.3	0.50
II.1-2				0.82
II.1-3				1.01
II.1-3				1.26
II.2-1	Kerosene	0.795	-2.7	0.50
II.2-2				0.82
II.2-3				1.01
II.2-4				1.26
II.3-1	n-Hexanol	0.819	39.75	0.50
II.3-2				0.82
II.3-3				1.01
II.3-4				1.26
II.4-1	Naphtha	0.785	7.8	0.50
II.4-2				0.63
II.4-3				0.95
II.4-4				1.10
II.5-1	m-Xylene	0.864	7.0	0.50
II.5-2				0.82
II.5-3				1.01
II.5-4				1.26

TABLE IV.4 SUMMARY OF TEST CONDITIONS FOR SPREADING TEST SERIES III
VOLATILE INSTANTANEOUS SPILLS IN BASIN

Run Number	Chemical	Specific Gravity	Spreading Coefficient (dyne/cm)	Vapor Pressure (millibars)	Spill Volume (liters)
III.1-1	n-Pentane	0.626	6.5	587.7	5
III.1-2					10
III.1-3					20
III.1-4					40
III.2-1	Heptane	0.684	1.6	47.7	4
III.2-2					10
III.2-3					20
III.2-4					40
III.3-1	Octane	0.703	0.3	13.9	5
III.3-2					10
III.3-3					20
III.3-4					40
III.4-1	m-Xylene	0.864	7.0	8.2	5
III.4-2					10
III.4-3					20
III.4-4					40
III.5-1	Ethyl Acetate	0.901	45.89	98.4	5
III.5-2					10
III.5-3					20
III.5-4					40

TABLE IV.5 SUMMARY OF TEST CONDITIONS FOR SPREADING TEST SERIES IV
VOLATILE CONTINUOUS SPILLS IN BASIN

Run Number	Chemical	Specific Gravity	Spreading Coefficient (dyne/cm)	Discharge Rate (liters/sec)
IV.1-1	n-Pentane	0.626	6.5	0.50
IV.1-2				0.82
IV.1-3				1.01
IV.1-4				1.26
IV.2-1	Heptane	0.684	1.6	0.50
IV.2-2				0.82
IV.2-3				1.01
IV.2-4				1.26
IV.3-1	Octane	0.703	0.3	0.50
IV.3-2				0.82
IV.3-3				1.01
IV.3-4				1.26
IV.4-1	m-Xylene	0.864	7.0	0.50
IV.4-2				0.82
IV.4-3				1.01
IV.4-4				1.26
IV.5-1	Ethyl Acetate	0.901	45.89	0.50
IV.5-2				0.82
IV.5-3				1.01
IV.5-4				1.26

TABLE IV.6 SUMMARY OF TEST CONDITIONS FOR SPREADING TEST SERIES V
FLOW CHANNEL TESTS

Run Number	Chemical (Sp.Gravity)	Spreading Coefficient (dyne/cm)	Discharge Rate (liters/sec)	Current m/sec
V.1-1	Octane (0.703)	0.3	0.038	0.134
V.1-2			0.050	0.189
V.1-3			0.100	0.241
V.1-4			0.149	0.290
V.2-1	Kerosene (0.795)	-2.7	0.038	0.134
V.2-2			0.050	0.189
V.2-3			0.100	0.241
V.2-4			0.149	0.290
V.3-1	n-Hexanol (0.819)	39.75	0.038	0.134
V.3-2			0.050	0.189
V.3-3			0.100	0.241
V.3-4			0.149	0.290
V.4-1	Naphtha (0.785)	7.8	0.025	0.119
V.4-2			0.050	0.189
V.4-3			0.100	0.241
V.4-4			0.100	0.290
V.5-1	m-Xylene (0.864)	7.0	0.038	0.134
V.5-2			0.050	0.189
V.5-3			0.100	0.241
V.5-4			0.149	0.290

wind and wave conditions that simulate the spill environment. The primary variables for these experiments were Reynolds number and wave roughness.

The test plan is summarized in Tables IV.7 through IV.10. Some minor alterations occurred in the test plan during the course of the experiments. The test chemicals for the wind-wave experiments were selected on the basis of test experience gained at SwRI during the first group of tests. In addition, some wave measurements for water only were taken for comparison to waves with a chemical slick.

IV.2 Test Facilities, Procedures, and Instrumentation

IV.2.1 Basin Tests: Spreading and Evaporation

Environmental Spill Facility. The concrete basin pictured in Figure IV.1, used for conducting the continuous and "instantaneous" spreading experiments was a 18.3m (60 ft) x 18.3m (60 ft) x 0.3m (1 ft) deep square pool located at SwRI. The basin was filled with fresh water through a 17.8 cm (7 inch) diameter water inlet in the middle of the basin. The basin was filled to a depth of 0.3m (1 ft) for each test. The basin could be emptied through a 15.2 cm (6 inch) diameter drain that was located at its center.

For the purpose of data collection, a rake assembly to measure spill diameters was constructed in the spill facility as shown in Figure IV.1. There were four rakes that spanned the basin along its diagonals. The rakes were numbered 1, 2, 3, and 4. Rake 1 is located in the upper lefthand corner of Figure IV.1. The remaining rakes were sequentially numbered in a clockwise direction. Each rake consisted of a 3.8 cm (1.5 inch) by 7.6 cm (3.0 inch) piece of wood that was secured to the bottom of the basin on which wooden pegs were mounted that extended through the water surface. The diameter of each peg was 0.64 cm (0.25 in). The center-most peg on each rake was located 0.6m (2 ft) from the center of the basin. The next ten pegs were at 0.3m (1 ft) intervals and the next 5 were at 0.6m (2 ft) intervals.

TABLE IV.7 SUMMARY OF TEST CONDITIONS FOR
EVAPORATION TEST SERIES VI,
WIND TUNNEL TESTS

Run Number	Chemical	Schmidt Number	Vapor Pressure (mb)	Wind Speed (m/s)
VI.1.2	Ethyl Acetate	1.81	98.4	2
VI.1.3				3
VI.1.4				4
VI.1.5				5
VI.2.2	Hexane(n)	2.15	161.8	2
VI.2.3				3
VI.2.4				4
VI.2.5				5
VI.3.2	Hexanol(n)	2.18	0.72	2
VI.3.3				3
VI.3.4				4
VI.3.5				5
VI.4.2	Octane(n)	2.60	13.9	2
VI.4.3				3
VI.4.4				4
VI.4.5				5
VI.5.2	Octanol(n)	2.51	0.086	2
VI.5.3				3
VI.5.4				4
VI.5.5				5

TABLE IV.8 SUMMARY OF TEST CONDITIONS FOR
EVAPORATION TEST SERIES VII
WIND-WAVE CHANNEL TESTS

Run Number	Chemical	Schmidt Number	Vapor Pressure (mb)	Wind Speed (m/s)	Mechanical Waves
VII.1.1	Octane(n)	2.60	13.9	2	No
VII.1.2	"	"	"	3.5	No
VII.1.3	"	"	"	5	No
VII.1.4	"	"	"	7.5	No
VII.1.5	Hexanol(n)	2.18	0.72	7.5	No
VII.2.1	Octane(n)	2.60	13.9	3.5	Yes
VII.2.2	"	"	"	5	Yes
VII.2.3	"	"	"	7.5	Yes

TABLE IV.9 SUMMARY OF TEST CONDITIONS FOR
DISSOLUTION TEST SERIES VIII
WIND TUNNEL TESTS

Run Number	Chemical	Schmidt Number	Solubility (ppm)	Wind Speed (m/s)
VIII.1.1	Ethyl Acetate	1120	87,000	2
VIII.2.1	Hexane(n)	1310	12.5	2
VIII.3.1	Octane(n)	1570	0.66	2
VIII.4.1	Hexanol(n)	1340	6,000	2
VIII.1.2	Ethyl Acetate	1120	87,000	5
VIII.2.2	Hexane(n)	1310	12.5	5
VIII.3.3	Octane(n)	1570	0.66	5
VIII.4.2	Hexanol(n)	1340	6,000	5

TABLE IV.10 SUMMARY OF TEST CONDITIONS FOR
DISSOLUTION TEST SERIES IX
WIND-WAVE CHANNEL TESTS

Run Number	Chemical	Schmidt Number	Solubility (ppm)	Wind Speed (m/s)	Mechanical Waves
IX.1.1	Octane(n)	1570	0.66	2	No
IX.1.2				5	Yes
IX.1.3				7.5	Yes
IX.2.3	Hexanol(n)	1340	6,000	7.5	Yes

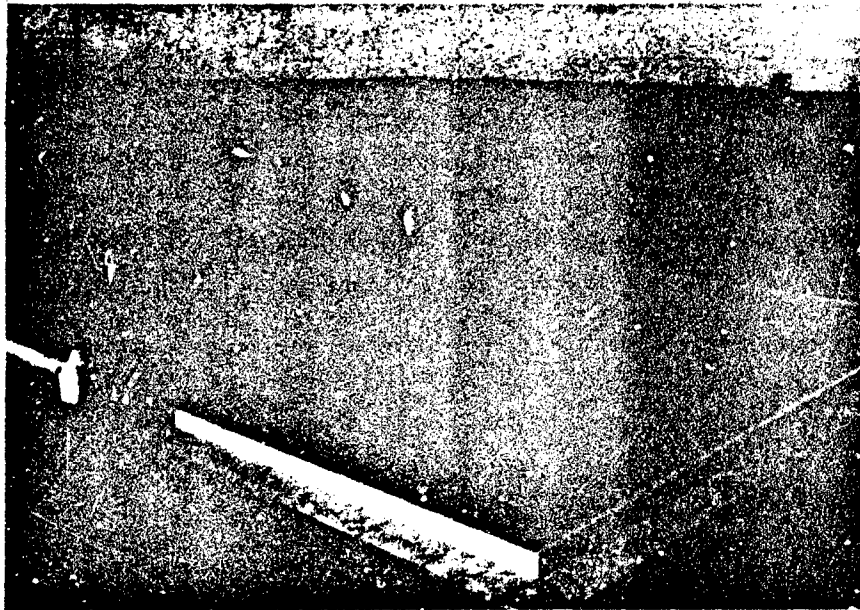


FIGURE IV.1 RAKE ASSEMBLY IN OUTDOOR TEST BASIN

Test Apparatus, Procedures and Instrumentation - Continuous Spill Experiments. For the continuous spill experiments a platform was built and placed in the center of the basin. Each platform leg was placed so that it bisected the angle formed by the rakes to minimize any disturbance in the area along the rakes.

The platform supported a holding tank, pump, a stroboscope, and the discharge tube. Each tested chemical was mixed with Red B. Automate^{*} Liquid Dye in the holding tank and held until the test began. To conduct a test, the pump was set at the speed pre-selected from the pump calibration curve to give the desired discharge rate. The valve to the holding tank was then opened. The rotational rate of the pump was determined by a stroboscope. The discharge rates were 0.5 l/s (8 gpm), 0.82 l/s (13 gpm), 1.01 l/s (16 gpm), and 1.26 l/s (20 gpm). The chemical was discharged through 7.62 cm (3 inch) diameter PVC pipe that ran along the platform, down a leg, along the basin bottom, then straight up at the center of the basin. The pipe extended out of the water 6.4 mm (0.25 inch). The chemical was discharged vertically with negligible vertical momentum.

During discharge of the chemical and dye mixture, the test data were recorded on a strip chart using a Honeywell Visicorder. A common voltage supply was utilized with four triggers that fed into four separate channels on the Visicorder. When the edge of the spill arrived at each peg on one of the rakes, the trigger for that rake was pushed. The events for each rake were marked on the strip chart recorder's light sensitive paper.

The event times for each rake were tabulated and used as input to obtain curves of slick radius vs. time. Then, the radius values of opposite rakes (1 and 3, 2 and 4) were added to obtain two graphs of diameter vs. time. The graph of the diameter least affected by any wind was used for comparison with the computer model predictions.

^{*} Red B. Automate Liquid Dye, Morton Chemical Co.

Test Apparatus, Procedures, and Instrumentation - Instantaneous

Spill Experiments. The same four-legged platform used for the continuous spill experiments was also used for these instantaneous spill experiments with some minor modifications. Replacing the holding tank, pump, stroboscope, and discharge tube was a system to approximate an "instantaneous" spill. This instantaneous spill apparatus consisted of an open tank without a bottom that was attached to the rod of a pneumatic cylinder as shown in Figure IV.2. The pneumatic cylinder was set so that in its fully extended position the spill tank was just off the basin bottom. While the cylinder was in its lowest position, the chemical/dye mixture was metered into the spill tank from the open top. Care was taken not to allow any chemical to be discharged at the bottom of the open spill tank. This procedure was possible because all of the chemicals studied were lighter than water and relatively immiscible and insoluble. To spill the chemical, a remote valve was used to activate the pneumatic cylinder and raise the spill tank in less than one second; as the tank was raised, the chemical was automatically released into the water without any significant momentum.

The procedures for data collection and reduction were the same as described above for the continuous spill experiments.

IV.2.2 Channel Spreading Tests

Flow Channel Facility. The flow channel used for the experiments of a continuous spill in a current is a 13.7m (45 ft) long, 2.4m (8 ft wide), and 1.5m (5 ft) deep channel with a 1.5m (5 ft) long, 3m (10 ft) deep sump at one end, located at SwRI. Water flow was achieved by pumping water from the sump area through a 20 cm (8 inch) diameter PVC pipe to the head of the channel. The water channel inlet area was constructed using a combination of a diffuser, weirs, fire bricks, screens, and rubberized hogs hair (shown in Figure IV.3) to yield a uniform flow field across the width of the channel. A weir was constructed at the upstream edge of the sump to limit the water depth and also isolate the sump from the rest of the flow channel. After allowing for the area necessary for flow straightening and sump isolation, the test section dimensions were 6.7m (22 ft) long by 2.4m (8 ft) wide. To aid in the flow visualization and

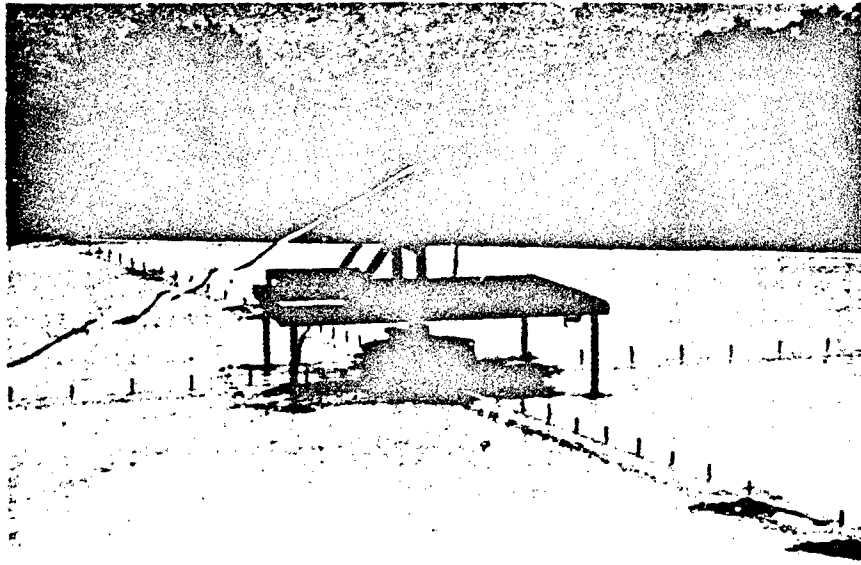


FIGURE IV.2 INSTANTANEOUS SPILL APPARATUS

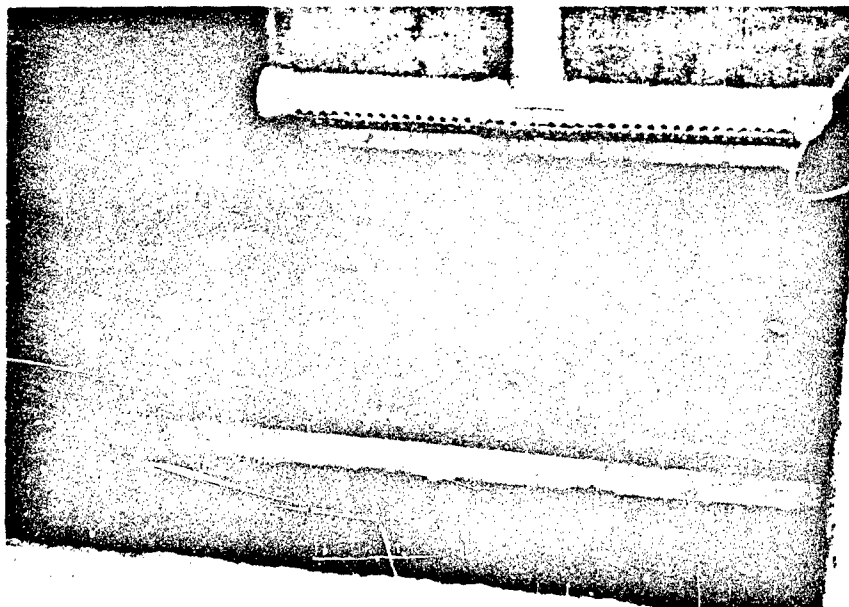


FIGURE IV.3 CHANNEL INLET AREA OF INDOOR CHANNEL

data collection, the channel floor was striped as shown in Figure IV.4 using graphic slit tape. For the first 3.05m (10 ft) of the test section, the stripes were spaced every 30.5 cm (1 ft) downstream and 15.2 cm (0.5 ft) cross-stream. For the last 3.65m (12 ft) of the test section, the stripes were spaced every 61 cm (2 ft) downstream and 30.5 cm (1 ft) cross-stream.

Water velocities in the channel from 12.0 cm/sec (0.39 ft/sec) to 29.0 cm/sec (0.95 ft/sec) were obtained by the use of an Aurora centrifugal pump driven by a hydraulic motor. Since the weir at the upstream edge of the sump was permanently installed, the water depth varied from about 15 cm (6 inches) to 23 cm (9 inches) over the range of flowrates necessary to achieve the water velocities mentioned above. It was determined that this change in depth had no significant impact on the experiments because only surface phenomena were of concern.

Test Apparatus, Procedures and Instrumentation. For the continuous spill experiments in the flow channel, various chemicals were mixed with "Red B. Automate Liquid Dye" and discharged from a discharge port located at the water surface in the upstream center of the channel width. The port was formed from either 2 cm or 5.5 cm diameter pipe configured to give a discharge aligned with the flow direction. The spill setup for these spills is shown in Figure IV.5. The chemical and dye were premixed in the pictured container and then pumped to the port at the discharge rates specified in the test plan using a variable speed motor and a 1/4" rotary gear pump.

During discharge of the chemical and dye mixture, the tests were filmed on video-tape. The films were then analyzed to determine the "thick slick" plume width as a function of distance from the discharge port. This information was graphed to yield a reproduction of the spreading of the chemical on the water surface, and thus to serve as a basis for comparison to the computer model predictions. Only data for that part of the spreading where the channel walls did not affect the results were analyzed. Thus, these tests simulate the spreading of a continuous spill in "open water" with a current.

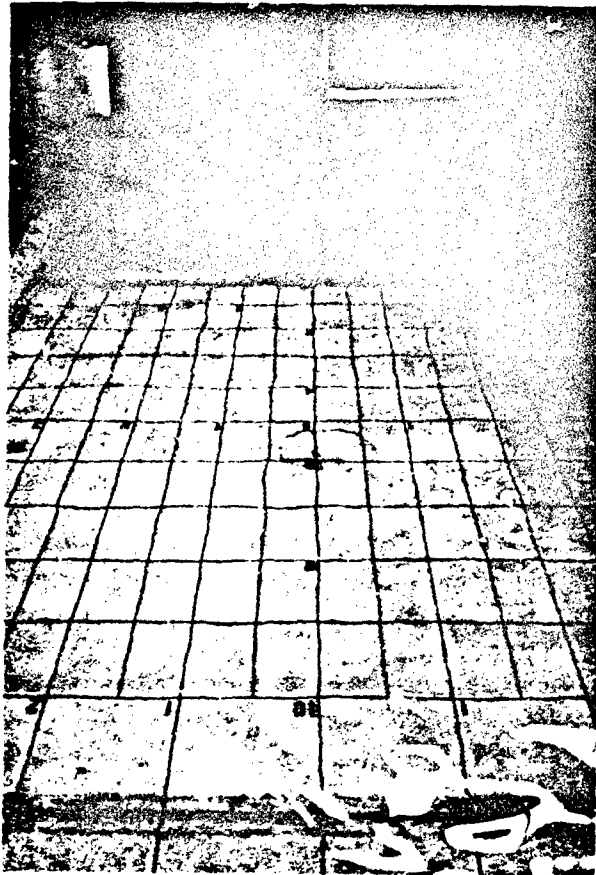


FIGURE IV.4 WATER CHANNEL WITH STRIPES FOR FLOW VISUALIZATION

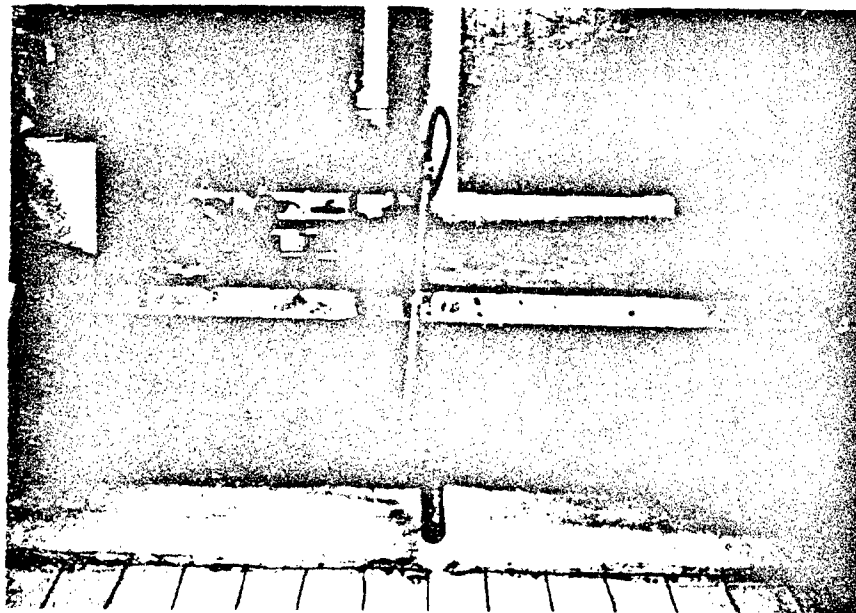


FIGURE IV.5 CONTINUOUS SPILL SETUP FOR CHANNEL EXPERIMENTS

IV.2.3 Wind Tunnel Tests: Evaporation

Theory. In the past, mass transfer by evaporation has been measured as the weight loss of chemical from a pan in a wind tunnel. The work of Pasquill [43] is a frequently referenced example of such experiments, and more recently pan evaporation experiments have been reported by Reijnhart and Rose [44] for pentane and toluene. In the present research, evaporation and wind shear stress were determined by measurement of the logarithmic profiles.

Experimentally, velocity and vapor concentration were measured as a function of height above the liquid surface. The relevant mass transfer constants were determined by a linear regression of the profile data in the following form:

$$U = a \ln z + b \quad (\text{IV.1})$$

$$C = a_c \ln z = b_c \quad (\text{IV.2})$$

where U , C , and z are measured quantities and the a 's and b 's are the slopes and intercepts from linear regression analysis. In non-dimensional form these equations are:

$$u_+ = U/u_* = A \ln z_+ + B \quad (\text{IV.3})$$

$$c_+ = C/c_* = A Sc_t \ln z_+ + B_c \quad (\text{IV.4})$$

where the intercepts are related to the roughness parameters of Equations (III.25) and (III.26) by

$$z_{0+} = \exp(-\kappa B) \quad (\text{IV.5})$$

and

$$z_{0c+} = \exp(-\kappa B_c / Sc_t) \quad (\text{IV.6})$$

The constants from boundary layer theory and the linear regression analysis are related as follows:

$$\text{for velocity: } u_* = a \kappa \quad (\text{IV.7a})$$

$$B = [b - U_s - a \ln(u_*/\nu)]/u_* \quad (\text{IV.7b})$$

$$\text{for concentration: } c_* = a_c \kappa / Sc_t \quad (\text{IV.8a})$$

$$B_c = (b - C_s)/c_* - A Sc_t [\ln(u_*/\nu)] \quad (\text{IV.8b})$$

By definition the friction velocity and concentration are:

$$u_* = \sqrt{\tau_0/\rho} \quad (\text{IV.9})$$

$$c_* = J_0/\rho u_* \quad (\text{IV.10})$$

These quantities are related to wind stress coefficient and Dalton number by

$$C_f/2 = (u_*/V_w)^2 \quad (\text{IV.11})$$

and

$$Da_* = c_*/(C_\infty - C_s) \quad (\text{IV.12})$$

where the saturation concentration, C_s , is a physical property calculated from the barometric pressure and liquid surface temperature.

Wind Tunnel. The wind tunnel for the pan evaporation experiments consisted of the following components:

- a. bell mouth entrance;
- b. rectangular test section with dimensions of 30.5 cm height, 61.0 cm width, and 484 cm length (12 x 24 x 190.5 inches);
- c. contraction section;

- d. Buffalo centrifugal blower which is rated at $4.7 \text{ m}^3/\text{s}$ (10,000 cfm) and is driven by a Dennison hydraulic motor;
- e. 20.3 cm (8 inch) diameter PVC plastic pipe; and
- f. evaporation pan with dimensions of 3.8 cm depth, 40.6 cm width, and 121.9 cm length (1.5 x 16 x 48 inches) and with a volume of 18.9 liters (5 gals).

Air for the wind tunnel was ingested at the bellmouth in the laboratory and exhausted by the blower to the outside air. The inlet to the blower was connected to the wind tunnel via the plastic pipe, and the air was transported from the blower outlet to the exterior of the laboratory by plastic pipe. Figure IV.6 shows the tunnel and instrumentation for the pan evaporation experiments.

This arrangement of the tunnel had three primary advantages. First, laboratory personnel were not exposed to the chemical vapors, and thus, the health hazard was reduced. Second, the concentration measurements were not contaminated from chemical vapors which would accumulate in the laboratory otherwise. The tunnel was sealed to minimize any leakage. Third, this design provided an additional method for the measurement of evaporation.

Mass transfer from evaporation was measured from an air sample taken from the plastic pipe downstream from the blower outlet. From the definition of Dalton number and conservation of mass, the Dalton number measured at the blower outlet is:

$$la_0 = (A_t/A_p) (C_0/C_s) \quad (\text{IV.13})$$

where A_t is the cross-sectional area of the test section, A_p is the surface area of the liquid in the evaporation pan, and C_0 is the concentration measured at the blower outlet. The following assumptions are inherent in Equation (IV.13):

- a. The flow was well mixed at the sampling station.
- b. Any air leakage in the wind tunnel between the sampling station and pan was small.

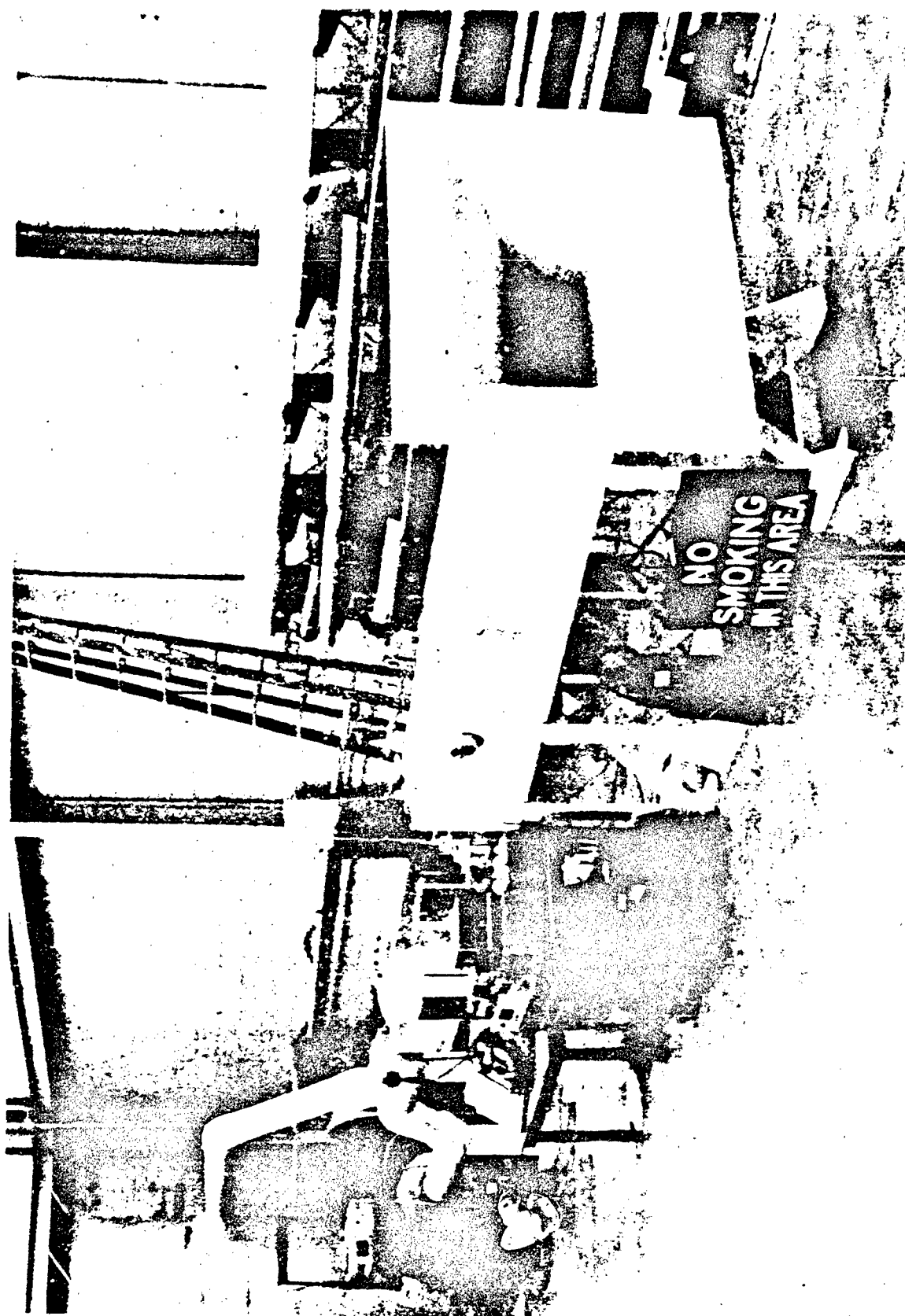


FIGURE IV.6 SwRI WIND TUNNEL

- c. Boundary layer displacement effect on the tunnel cross-sectional area was small; however, an effective area could have been applied.

The tunnel was constructed primarily of wood; however, the two sides of the test section at the pan location were Plexiglas. The pan was constructed of stainless steel sheet metal. A manual gravity feed and drain system was connected to the pan which included 6.4 mm (0.25 inch) diameter stainless steel tubing, fittings, ball valves, 19 liter (5 gal) reservoir, and sight gage. During an experiment the liquid level in the pan was maintained manually to within ± 0.5 mm. The liquid surface was typically 5 mm below the tunnel floor.

A set of eight baffles was installed in the pan below the liquid surface for the prevention of surface waves on the chemicals. The baffles were not necessary for water whose surface tension is more than twice that of the chemicals tested. A 35 mm square horse-hair filter was also installed across the width of the pan at its downstream edge for damping surface waves. Figure IV.7 shows close-up views of the pan and test section area during a typical experiment.

Instrumentation. The following is a list of the commercial equipment for the evaporation experiments.

- a. TSI 1050 constant temperature anemometer.
- b. DISA traversing mechanism including a DISA 52B01 sweep drive unit, DISA 55E40 traversing unit, and stepper motor.
- c. TSI 1076 rms voltmeter.
- d. MKS Baratron model 170 with a 1 Torr pressure transducer.
- e. TSI 1125 calibrator.
- f. DISA 55P05 boundary layer probe.
- g. Century OVA-128 organic vapor analyzer.

The first six items were primarily for the measurement and calibration of velocity. The organic vapor analyzer (OVA) and the DISA traversing system were used in the measurement of concentration profiles.

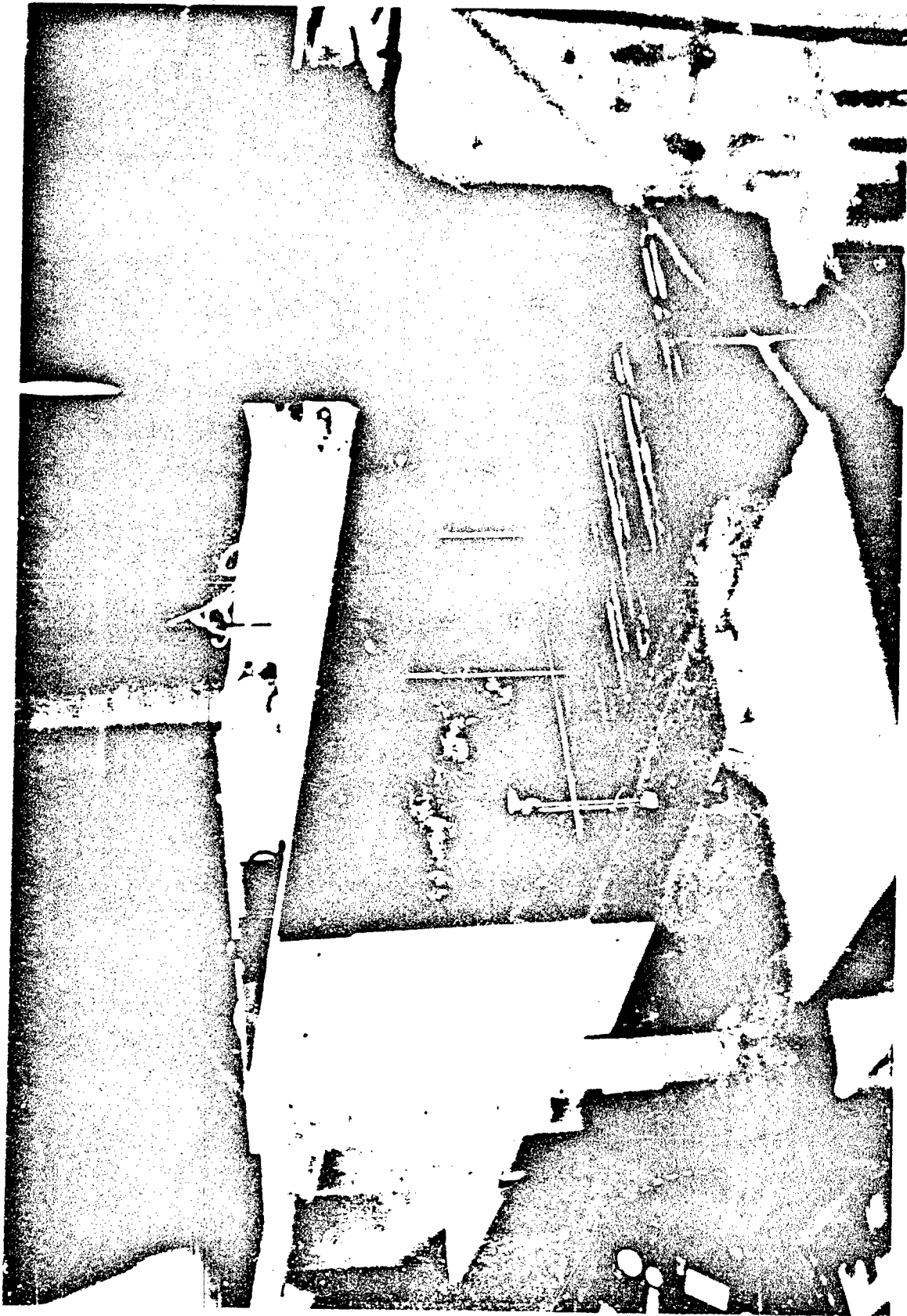


FIGURE IV.7 VIEW OF WIND TUNNEL TEST SECTION AND LIQUID PAN

The wind tunnel speed was set by dynamic pressure measurements with the MKS Baratron. The velocity was calculated from Bernoulli's equation

$$V_w = [2 (p_a - p_i) / \rho_a]^{1/2} \quad (\text{IV.14})$$

where p_a is the barometric pressure which in the present case is the same as the total pressure, and p_i is the tunnel wall static pressure at station i . Since the MKS has a differential pressure transducer, $(p_a - p_i)$ was measured directly. Experimentation indicated that velocities from this method at station 3 were closer to the hot-wire measurements than those from a Pitot-static probe. Table IV.11 is a list of transducer locations and the pan location relative to the test section entrance. A scale drawing of the test section with static pressure hole and hot-wire locations is shown in Figure IV.8. Also, the nondimensional pressure gradient for flow over octane is presented in this figure for the test section.

The pressure gradient is defined as:

$$(1/q) (dp/dx) = -C_p/\Delta x \quad (\text{IV.15})$$

where the pressure coefficient, C_p is

$$C_p = (p_{i+1} - p_i) / q \quad (\text{IV.16})$$

p_i is the pressure at station i , q is the dynamic pressure, $\rho_a V_w^2 / 2$, and $\Delta x = x_{i+1} - x_i$. The physical properties which were not measured directly such as density and viscosity were computed by the methods in Appendix A from the measured temperatures and barometric pressure. Room air temperature and liquid surface temperature were measured with Type T thermocouples while barometric pressure was monitored with an aneroid barometer from Weathermeasure Corporation. The error in velocity from errors in temperature and barometric pressure was less than 0.5%.

The velocity profiles were measured with a TSI 1050 constant temperature anemometer and DISA 55P05 hot-wire probe. The hot-wire anemometer was calibrated with a TSI 1125 calibration jet. Voltages from the

TABLE IV.11 TRANSDUCER LOCATIONS

Station (cm)	x (in)	Item
274.3	108	No. 1 static pressure hole
302.3	119	Inside leading edge of pan
335.3	132	No. 2 static pressure hole
396.2	156	No. 3 static pressure hole
408.9	161	Hot-wire sensor
408.9	161	Pitot-static probe tip
408.9	161	Pan thermocouple
411.8	162.1	Liquid sampling probe tip
413.4	162.8	Gas sampling probe tip
415.3	163.5	DISA traversing mechanism guide tube
424.2	167	Inside trailing edge of pan
457.2	180	No. 4 static pressure hole

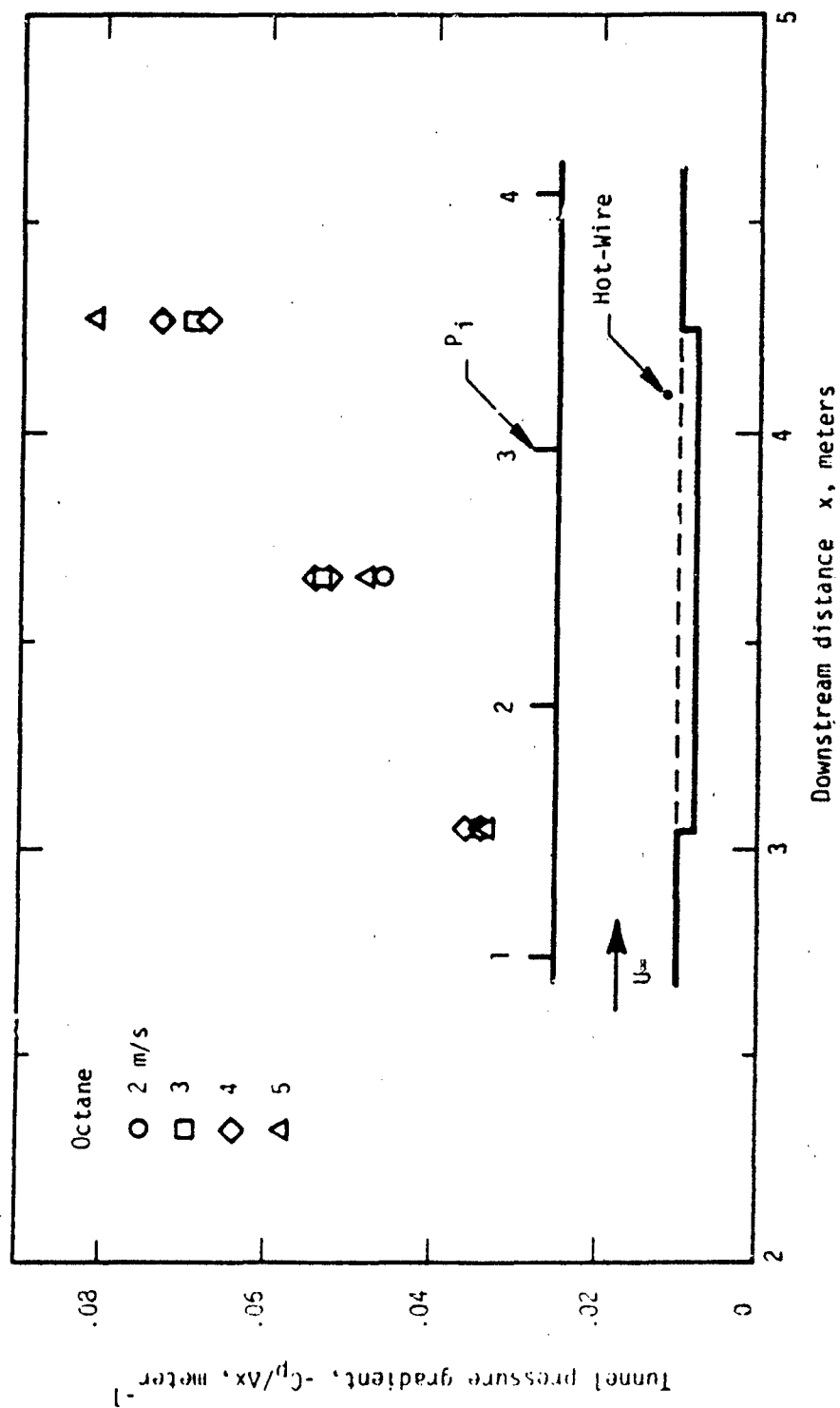


FIGURE IV.8 WIND TUNNEL PRESSURE GRADIENT MEASUREMENTS FOR FLOW OVER OCTANE(n)

anemometer were measured with a TSI 1076 voltmeter. King's law in the following form was applied to the calibration data:

$$E_b^2 = A + B V_w^n \quad (IV.17)$$

where A , B , and n are constants determined by linear regression analysis and E_b is the bridge voltage. Usually the exponent n has a value of $0.45 < n < 0.5$. The exponent n was selected so that the correlation coefficient returned in the linear regression analysis was a maximum. A typical calibration curve is shown in Figure IV.9. The hot-wire was operated at 200°C which was below the ignition temperature of the chemicals being tested. The relative turbulence intensity was computed from a linear perturbation of Equation (IV.17)

$$\sigma_u/V_w = 2 \sigma_e E_b / [n(E_b^2 - A)] \quad (IV.18)$$

where σ_u is the rms or standard deviation of the velocity u , and σ_e is the measured rms voltage.

Concentration measurements were taken with a Century OVA-128 total hydrocarbon analyzer which has a hydrogen flame ionization detector. The OVA was calibrated for each chemical used. The calibration was of the form

$$X = A X_0^n \quad (IV.19)$$

where X is the volume fraction in ppm (parts per million), X_0 is the OVA measurement, and A and n are constants determined by linear regression analysis. Table IV.12 is a table of calibration constants, and Figure IV.10 is a typical calibration curve. The meter for the OVA was analog with a linear range of 0 to 10 and a resolution of 0.1. The instrument included a scale factor of 1, 10, and 100 ppm, or it had a maximum range of 1000 ppm. For those measurements outside the range of the OVA, a diluter was used which was also calibrated. The volume fraction, X , in Equation (IV.19) is related to the mass fraction, C , in Equations (III.19) and (III.26) by

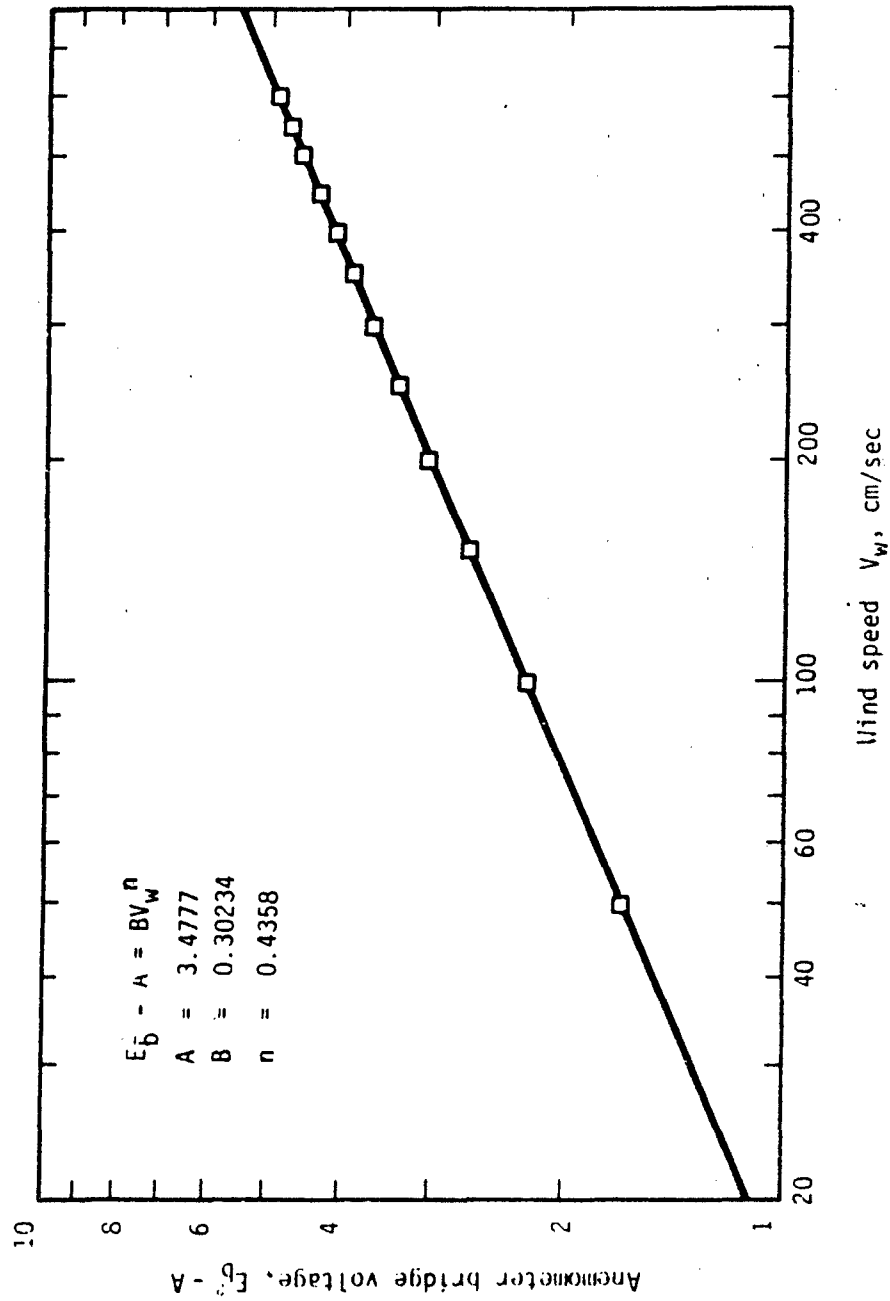


FIGURE IV.9 TYPICAL CALIBRATION CURVE FOR DISA 55P05 BOUNDARY-LAYER PROBE WITH AN OPERATING TEMPERATURE OF 200°C. STRAIGHT LINE IS A LINEAR REGRESSION WITH A CORRELATION OF 0.999989

TABLE IV.12 CALIBRATION CONSTANTS FOR CENTURY
OVA-123 ORGANIC VAPOR ANALYZER

Chemical	Date	Coefficient A	Exponent n	Correlation Coefficient	Dilution Ratio
Ethyl Acetate	07-16-82	1.276	0.9468	0.9992	11.5
	09-07-82	1.082	1.004	0.9995	12.1
	09-08-82	0.018	1.018	0.9996	11.9
	09-08-82	1.302	0.9523	0.9987	11.5
Hexane	11-30-82	1.272	0.9366	0.9992	12.54
Hexanol	09-21-82	1.120	1.100	0.9974	
	02-24-83	1.037	1.078	0.9995	
	All	1.144	1.078	0.9967	
Octane	07-08-82	0.684	0.9700	0.9946	18.1
	10-05-82	1.097	0.9416	0.9978	11.43
	02-24-83	0.8438	0.9946	0.9971	
	10-05-82 & 02-24-83	1.015	0.9574	0.9971	11.43
Octanol	10-26-82 & 12-03-82	1.593	0.8909	0.9793	

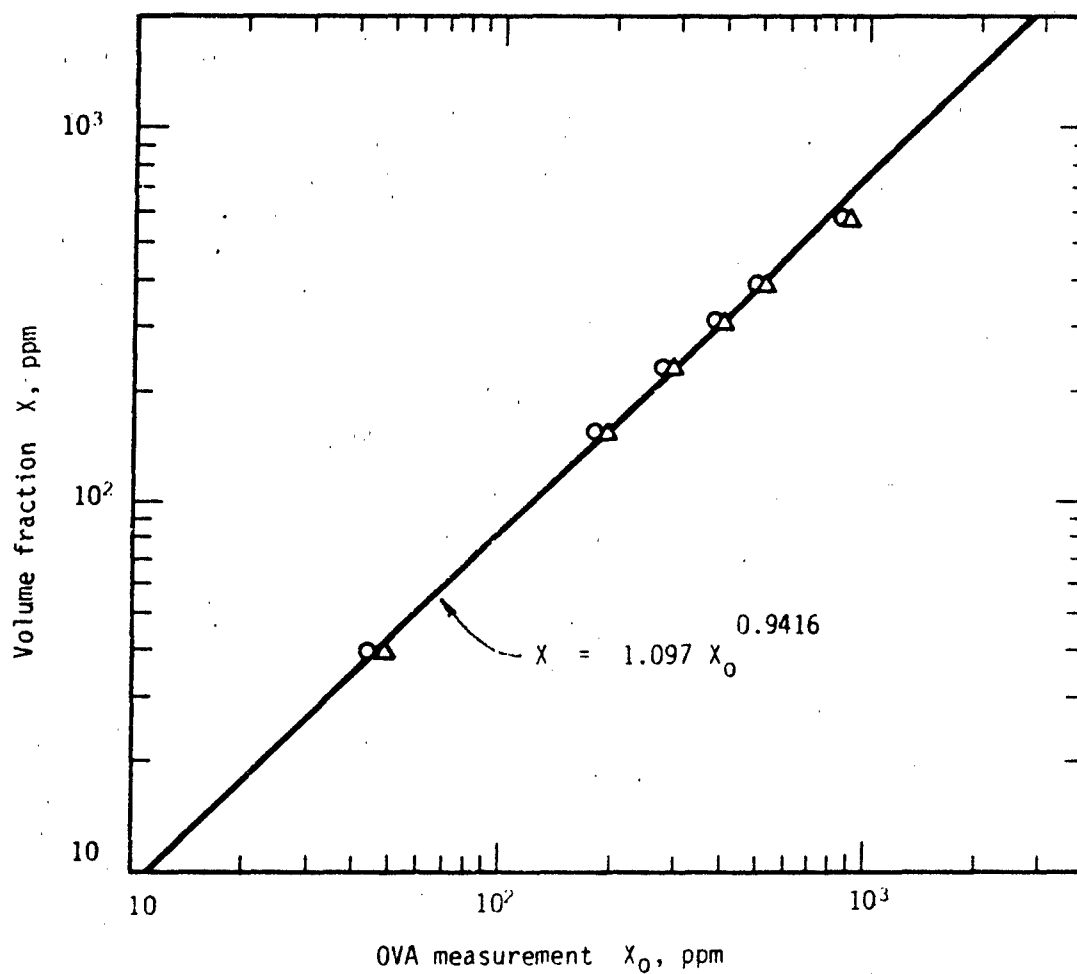


FIGURE IV.10 TYPICAL CALIBRATION CURVE OF CENTURY OVA-128 ORGANIC VAPOR ANALYZER FOR OCTANE(n). STRAIGHT LINE IS A LINEAR REGRESSION WITH A CORRELATION OF 0.9978

$$X = C M_a / M$$

(IV.20)

where M_a is the molecular weight of air, and M the molecular weight of the chemical.

A schematic of the gas sampling system for the concentration profile measurements is shown in Figure IV.11. A gas sample was withdrawn from the wind tunnel through the sampling probe by a Metal Bellows Corp. pump. The flowrate was adjusted by a needle valve and measured by a calibrated Matheson rotameter. The sample gas was collected in two-liter plastic bags and analyzed with the OVA. The flowrate of the sampling system was adjusted to the local mean velocity on the basis of velocity profile measurements with the hot-wire anemometer. The vertical position for the concentration and velocity profile measurements was set by the DISA traversing system which has a resolution of 0.02 mm.

The gas sampling probe was designed and built specifically for this project. The probe consisted of three stainless-steel tubes with an outside diameter of 1.91 mm (0.075 in) and inside diameter of 1.36 mm (0.0535 in). The tubes were separated by 19.1 mm (0.75 in) horizontally with the entrances in the same plane. The three tubes were routed through a 6 mm (0.237 in) diameter stainless steel tube and manifolded by teflon tubing at the exit of the main probe shaft. The sampling tubes were bent so that their lengths between the probe tip and main shaft were the same and, consequently, so that the pressure drops were nearly the same.

IV.2.4 Wind Tunnel Tests: Dissolution

Theory. In the present program, only the model for dissolution on lakes and coastal waters was investigated. Measurement of mass transfer by the profile method was not feasible, however, because of the very thin concentration boundary layer in the water for "insoluble" chemicals. The concentration boundary layer thickness, from Shaw and Hanratty [36], is (for large Reynolds number and Schmidt number):

$$\delta_{c+} = (Da_* Sc_w)^{-1} \quad (IV.21)$$

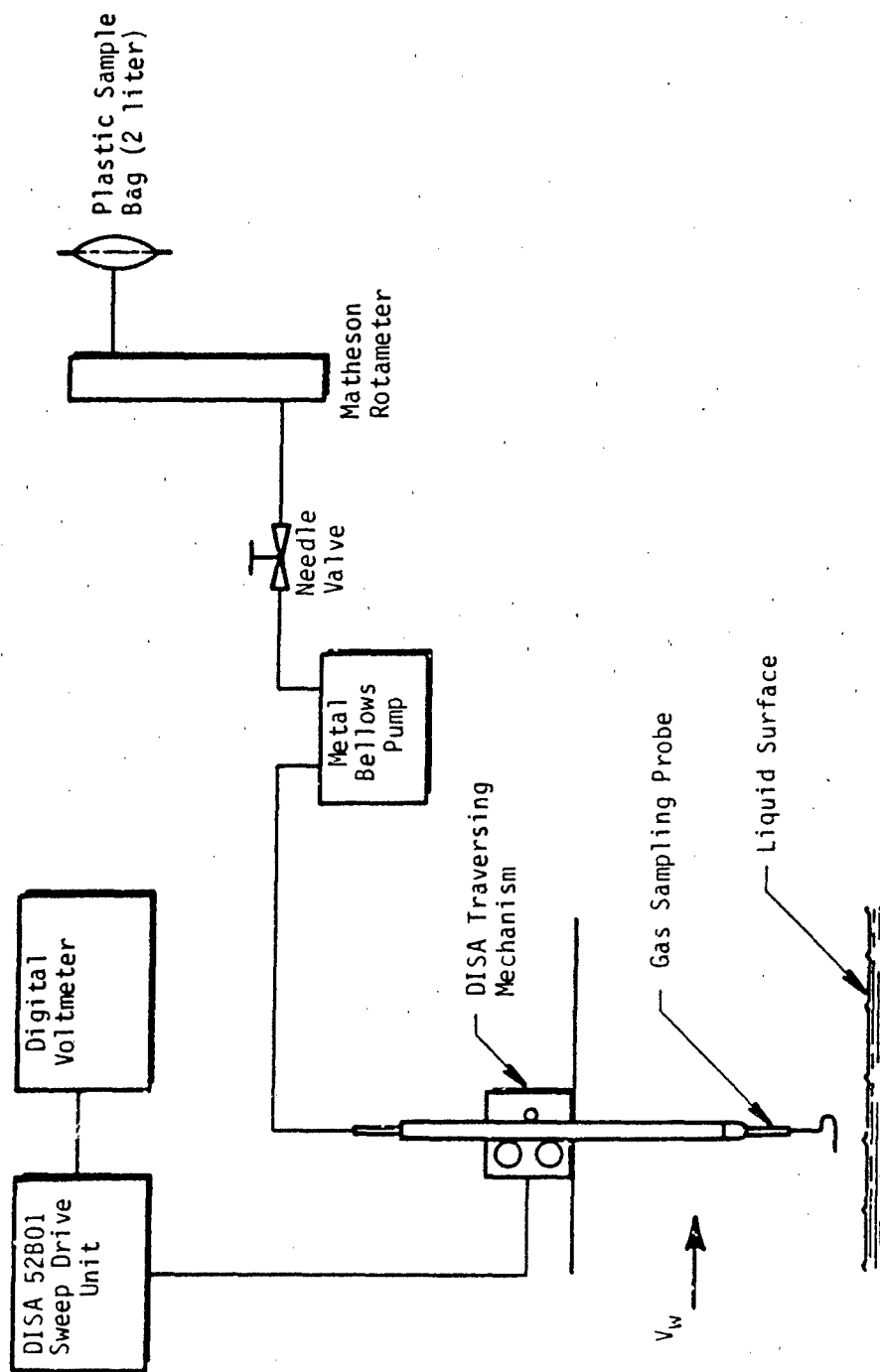


FIGURE IV.11 SCHEMATIC OF GAS SAMPLING SYSTEM FOR CONCENTRATION PROFILE MEASUREMENTS

where the Dalton number is given in Equation (III.34). In their experimental results $K = 0.0889$ and $n = 0.704$. As an estimate, the concentration boundary-layer thickness, δ_{C+} , for $Sc = 1000$ is 1.46, or in physical units is 0.1076 mm (3 mils) on the basis of water boundary-layer measurements by Lin, et al. [45] where u_{*w} was 1.92 cm/s for a wind speed of 10 m/s and fetch of 6m. Consequently, a successful verification with available instrumentation would be the detection of no chemical in the water within 6.4 mm of the free surface, the location of the first probe. Significant chemical in the water would indicate that another mechanism is more important than boundary layer processes in dissolution.

Wind Tunnel. Minor modifications were made to the chemical feed system of the evaporation tests. The feed system for the dissolution experiments uniformly dispensed chemical on the water surface upstream and withdrew the chemical at the downstream edge of the pan. This method of chemical dispersal on the water surface was selected after some experimentation. Other methods would have allowed dispersal without removal of the chemicals, but chemical would accumulate downstream and waves would grow. Also, more chemical would be required to cover the surface. Removal of the chemical downstream allowed a more uniform slick thickness through control of both the inflow and outflow, and consequently, the spill was modeled more accurately.

The chemical was dyed with a mixture of one part per 5,000 of the red dye from the spreading experiments. The dye served two purposes. First, the dye indicated when the surface was completely covered by the chemical, and second, the dye aided visually in the separation of the chemical from the water during recovery of the chemical at the downstream end of the pan.

Instrumentation. A liquid sampling probe was built from the same tubing as the gas sampling probe. The probe was a conventional rake arrangement of four tubes with their entrances in a vertical plane at 6.4 mm (0.25 inch) intervals, with the top probe positioned 6.4 mm below the free surface. Liquid samples of 8 cm³ each were withdrawn through teflon tubing by a 10 cm³ glass hypodermic syringe. Samples were withdrawn at 15-minute intervals for one hour. Preliminary testing showed that the top probe had to be at least 6.4 cm below the surface in order to avoid surface disturbances.

The liquid samples were then analyzed for chemical concentration. The differences in solubilities of the chemicals tested required two analysis methods. Water samples with ethyl acetate and hexanol were analyzed with a Beckman Carbonaceous Analyzer (NDIR) which is a total organic carbon combustion-infrared device. The octane and hexane, whose solubilities are quite low, were analyzed by the microextraction method and a gas chromatograph.

IV.2.5 Wind-Wave Channel Tests: Dissolution and Evaporation

Wind-Wave Channel. Evaporation and dissolution experiments were performed in the wind-wave channel at Flow Industries, Inc., in Kent, Washington. The theory and experimental methods for these experiments were essentially the same as described in the previous two sections. The wind-wave channel consisted of a wave tank with dimensions of 9.1m length, 1.2m width, and 0.9m depth, and it included a mechanical wave maker. A wind tunnel of equal width was located above the wave tank with a variable height test section which was set at 65 cm for these experiments. The test station was 5.5m from the wind tunnel entrance. Additional details on the channel, its performance, and instrumentation are contained in Lin, et al. [45].

The chemical feed system was slightly different from that described in [45]. The system was originally designed as a once-through system for the chemical. It was modified so that chemical could be continuously fed through the system. A slight amount of dye was added to the chemical to make the water/chemical interface readily visible in the recovery tanks.

Instrumentation. The instrumentation for the wind-wave channel experiments was similar to that previously described. The liquid and gas sampling systems were the same; however, the liquid sampling probe was replaced by a larger rake. The rake consisted of six sampling tubes with 3.2mm (1/8 in.) outside diameter. The vertical spacing between tube centerlines was 25.4mm (1 in.).

All probes for the traverse in air were mounted on one traversing mechanism. The probes included the following:

- a. Two TSI 1210 hot-wire probes (Tungsten T1.5 sensor)
- b. Thermistor for air temperature
- c. Pitot-static probe
- d. Gas sampling probe

The hot-wire anemometer was a TSI 1054B. The water surface temperature was monitored with a thermistor. The flow of chemical onto the water surface was controlled and measured with a Dwyer rotameter. The tunnel speed and hot-wire calibration were determined by a Dwyer micromanometer and Pitot-static probe.

The wave heights were measured with a photodiode wave height gauge which consisted of the following components:

- a. Reticon Model LC600V256-1 camera
- b. Reticon RS605 Line Scan Controller
- c. Spectra Physics 164 argon ion laser

The laser was operated at approximately 3 Watts of power, and the water was dyed with a fluorescent dye. Since only the water was illuminated, the wave heights were actually measured at the chemical/water interface. The resolution of the gauge for these experiments was 0.25 mm.

All data were processed with a digital data acquisition system and computer. The data provided included the mean and rms values in physical units of the following:

- a. Velocities from two hot-wires
- b. Air and water surface temperatures
- c. Position of traversing mechanism, and
- d. Wave height.

Approximately 30 seconds of data were averaged. All measurements but wave height were simultaneous. Since the wave height measurements were digital and the other measurements analog, two different software routines were required for the data acquisition. Plots of the data (signal vs. time) were also provided by the data acquisition system.

IV.3 Data Collection (Typical Results)

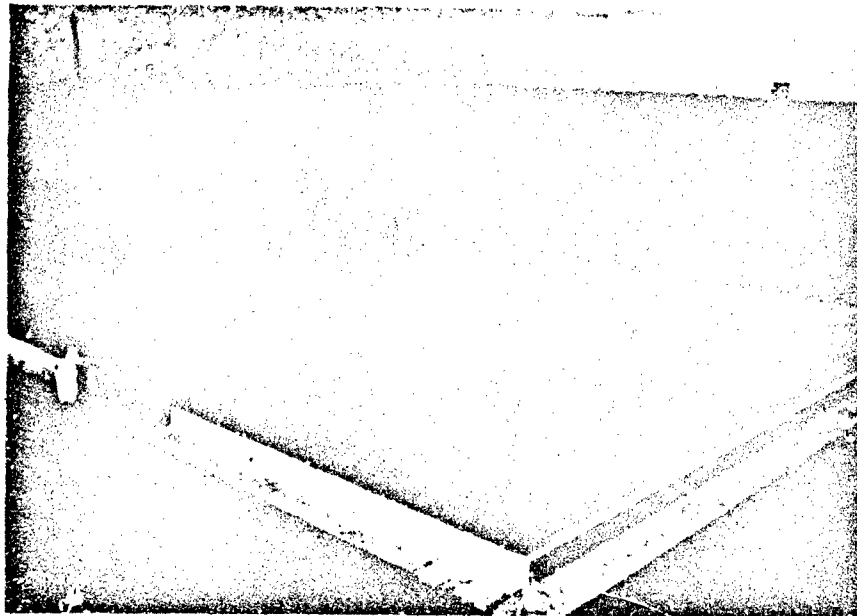
IV.3.1 Spreading Tests

Only a general overview of these experiments mainly based on flow visualization will be presented in this section. For detailed information about the results of each experiment, see Appendices A through E of the Test Data Volume of the Final Report.

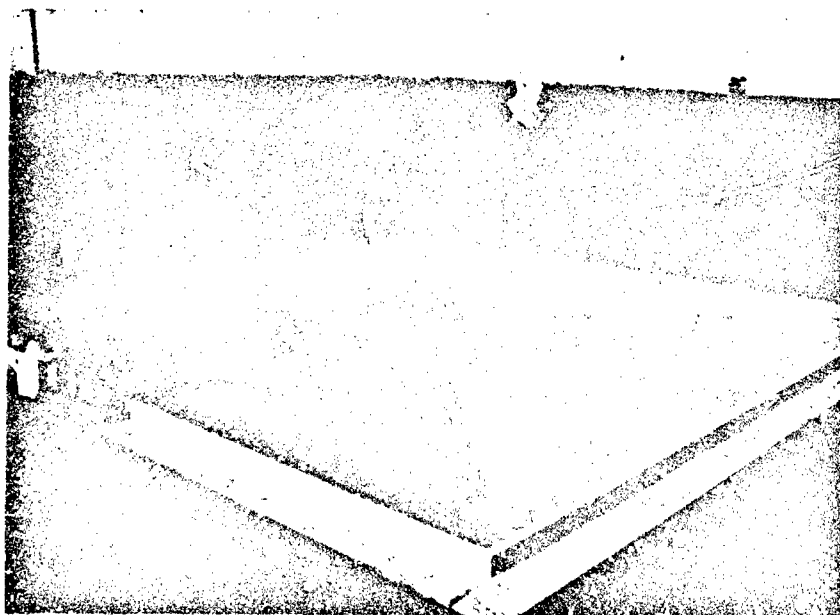
Instantaneous Spills in Basin. The series of photographs labeled Figure IV.12 show a time lapse sequence of a 60 liter instantaneous spill of naphtha. As can be seen, the chemical spreads axisymmetrically from the spill point. The outer edge of the thick slick was very easy to distinguish at the beginning of the spill. Later, when the slick was considerably thinner, a thin slick began forming which made it more difficult to distinguish the edge of the thick slick as shown in Figure IV.13. At that point, the data collection was stopped. From the data obtained, a graph of slick diameter as a function of time was drawn as shown in Figure IV.14, for comparison with the computer model predictions.

These results are typical of the non-volatile instantaneous spills studied. The results for all of the non-volatile instantaneous spills in the basin are contained in Appendix A of the Test Data Volume of the Final Report.

Continuous Spills in Basin. The series of photographs labeled Figure IV.15 show a time lapse sequence of a continuous spill of naphtha at a spill rate of 0.95 liters/ second. The slicks spread much the same as the instantaneous spills described above. The major difference was that a thin slick formed almost immediately on the outer edges of the slick. This made it more difficult to document the thick slick spreading rate. From the data obtained, a graph of slick diameter as a function of time was drawn, as shown in Figure IV.16, for comparison with the computer model predictions.

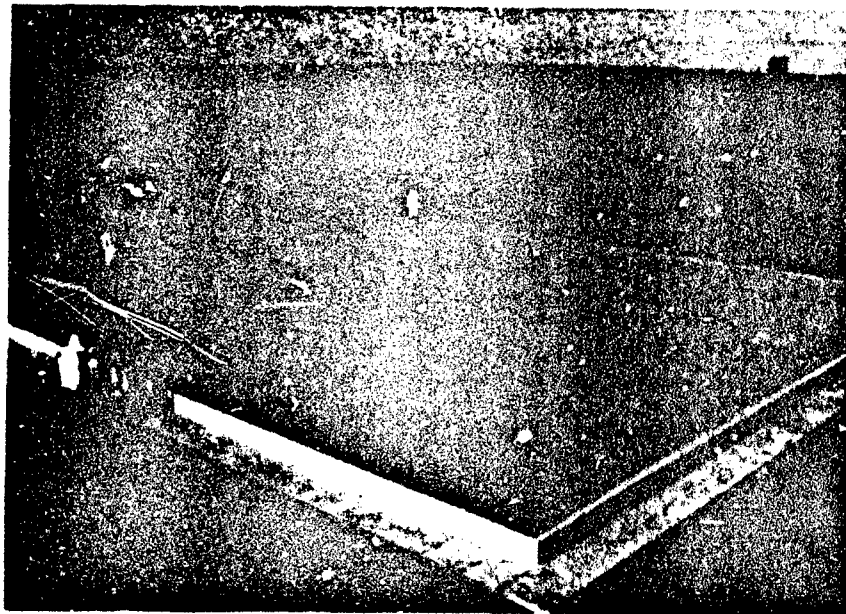


(a)

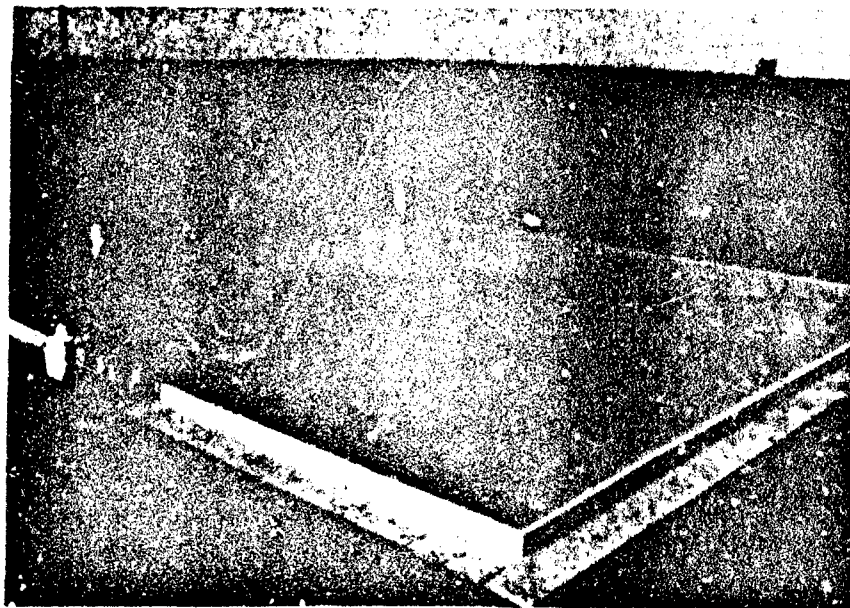


(b)

FIGURES IV.12 (a,b) 60-LITER NON-VOLATILE
INSTANTANEOUS NAPHTHA SPILL



(c)



(d)

FIGURES IV.12 (c,d) 60-LITER NON-VOLATILE
INSTANTANEOUS NAPHTHA SPILL

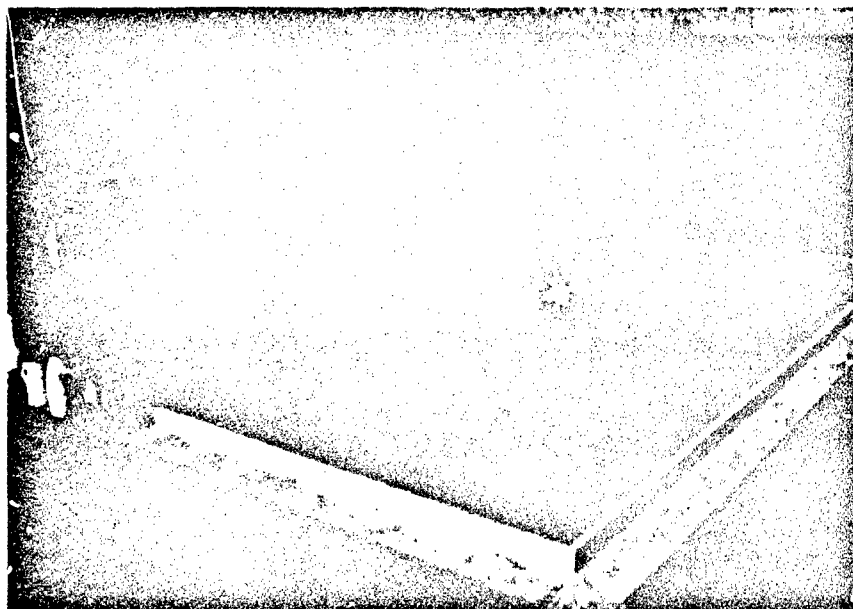


FIGURE IV.13 FINAL SPREADING STAGE OF AN
INSTANTANEOUS SPILL

I.4-5 60. LITER NON-VOLATILE
INSTANTANEOUS NAPHTHA SPILL

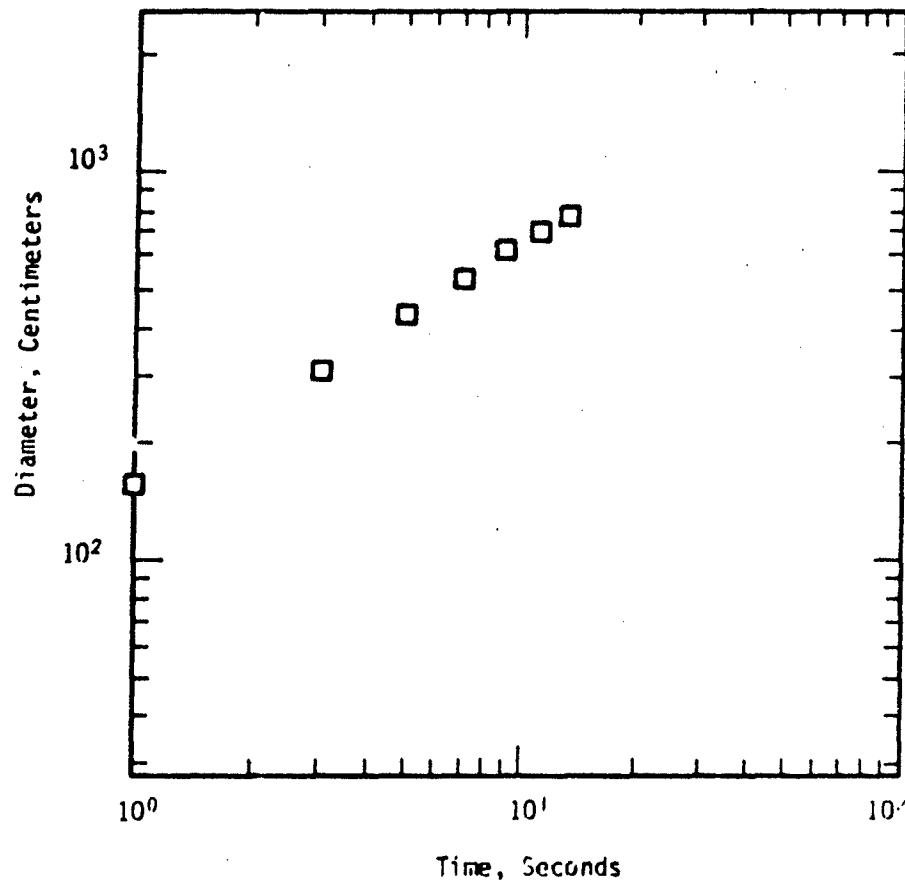
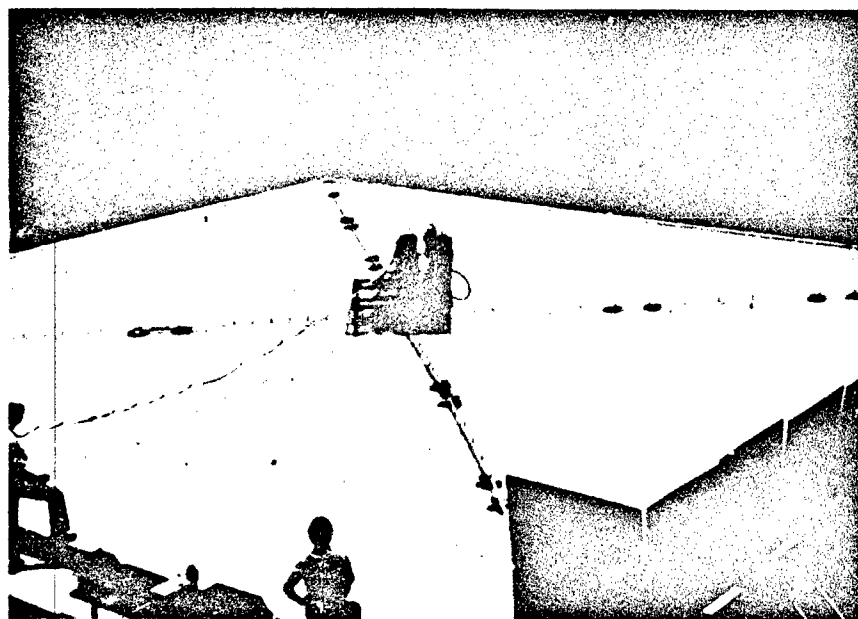
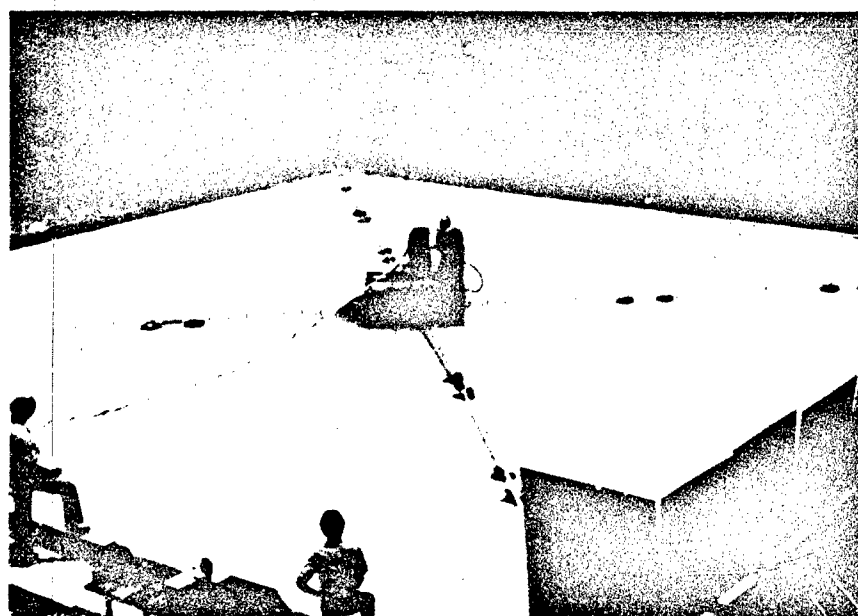


FIGURE IV.14 INCREASE OF SLICK SIZE WITH TIME

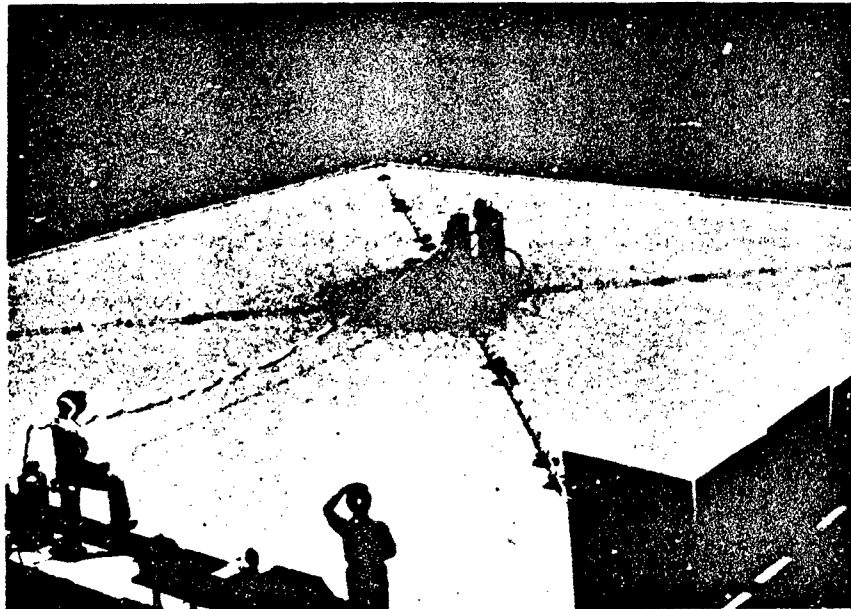


(a)

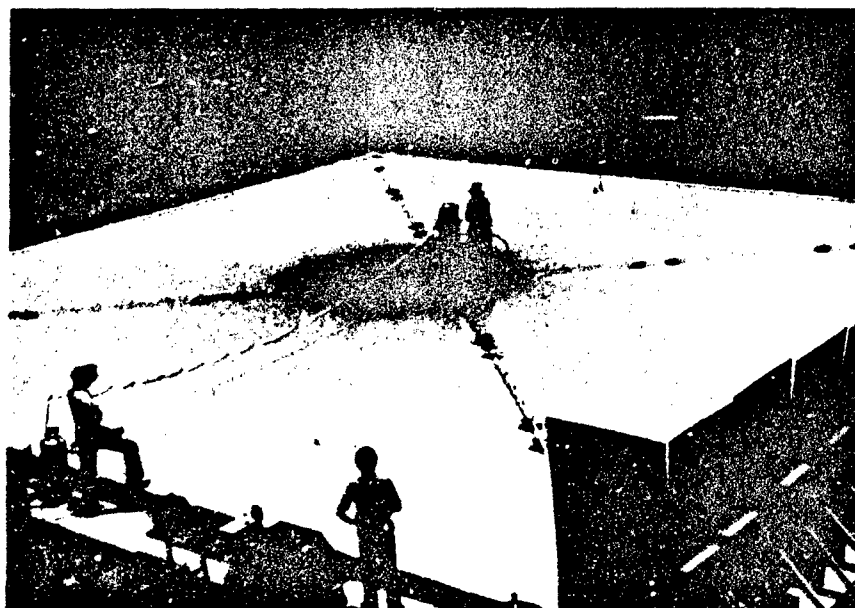


(b)

Figures IV.15 (a,b) 0.95 LITER/SECOND NON-VOLATILE
CONTINUOUS NAPHTHA SPILL



(c)



(d)

FIGURES IV.15 (c.d) 0.95 LITER/SECOND NON-VOLATILE
CONTINUOUS NAPHTHA SPILL

II.4-3 0.95 L/SEC NON-VOLATILE
CONTINUOUS NAPHTHA SPILL

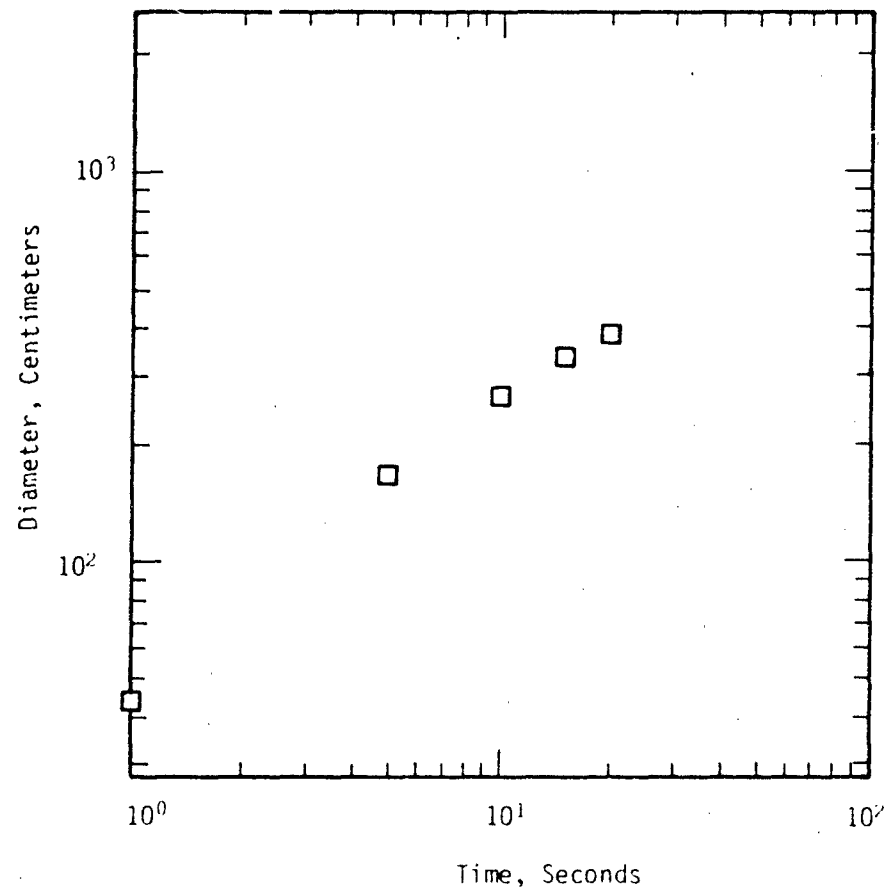


FIGURE IV.16 INCREASE OF SLICK SIZE WITH TIME

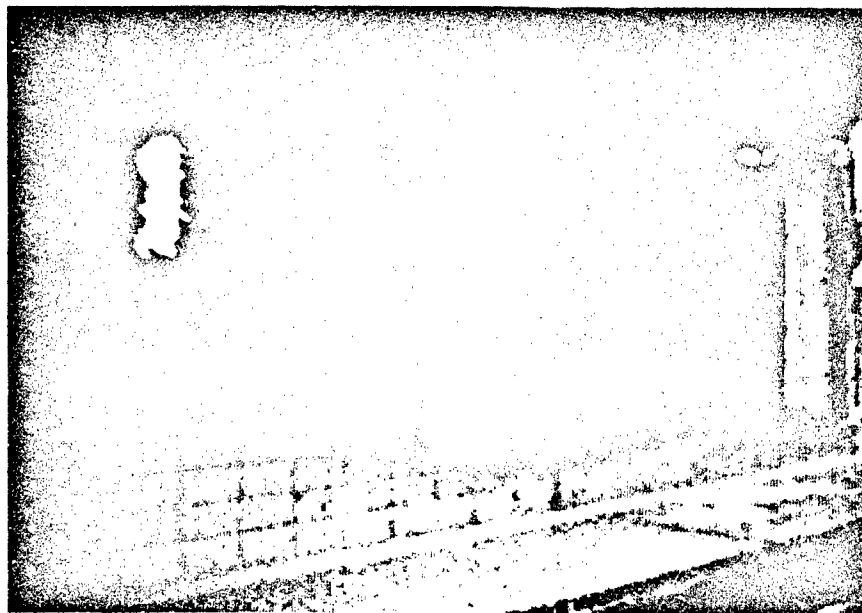
These results are typical of the non-volatile continuous spills studied. The results for all of the non-volatile continuous spills in the basin are contained in Appendix B of the Test Data Volume of the Final Report.

Continuous Spills in Channel. Figures IV.17 are photographs of the development of four different continuous spills of m-Xylene in the channel. The table below summarizes the flow conditions for the pictures in this figure.

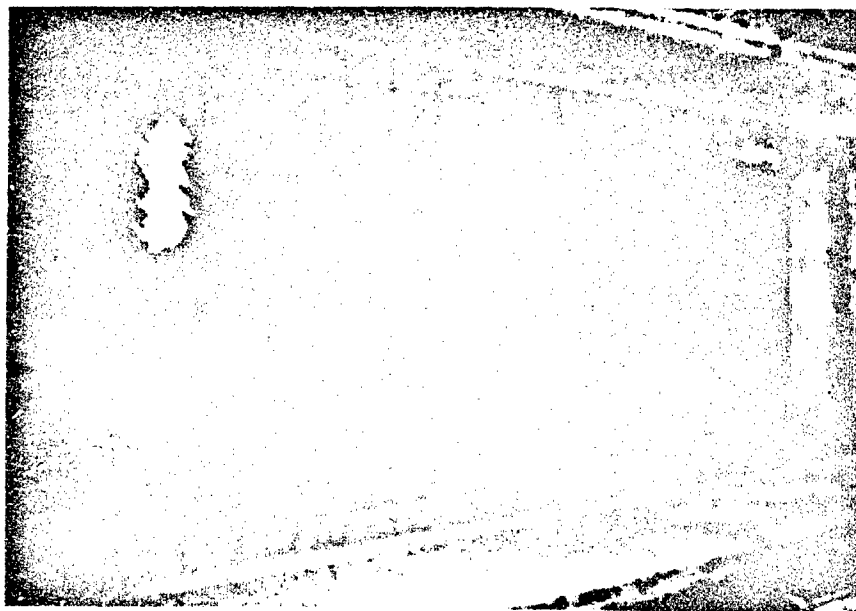
Flow Conditions	River Speed (cm/sec)	Discharge Flowrate (liter/sec)
A	13.4	0.038
B	18.9	0.050
C	24.1	0.100
D	29.0	0.149

These river speed/discharge flowrate combinations were chosen to maximize the length of the channel over which spreading could occur without any influence of the walls. Data collection of this slick width downstream of the spill location was stopped when the thin slick hit the channel walls. The thin slick is indistinguishable in the photographs of Figure IV.17. From the data obtained, a graph of slick width vs. downstream distance was drawn for comparison with the computer model predictions. Figures IV.18 through IV.21 show these graphs for the four m-Xylene spills discussed above.

These results are typical of the continuous spills in the channel that were studied. The results for all of the continuous spills in the channel are contained in Appendix E of the Test Data Volume of the Final Report.

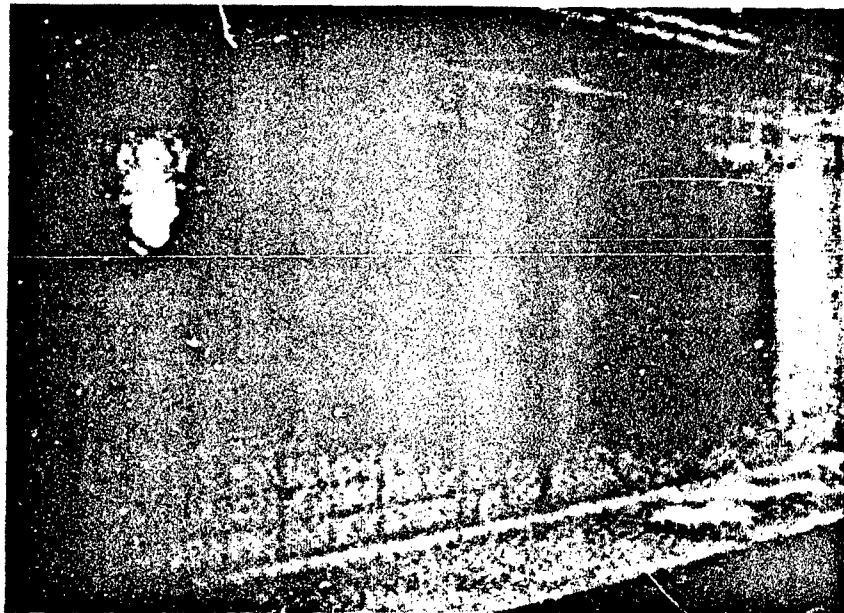


A

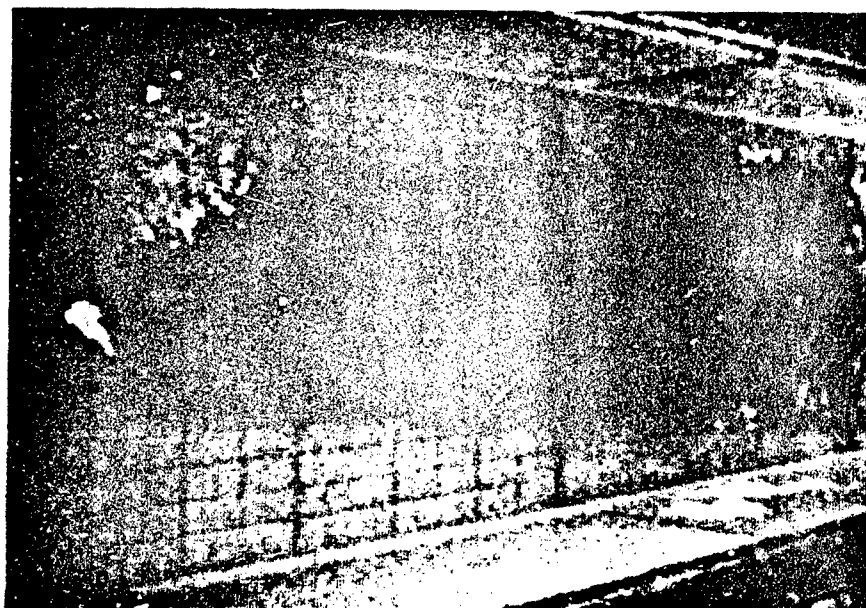


B

FIGURES IV.17 (A,B) CONTINUOUS SPILLS OF m-XYLENE
IN A FLOWING RIVER



C



D

FIGURES IV.17 (C,D) CONTINUOUS SPILLS OF m-XYLENE
IN A FLOWING RIVER

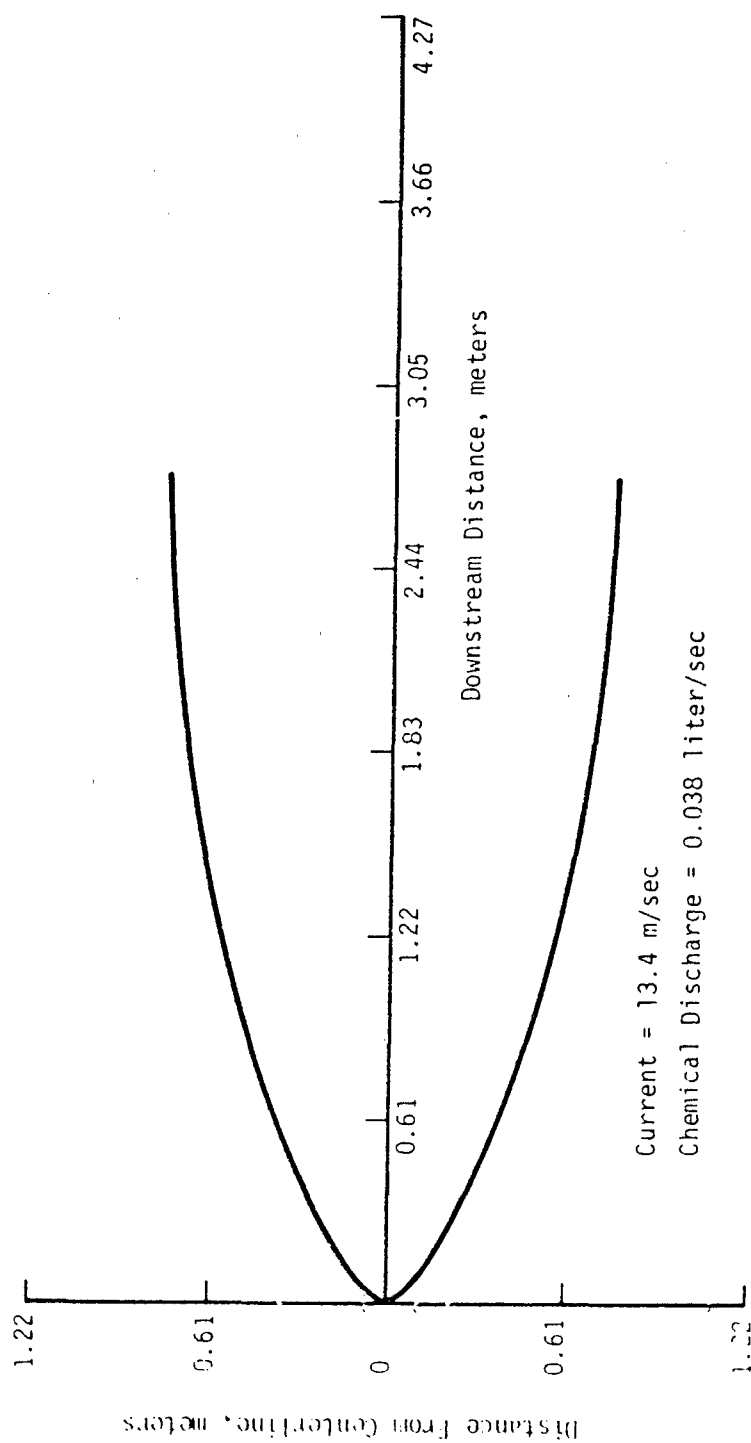


FIGURE IV.18 SLICK SPREADING OF m-XYLENE FOR FLOW CONDITION A

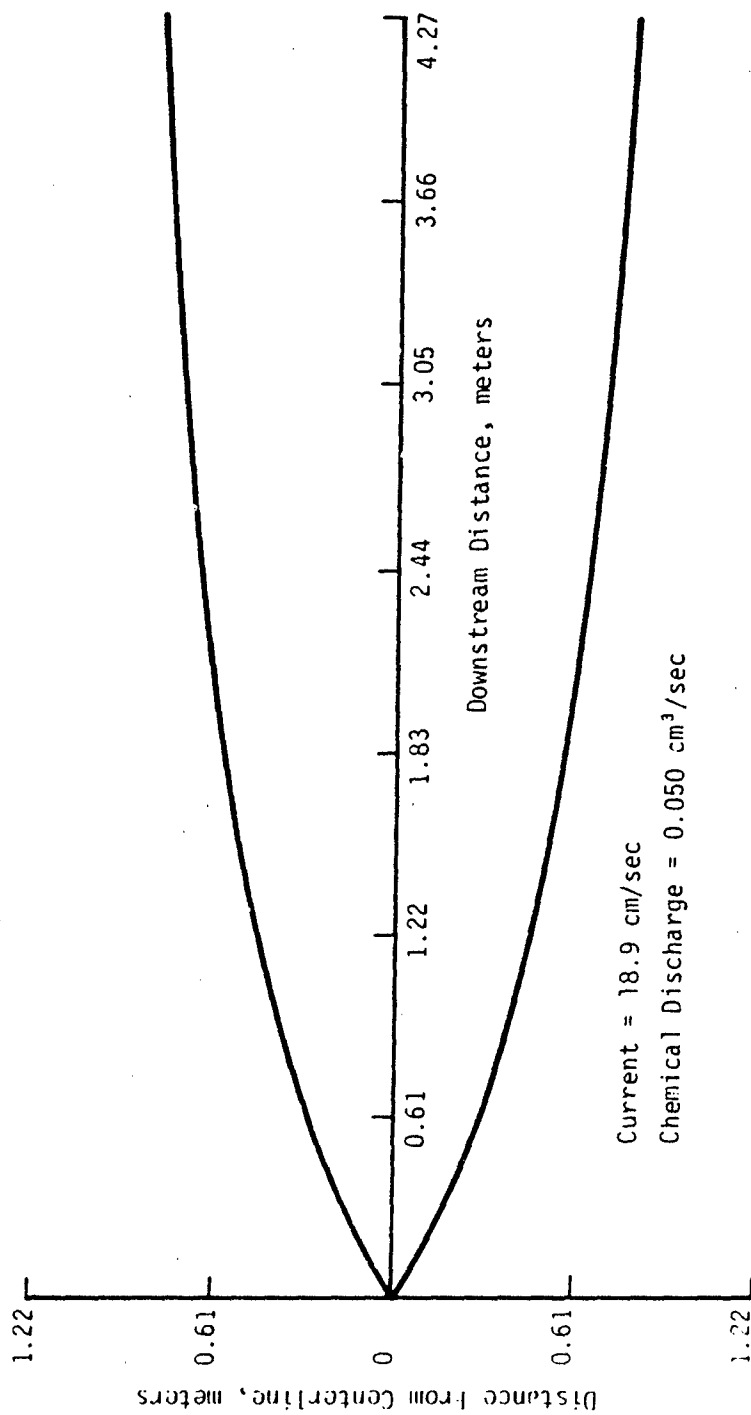


FIGURE IV.19 SLICK SPREADING OF m-XYLENE FOR FLOW CONDITION B

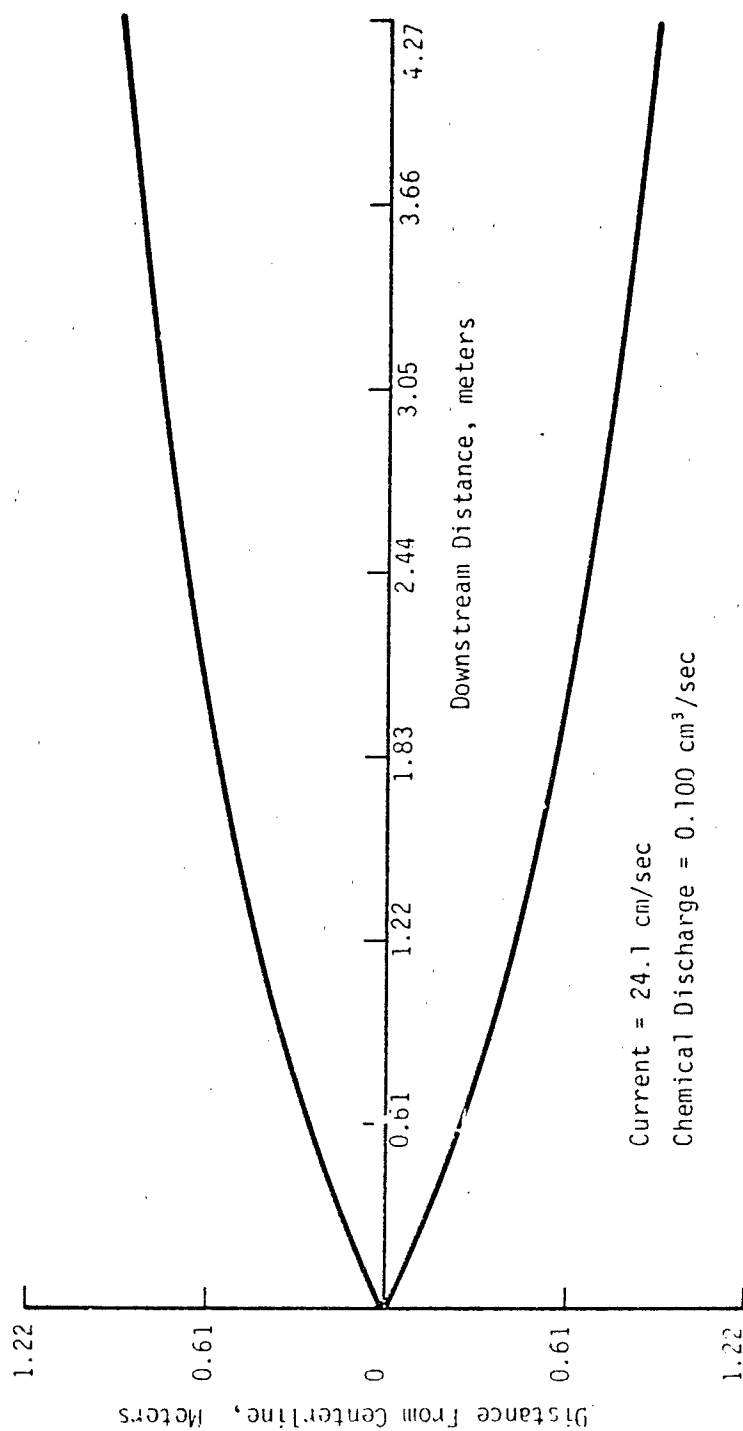


FIGURE IV.20 SLICK SPREADING OF n-XYLENE FOR FLOW CONDITION C

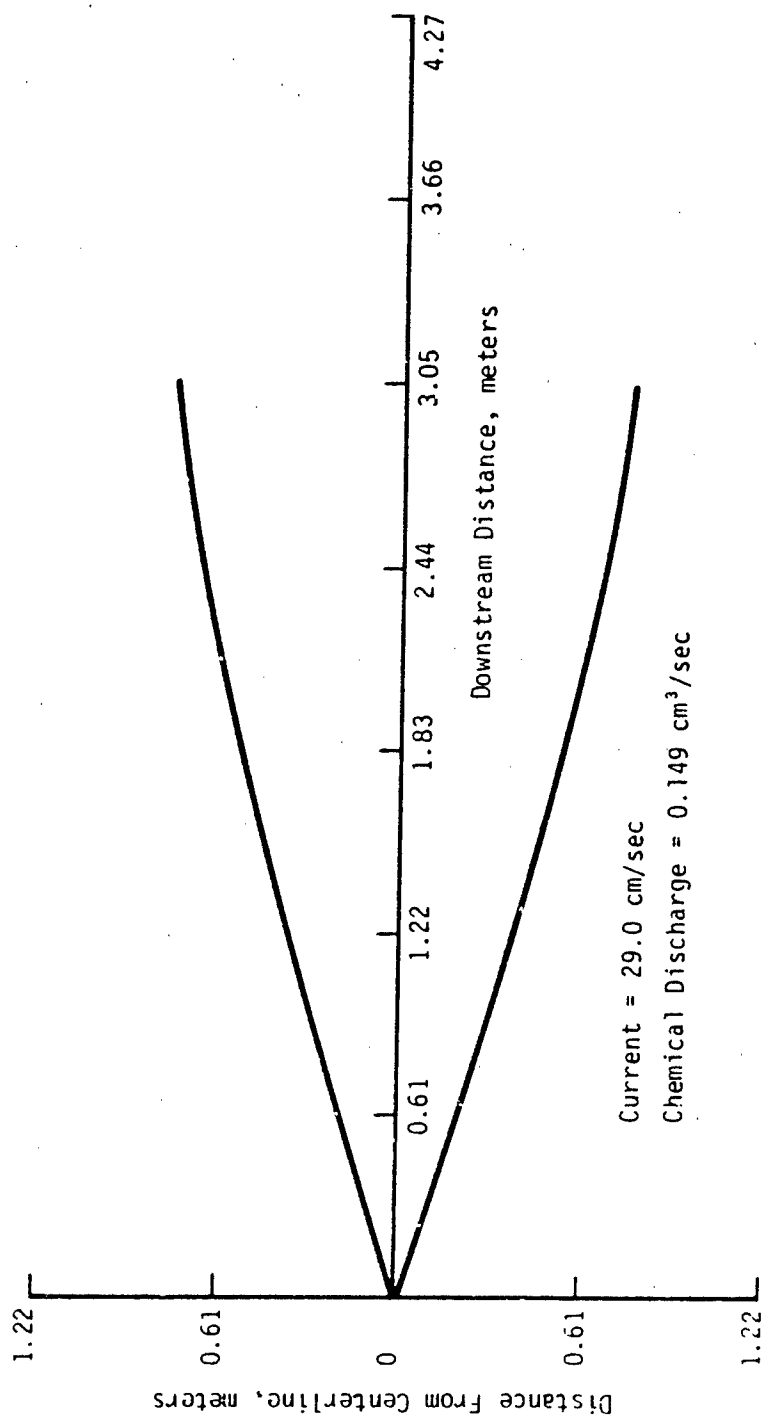


FIGURE IV.21 SLICK SPREADING OF m-XYLENE FOR FLOW CONDITION D

IV.3.2 Evaporation Tests

Velocity Profile Measurements. Since the friction velocity and boundary layer thickness were required for calculation of Dalton number in Equation (III.27), the velocity profiles were measured for model validation. The results of the velocity profile measurements are summarized in Table IV.13. The data in the table includes the wind velocity, friction velocity, friction coefficient, intercept, roughness parameter, the correlation coefficient for the linear regression, the average coefficient for the 1/7 power-law velocity profile, and the boundary layer thickness. The results are compared to those of a standard smooth flat plate. The boundary layer thickness was computed from the 1/7 power-law profile where $u/V_w = 0.99$.

Representative velocity profiles are presented in Figures IV.22 and IV.23 for the pan evaporation and wind-wave experiments, respectively. For the pan evaporation experiments, the surface velocity, U_s , was assumed to be zero. In the wind-wave experiments, the surface velocity was assumed to be

$$U_s/u_* = 0.55 \quad (IV.22)$$

in accordance with the recommendation of Street, et al. [46]. Another possible method is from conservation of momentum across the air-water interface for a 1/7 power-law velocity profile. The result is

$$V_w/U_s = (\rho/\rho_a)^{5/9} (v/v_a)^{1/9} \quad (IV.23)$$

At standard pressure and a temperature of 20°C, the surface velocity is

$$V_w/U_s = 30.96 \quad (IV.24)$$

Either result is consistent with previous experiments in the wind-wave channel [45]

The velocity profiles were typical of flows over a smooth surface with some exceptions. The profiles over the mechanically driven waves

TABLE IV.13 SUMMARY OF VELOCITY PROFILE MEASUREMENTS

Surface	Facility	V_w (cm/s)	u_* (cm/s)	$10^3 C_f/2$	B	z_{0+}	Correlation Coefficient	u_+/y_+	δ_+
Sheet	--	--	--	--	5.1(1)	0.13	--	8.16(2) 8.74	
Aluminum	SWRI	526	28.4	2.917	2.11	0.43	0.9844	7.11	761
Water	SWRI	446	23.6	2.782	3.96	0.20	0.9963	7.88	435
Ice and	SWRI	191	10.1	2.829	3.93	0.21	0.9773	7.79	443
		294	14.2	2.325	4.57	0.16	0.9549	8.23	600
Ice and	SWRI	387	15.2	1.548	8.54	0.033	0.9225	10.23	542
		467	23.4	2.520	2.45	0.38	0.9910	7.28	1,068
Mexanol/Water	Flow Research	730	44.6	3.740	-6.67	14.4	0.9895	4.09	12,003
Octane	SWRI	195	10.5	2.913	3.85	0.21	0.9615	7.94	350
		304	14.6	2.300	5.11	0.13	0.9764	8.40	539
		392	19.9	2.581	3.56	0.24	0.9685	7.67	681
		485	23.6	2.371	4.05	0.20	0.9862	8.03	670
Octane/Water	Flow Research	208	8.92	1.835	5.30	0.12	0.9801	8.59	862
		342	13.0	1.455	6.74	0.068	0.9981	9.36	1,082
		*357	13.6	1.439	6.10	0.087	0.9961	9.02	1,461
		519	20.8	1.605	3.97	0.20	0.9985	8.00	2,296
		*482	21.3	1.952	2.35	0.39	0.9904	7.33	2,098
		729	28.1	1.489	4.97	0.14	0.9954	8.29	2,338
		*725	22.6	0.975	9.94	0.019	0.9490	10.24	2,410

(1) Monin and Yaglom [49]

(2) Hinze [50]

* Wavemaker

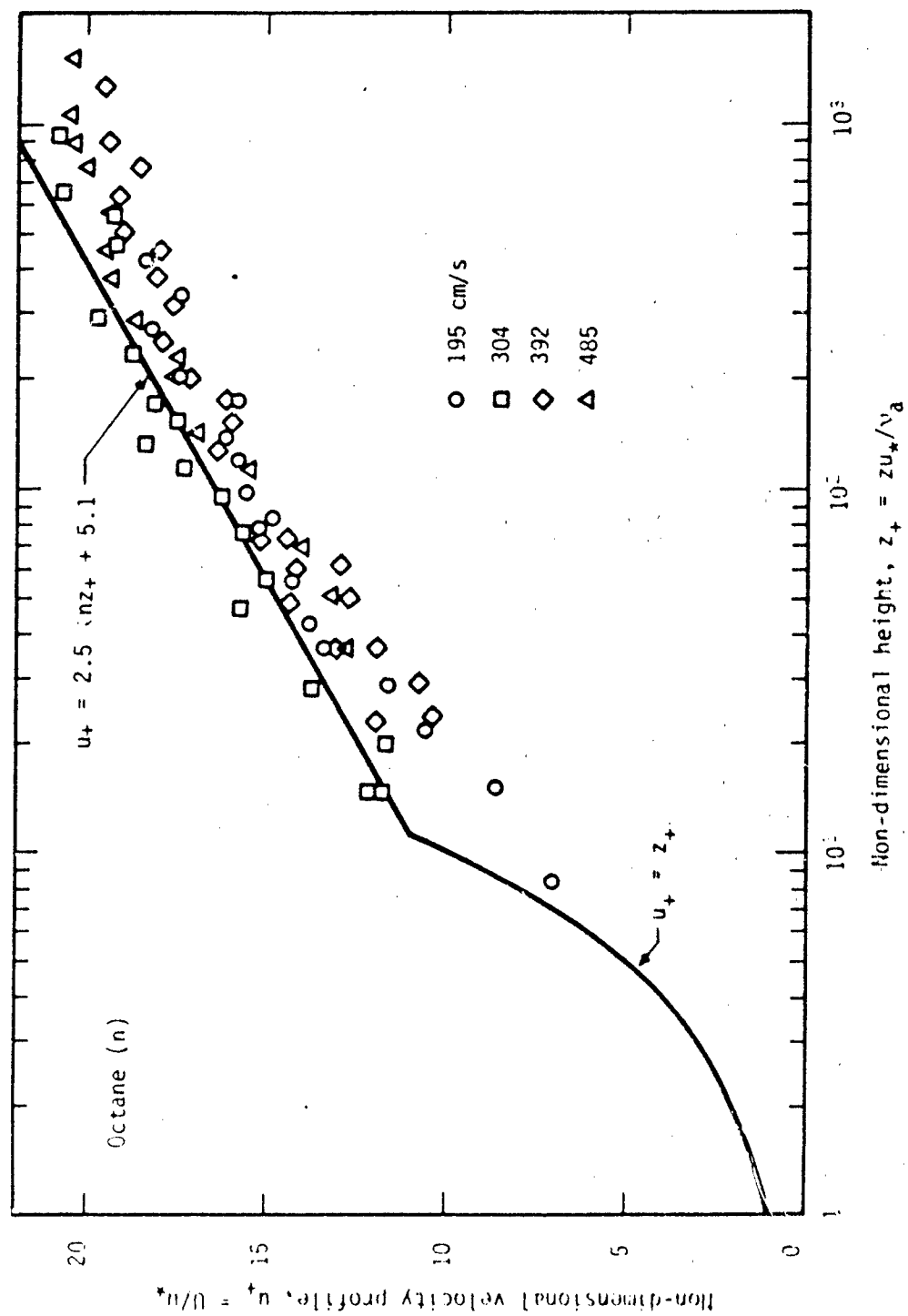


FIGURE IV.22 VELOCITY PROFILES OVER OCTANE IN PAN EVAPORATION EXPERIMENTS

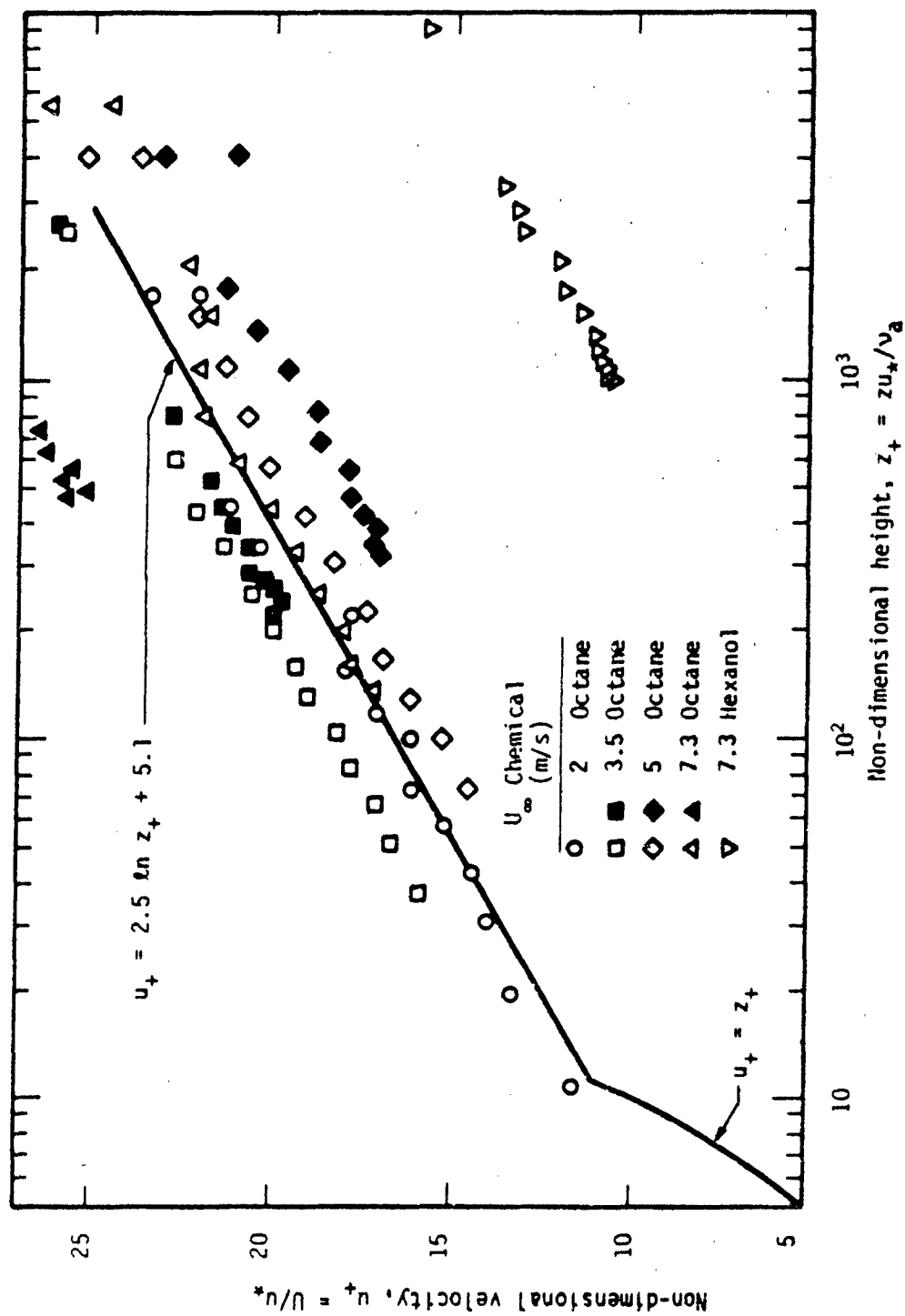


FIGURE IV.23 VELOCITY PROFILES FOR CHEMICAL SLICKS IN FLOW RESEARCH WIND-WAVE CHANNEL.
FILLED SYMBOLS ARE WITH MECHANICAL WAVE MAKER.

were anomalous. In particular, the flow at 725 cm/s with the wavemaker had an exceptionally low friction coefficient. The friction coefficient in this case is possibly in error from a wave induced velocity component.

In other cases, the friction velocities are also apparently low. For example, at 729 cm/s without the wavemaker, the friction velocity is 28.1 cm/s whereas Lin, et al. [45] reported 38 cm/s at a tunnel velocity of 7 m/s.

Another exception is the flow over hexanol at 730 cm/s in the wind-wave channel. Figure IV.24 is a plot of the friction coefficients of all experiments in comparison to a smooth surface. As the figure indicates, the friction coefficient over hexanol in the wind-wave channel was unusually high. However, this result, which implies flow over a rough surface, is also consistent with the wave height measurements and flow visualization experiments. The wave heights were increased in the flow over hexanol whereas the octane dampened the waves. This phenomenon is associated with the spreading coefficient of the chemical on water.

Wave Height Measurements and Slick Thickness. One of the objectives of the wind-wave experiments was to measure the effect of waves in mass transfer from evaporation. The results of the wave height measurements are summarized in Table IV.14. The interesting result in this table is a comparison of the rms wave heights for water, octane, and hexanol at 7.5 m/s for wind waves only. The octane dampens the waves while hexanol increases the wave height.

The wave heights in non-dimensional inner-scale variables are also included in Table IV.14. Both rms and mean wave heights are included in the table. The rms was measured, but the evaporation model, Equation (III.27), contains the mean wave height. According to Street [29], the mean and rms wave heights are related by

$$h_{m+} = (2\pi)^{\frac{1}{2}} n_+ \quad (IV.25)$$

The frequency and peak-to-peak amplitude of the mechanically-generated waves were 1.6 Hz and 3 cm, respectively.

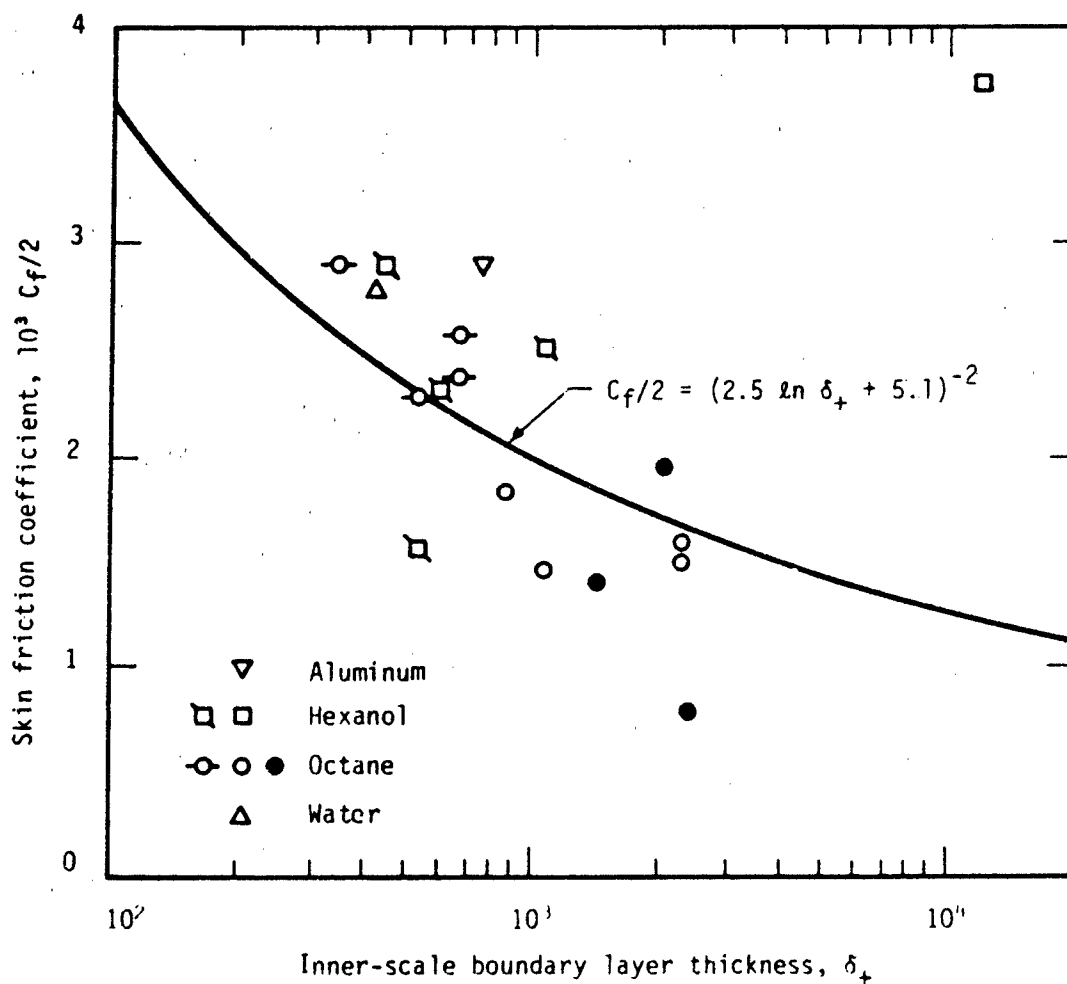


FIGURE IV.24 SKIN FRICTION COEFFICIENT MEASUREMENTS FROM PROFILE METHOD. SYMBOLS WITH SLASH ARE FOR PURE CHEMICAL WHILE OTHERS ARE FOR SLICK ON WATER, AND CLOSED SYMBOLS ARE FOR WAVE MAKER. LINE IS FOR SMOOTH SURFACE.

TABLE IV.14 WAVE HEIGHT MEASUREMENTS

Surface	V_w (cm/s)	RMS Wave Height η (cm)	η_+	h_{m+} (1)
Octane	208	0.01	0.54	1.36
	342	0.01	0.86	2.15
	* 482	0.916	128.	320.
	519	0.0741	10.2	25.5
	* 357	0.971	86.1	216.
	729	0.0779	14.1	35.4
	* 725	1.037	151.	379.
Hexanol	730	0.647	186.	467.
Water	* 760	1.53	421. (2)	1055.
Water	760	0.558	153. (2)	385.
* Wavemaker (1) $h_{m+} = (2\pi)^{\frac{1}{2}} \eta_+$ (2) Estimated from Lin, et al. [45]				

For the wind-wave experiments, slick thickness may be an important parameter in evaporation and dissolution. Slick thickness was estimated by conservation of mass from the following:

$$h = Q / (U_s w) \quad (IV.26)$$

where Q is the measured flowrate of the chemical onto the water surface, w is the tunnel width, and the surface velocity, U_s , is estimated from Equation (IV.22) or (IV.24). The primary assumption in Equation (IV.26) is that the slick moves uniformly as slug flow. The average slick thickness with two different estimates of surface velocity is tabulated for all the experiments in Table IV.15.

Normally, both octane and hexanol have positive spreading coefficients. Consequently, they will continue to spread until they form a monolayer. However, in the case of hexanol, a thin layer spreads very rapidly and locally changes the surface tension of the water. Thus, the spreading coefficient of hexanol becomes negative, and hexanol forms lenses. The minimum thickness for an infinitely large slick is given by Equation (III.15). From this equation, the minimum thickness for a hexanol slick is 2 mm. Since the average thickness was estimated to be only 0.04 mm, only a small fraction of the surface was covered by lenses. The surface area covered by lenses could be estimated from [19] if an average lens diameter were assumed.

Slick thickness for these experiments can be controlled by the flowrate of the feed system. The flowrate of hexanol was less than the octane in these experiments because the flowrate was limited by the higher viscosity of the hexanol.

Evaporation Concentration Profiles. The results for the concentration measurements are summarized in Table IV.16. Typical concentration profiles are shown in Figures IV.25 and IV.26 for the pan evaporation experiments and wind-wave experiments, respectively. In general, the curves are relatively linear and yield reasonable values of the Dalton number. No trends have been discovered on the value of the intercept, B_c .



TABLE IV.15 ESTIMATED AVERAGE SLICK THICKNESS
FOR WIND-WAVE EXPERIMENTS

Surface	V_w (cm/s)	Chemical Flowrate (l/min)	$U_s^{(1)}$ (cm/s)	h (mm)	$U_s^{(2)}$ (cm/s)	h (mm)
Octane	208	5.3	4.91	0.15	6.73	0.11
	342	8.8	7.17	0.17	11.0	0.11
	* 482	8.8	11.7	0.10	15.6	0.079
	519	8.8	11.4	0.11	16.8	0.073
	* 357	8.8	7.46	0.16	11.5	0.11
	729	9.7	15.5	0.087	23.5	0.057
Octane	* 725	10.6	12.4	0.12	23.4	0.063
Hexanol	730	6.6	24.5	0.037	23.6	0.039
(1) $U_s/u_* = 0.55$ (2) $V_w/U_s = 30.96$ * Wavemaker						

TABLE IV.16 SUMMARY OF EVAPORATION CONCENTRATION PROFILE MEASUREMENTS

Surface	Facility	V_w (cm/s)	Sc	$-X_*$ (ppm)	Da_*	B_c	Z_{oc+}	Correlation Coefficient	$10^3 Da_0$	Da_{*0}
Ethyl acetate	SwRI	202	1.82	1856	0.0253	27.1	2.86×10^{-6}	0.9362	1.853	0.0343
		202	1.82	2072	0.0282	23.4	1.65×10^{-5}	0.9888	1.765	0.0327
		301	1.82	1924	0.0287	22.1	3.02×10^{-5}	0.9945	1.944	0.0405
		403	1.82	1512	0.0244	27.2	2.71×10^{-6}	0.9918	2.000	0.0394
		501	1.82	1815	0.0321	17.4	2.80×10^{-4}	0.9958	1.994	0.0410
Hexane		203	2.16	2941	0.0290	22.7	2.28×10^{-5}	0.9864	3.407	0.0631
		302	2.16	4517	0.0495	8.28	2.03×10^{-2}	0.9750	2.308	0.0481
		403	2.16	3495	0.0417	10.73	6.42×10^{-3}	0.9941	2.374	0.0467
		498	2.16	3258	0.0468	7.67	2.70×10^{-2}	0.9953	2.443	0.0502
Hexanol		201	2.19	34.2	0.0348	16.5	4.28×10^{-4}	0.9381	1.521	0.0282
		303	2.19	47.7	0.0415	11.7	4.03×10^{-3}	0.9755	1.403	0.0293
		402	2.19	39.4	0.0407	11.9	3.69×10^{-2}	0.9959	1.946	0.0383
		500	2.19	63.9	0.0655	2.34	0.333	0.9530	2.418	0.0497
Hexanol/Water	Flow Research	730	2.19	12.6	0.0177	38.6	1.27×10^{-8}	0.9750	--	--
Octane	SwRI	200	2.61	794.	0.0463	9.95	9.27×10^{-3}	0.9864	1.561	0.0289
		302	2.61	654.	0.0451	9.71	1.04×10^{-2}	0.9913	1.678	0.0350
		400	2.61	692.	0.0497	7.52	2.90×10^{-2}	0.9892	1.782	0.0351
		501	2.61	432.	0.0336	16.0	5.46×10^{-4}	0.9909	2.312	0.0475
		501	2.61	468.	0.0352	14.7	1.33×10^{-6}	0.9885	2.241	0.0460
Octane/Water	Flow Research	200	2.60	219	0.0219	31.2	4.28×10^{-7}	0.9947	--	--
		342	2.60	281	0.0202	34.2	1.03×10^{-7}	0.9975	--	--
		* 357	2.60	222	0.0164	44.7	7.33×10^{-10}	0.9742	--	--
		501	2.60	361	0.0296	20.6	6.06×10^{-5}	0.9897	1.949	0.0400
		520	2.60	290	0.0213	30.9	4.85×10^{-7}	0.9969	--	--
Octanol	SwRI	* 482	2.60	232	0.0228	27.0	3.02×10^{-6}	0.9975	--	--
		* 729	2.60	225	0.0157	46.7	2.80×10^{-10}	0.9950	--	--
		* 725	2.61	206	0.0150	50.2	5.54×10^{-11}	0.9778	--	--
Octanol	SwRI	202	2.36	1.67	0.0149	52.3	2.67×10^{-11}	0.8569	--	--
		301	2.36	2.70	0.0240	29.0	1.11×10^{-6}	0.9848	--	--
		400	2.36	1.60	0.0143	55.2	5.21×10^{-12}	0.8176	--	--
		500	2.36	2.36	0.0200	35.1	3.64×10^{-8}	0.9705	--	--

* Wavemaker

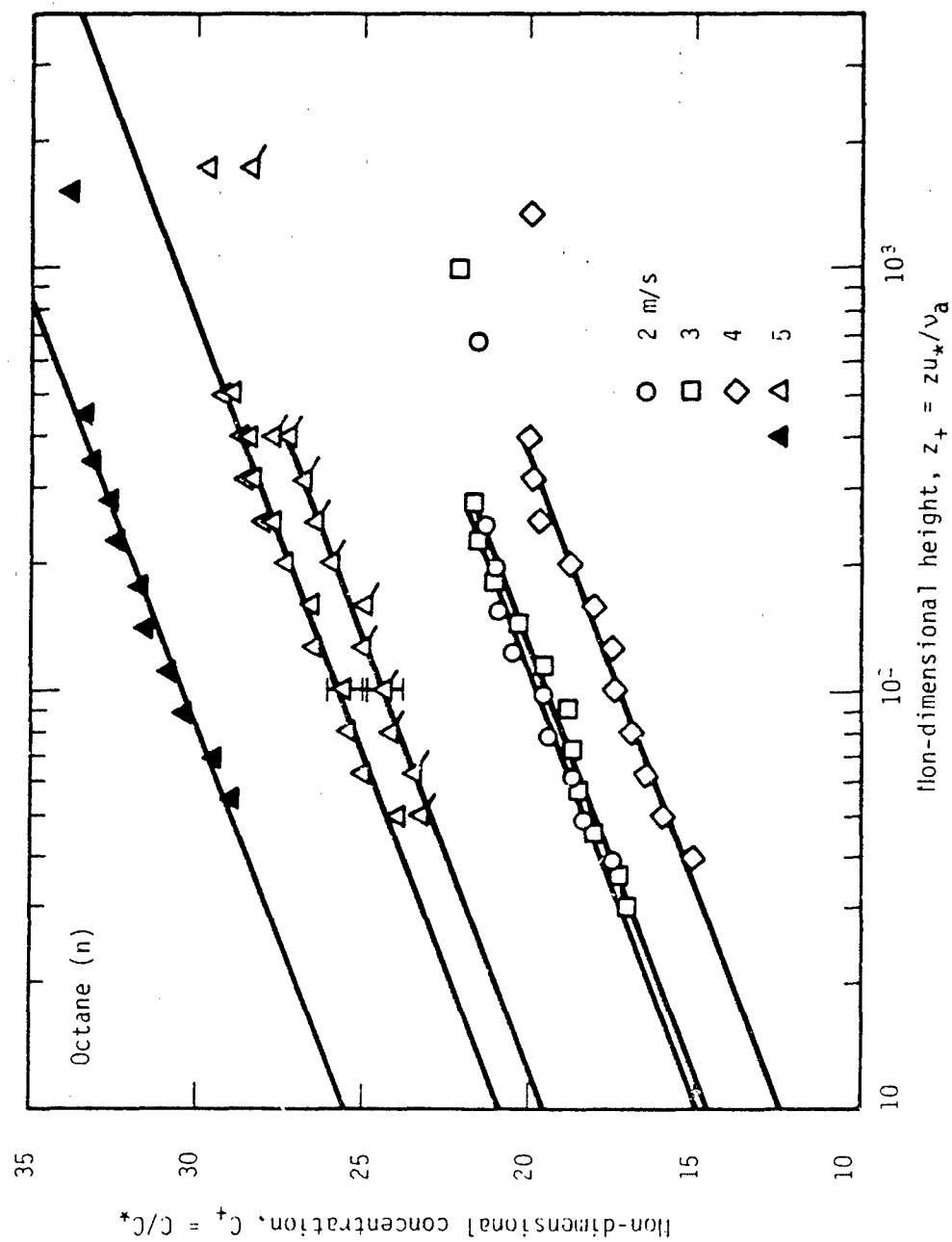


FIGURE IV.25 CONCENTRATION PROFILES FOR OCTANE IN PANI EVAPORATION EXPERIMENTS.
CLOSED SYMBOLS ARE FOR OCTANE ON WATER

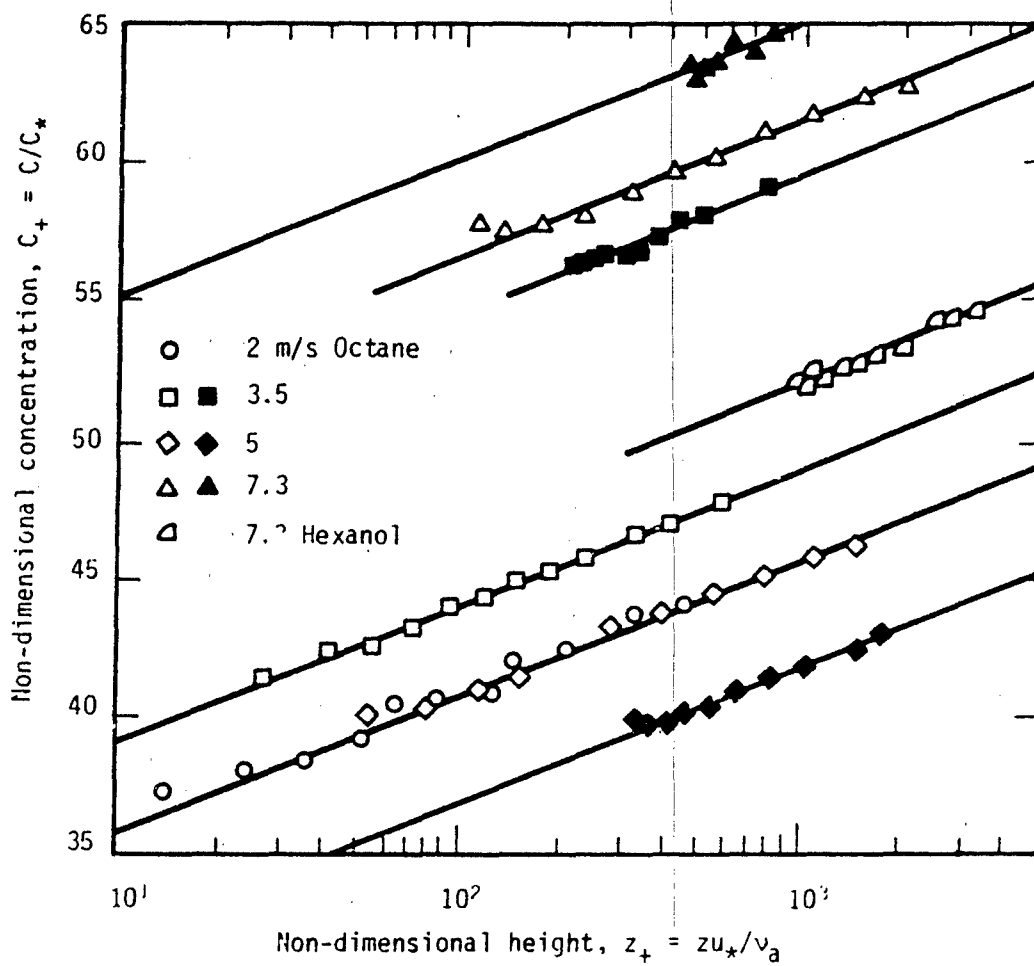


FIGURE IV.26 CONCENTRATION PROFILES FOR WIND-WAVE CHANNEL EXPERIMENTS.
CLOSED SYMBOLS ARE FOR WAVEMAKER

The quality of the data was checked through repetition of the experiments. One such check is the two concentration profiles for a wind speed of 5 m/s. Although the repeat data are not within the error bars of the measurement, the data are reasonably close. The error bars are $\pm 2\sigma$, or 20-to-one odds, and the standard deviation of the concentration measurements was established by an average of twenty consecutive measurements at one location. According to Moffat [47], this procedure will determine the accuracy of the standard deviation within $\pm 5\%$. The standard deviation was measured to be 8% of the mean concentration of octane at two locations, one in the boundary layer and one at the downstream sampling station.

Values of the Dalton number for all pan evaporation experiments are shown in Figure IV.27 in comparison to the theories of Street [29] and Yaglom and Kader [28] for smooth flow. This figure indicates that Schmidt number effects are not discernible in these experiments. Also, no relationship can be identified between the results of the two methods of mass transfer measurement; however, in most cases the results are the same within experimental error.

The results for octane in the pan evaporation experiments are presented in Figure IV.28. The primary purpose of this figure is to indicate the magnitude of uncertainty in the measurements. The error bars are again for $\pm 2\sigma$. The uncertainty for the profile measurements was determined from the standard deviation of the slope in the linear regression analysis. The uncertainty for the downstream concentration measurement was computed from an average of 20 bag samples. The error bars for the two measurements of Dalton number usually overlap. Also, the error bars are smaller for the more volatile chemicals such as ethyl acetate, and larger for the less volatile such as hexanol and octanol. The results for the octane on water experiments are comparable to the pure octane experiments.

Dalton numbers from the the two test facilities are compared in Figure IV.29 for the profile method. The uncertainty in the wind-wave experiments tends to be less, and the Dalton numbers are smaller. The lower Dalton numbers may be associated with slick thickness. The slick thickness of octane on water for the pan evaporation experiments was probably much thicker than in the wind-wave experiments. Since the Dalton number of hexanol is similar to that of octane, the water surface must

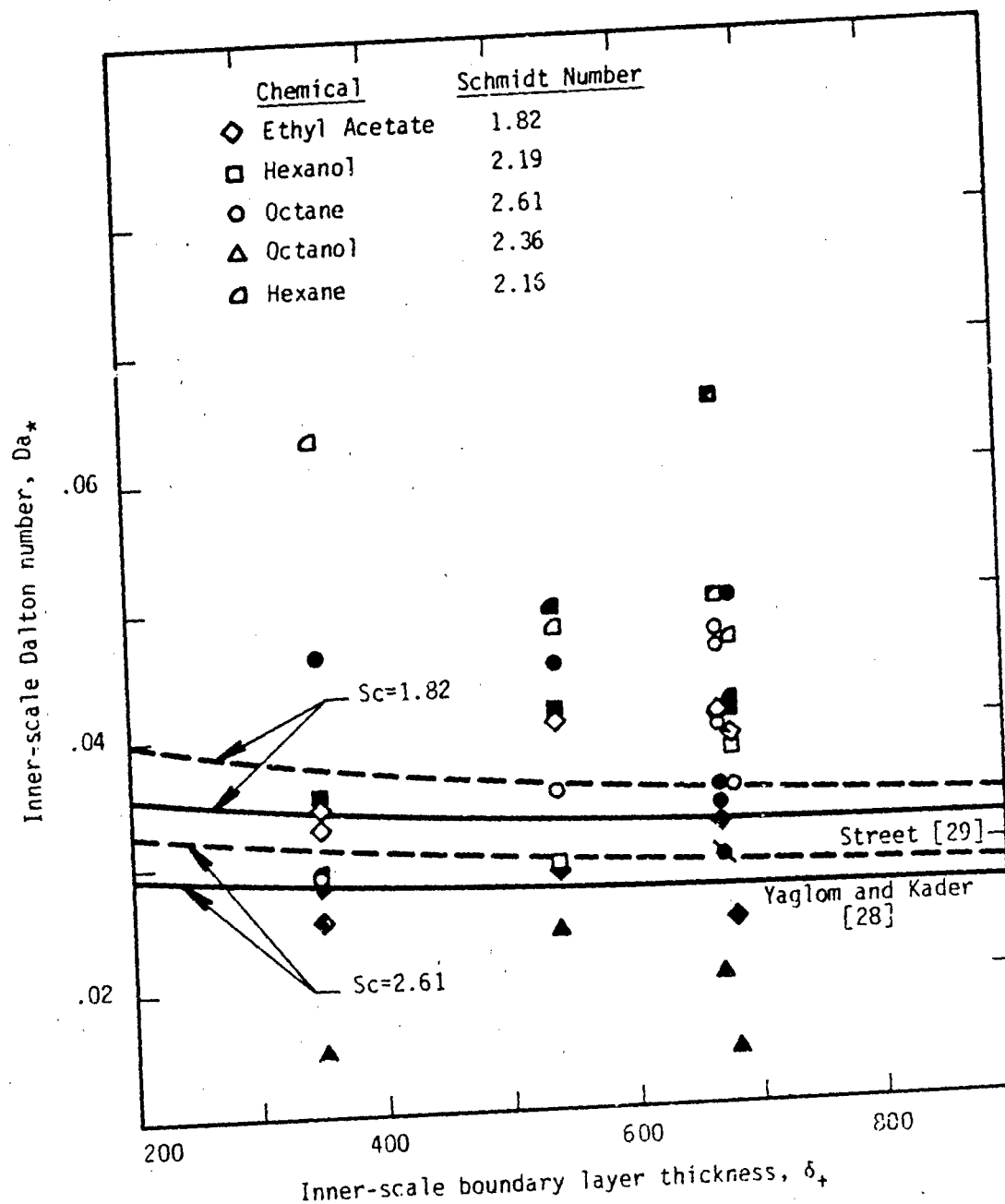


FIGURE IV.27 COMPARISON OF DALTON NUMBERS FOR VARIOUS CHEMICALS IN PAN EVAPORATION EXPERIMENTS. CLOSED SYMBOLS ARE FOR PROFILE METHOD; OPEN SYMBOLS ARE FROM TUNNEL EXHAUST MEASUREMENTS; AND SYMBOLS WITH SLASH ARE CHEMICAL ON WATER EXPERIMENTS.

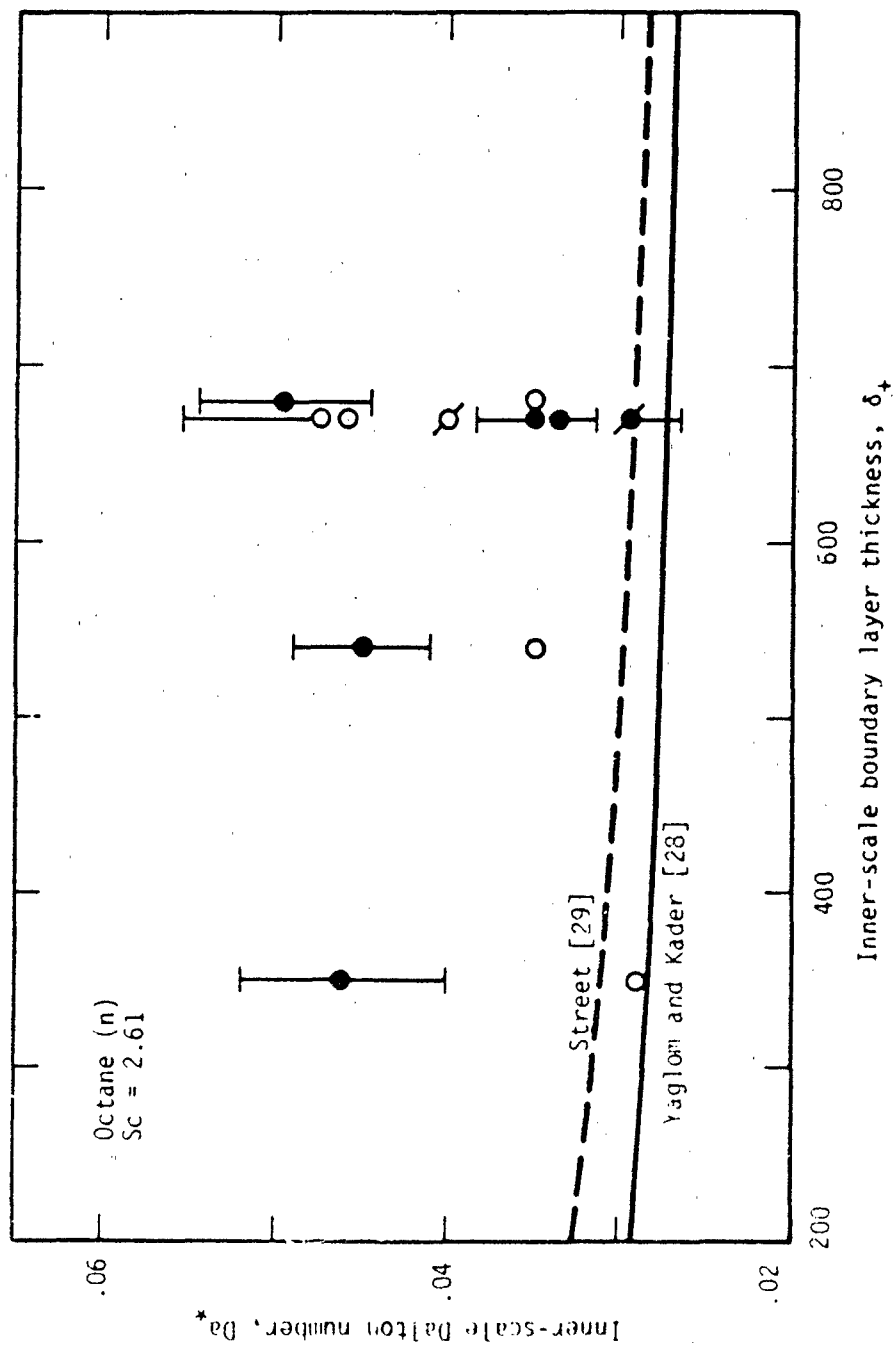


FIGURE IV-28 DALTON NUMBER WITH 2σ ERROR BARS FOR OCTANE IN PAN EVAPORATION EXPERIMENTS. SOLID SYMBOLS ARE FROM PROFILE METHOD, AND OPEN SYMBOLS FROM TUNNEL EXHAUST CONCENTRATION MEASUREMENTS. SYMBOLS WITH SLASH ARE FOR OCTANE ON WATER EXPERIMENTS.

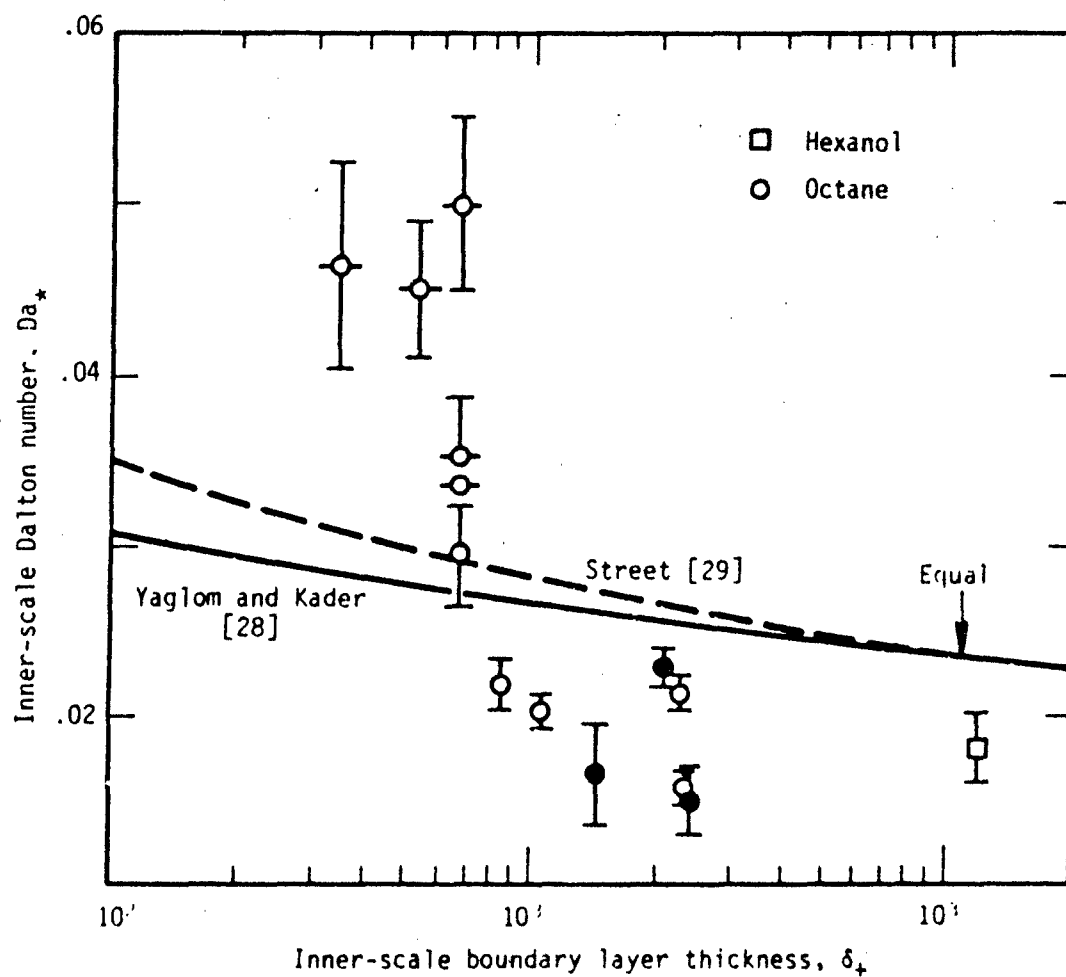


FIGURE IV.29 COMPARISON OF DALTON NUMBERS FOR PAN EVAPORATION AND WIND-WAVE EXPERIMENTS. CLOSED SYMBOLS ARE FOR WAVEMAKER, AND SYMBOLS WITH HORIZONTAL SLASH ARE PURE CHEMICALS

have been covered in a thin film during lens formation; otherwise, the Dalton number would have been much smaller.

The effect of roughness on Dalton number is emphasized in Figure IV.30. The Dalton number is plotted as a function of wave height for the experimental data and for the theories of Street [29] and Yaglom and Kader [28], in which $\delta_+ = 2000$ and $Sc = 2.61$ were used in Equation (III.27). The data are consistent with the hypothesis that mass transfer will diminish in flows over rough surfaces.

During the pan evaporation experiments, substantial cooling occurred. The liquid temperature attained steady state before data acquisition. The liquid surface temperature was used in the calculation of the saturation concentration. The temperature of the chemicals tested as a function of wind speed is presented in Figure IV.31. This cooling has two important effects: boundary layer stabilization and errors in velocity for the hot-wire. In the concentration calculations for these experiments, the friction velocity from the velocity measurements over octane were used. Cooling was not detected in the wind-wave experiments.

IV.3.3 Spreading and Evaporation Tests in Basin

The procedures used for the spreading and evaporation tests in the basin were similar to the non-volatile spreading tests in the basin discussed earlier in Section IV.3.1. These tests, which included evaporation, differed from the non-volatile tests in two ways:

- (1) Since a wind was necessary for evaporation, the entire slick tended to move with the wind while spreading. Although the slicks stayed relatively symmetric, they no longer were centered in the basin, and special treatment was necessary to determine the average slick diameters over time.
- (2) The evaporation of the chemicals caused the outer edges of the slick to form irregular fingers rather than being smooth. Estimation of each average radii was necessary during the data collection to collect meaningful slick diameter data.

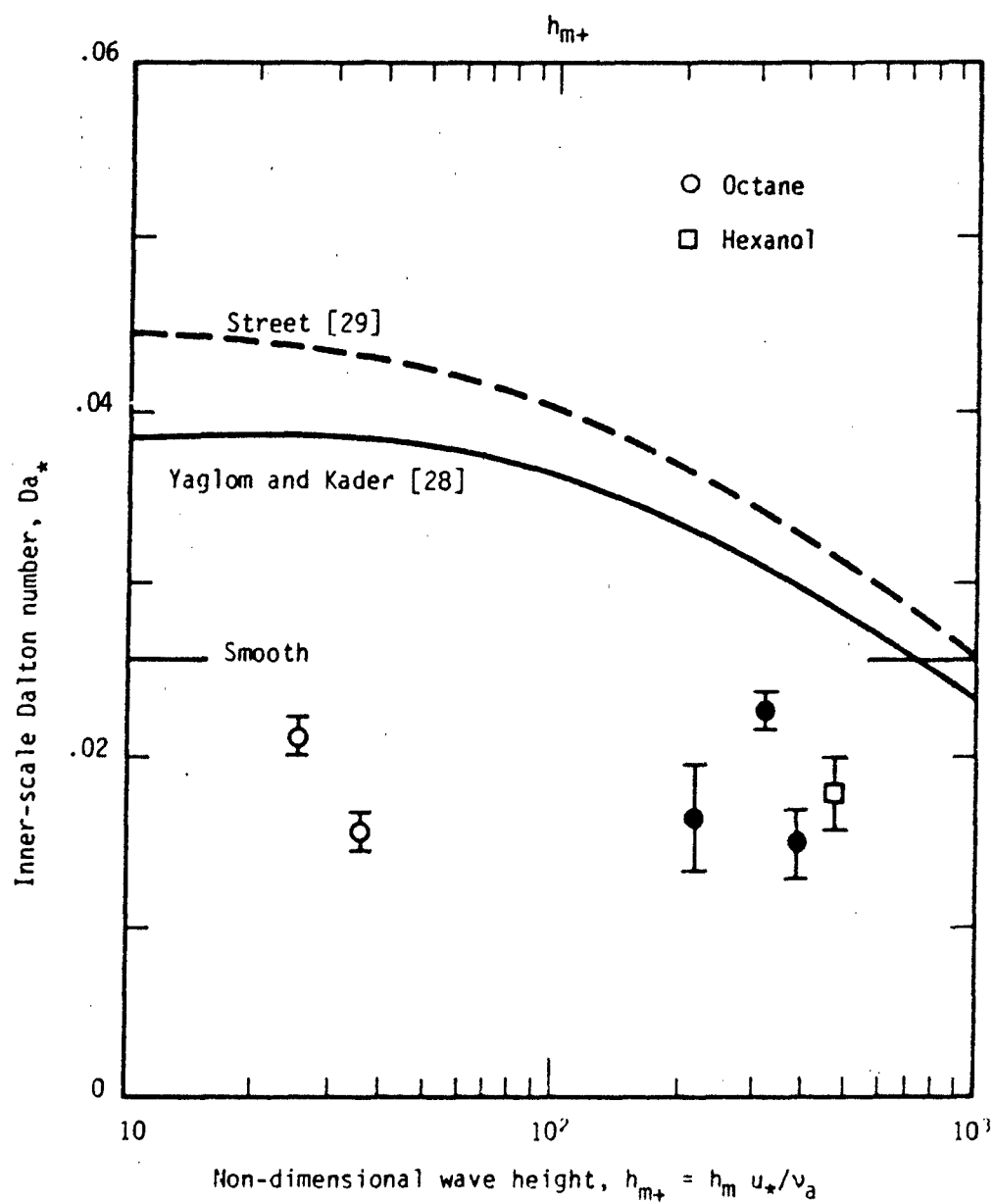


FIGURE IV.30 DALTON NUMBER AS A FUNCTION OF WAVE HEIGHT. LINES ARE THEORY FOR $\delta_* = 2000$ and $Sc = 2.61$. CLOSED SYMBOLS ARE FOR MECHANICAL WAVES.

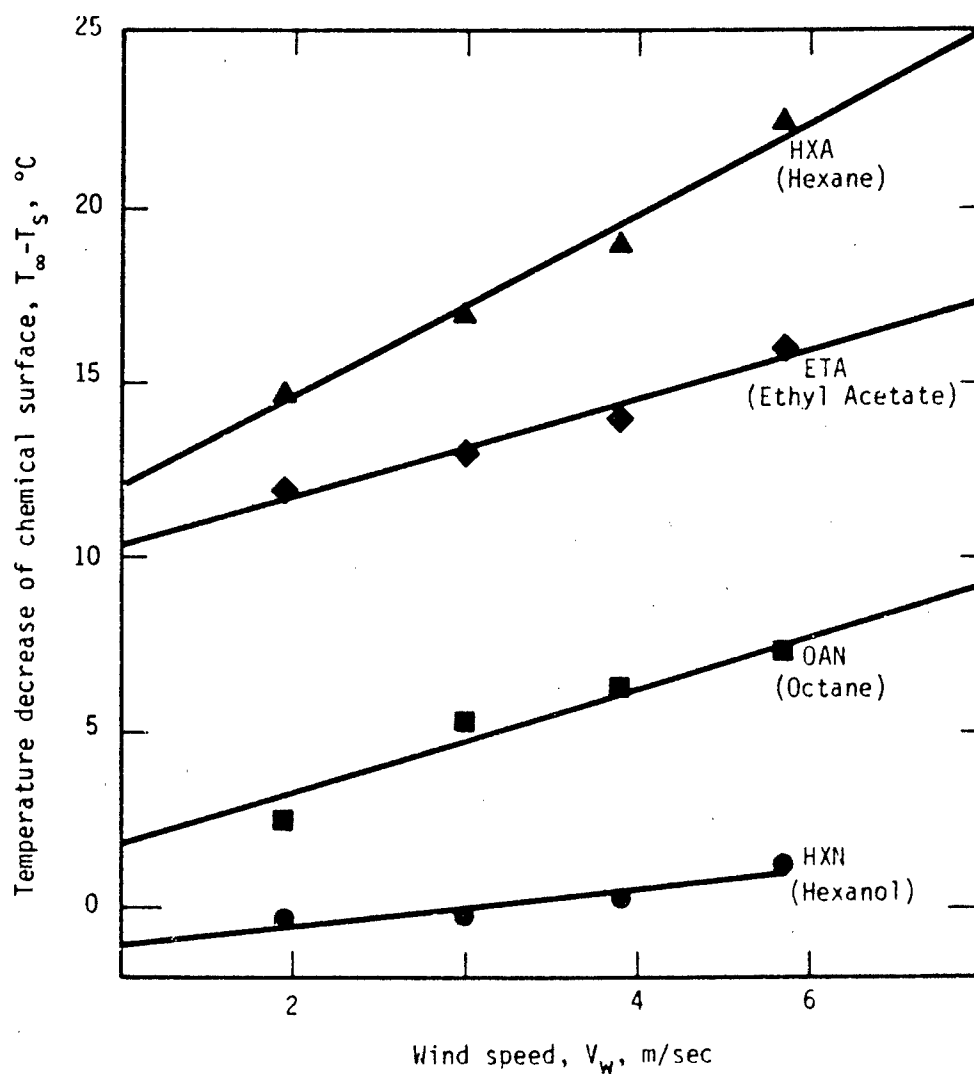


FIGURE IV.31 STEADY STATE LIQUID SURFACE TEMPERATURE FOR VARIOUS CHEMICALS FROM EVAPORATIVE COOLING IN PAN EVAPORATION EXPERIMENTS

The data collected for the spreading and evaporation tests in the basin were graphed in the form of average slick diameter as a function of time. The results for all of the volatile instantaneous spills are contained in Appendix C of the Test Data Volume of the Final Report. The results for all of the volatile continuous spills are contained in Appendix D of the Test Data Volume.

IV.3.4 Dissolution Tests

Wind Tunnel. Four chemicals (ethyl acetate, hexane, hexanol, and octane) were tested for dissolution in water in the wind tunnel as a function of wind speed. The measured solubilities are listed in Table IV.17

TABLE IV.17 SOLUBILITY

Chemical	Measured Solubility (ppm)	Literature Solubility
Ethyl Acetate	64,387	87,000
Hexane	7	9.5
Hexanol	6,149 6,305	6,000
Octane	2	0.43 - 0.88

in comparison to values from the literature. The solubilities of hexane and octane were much lower than that listed in Appendix A; however, they are in agreement with those reported by Mackay and Shiu [48]. The results of the dissolution tests are summarized in Table IV.18. Since the concentration profiles were fairly uniform, only an average value (over the 31.7 mm depth of the probe) is presented for each time interval. Octane and hexane were virtually insoluble. A maximum of one percent of the solubility limit for octane was measured in a 60-minute period while 15% was the maximum for hexane. Dissolution rate was a strong function of wind speed for ethyl acetate. Ethyl acetate reached 100% of its solubility in 60 minutes at 5 m/s while hexanol attained 77% saturation under the same conditions.

TABLE IV.18 RESULTS OF DISSOLUTION TESTS IN SWRI WIND TUNNEL

Average of 4 Concentration Measurements
Over a Depth of 25 to 30 mm.

Chemical	V_w (m/s)	Saturation (%)	Time (min)
Ethyl Acetate	2	20.1	15
↓	2	29.7	30
↓	2	38.5	45
↓	2	44.2	60
↓	5	46.0	15
↓	5	72.0	30
↓	5	89.3	45
Ethyl Acetate	5	100.0	60
Hexane	5	5.7	15
↓	5	9.3	30
↓	5	9.6	45
Hexane	5	14.6	60
Hexanol	2	38.2	15
↓	2	58.9	30
↓	2	66.4	45
↓	2	65.7	60
↓	5	42.5	15
↓	5	62.0	30
↓	5	68.8	45
Hexanol	5	77.3	60
Octane	5	0.7	15
↓	5	1.3	30
Octane	5	0.4	45

Wind-Wave Channel. The more interesting dissolution results were from the wind-wave channel. Again, octane was essentially insoluble, but the hexanol was uniformly dispersed in the upper layer of water. The concentration profiles are shown in Figure IV.32 for a wind speed of 7.5 m/s and with mechanical waves. The profiles were averaged and plotted as a function of time in Figure IV.33. The difference in concentration with its saturated value decays in time like a diffusion process. The time constant is 0.0164 min^{-1} .

The dissolution process was investigated further by flow visualization. Sufficient dye was added to the hexanol so that it was readily visible on the water surface. Hexanol lenses formed on the surface with diameters of approximately 5 mm. Hexanol droplets were dispersed into the water by wind waves. Neither mechanical waves nor breaking waves were required for the droplet dispersion. At 7.5 m/s, the drops were dispersed to a depth of 10 to 15 cm. In contrast, the octane formed a uniform sheet on the water surface, and no droplets were formed.

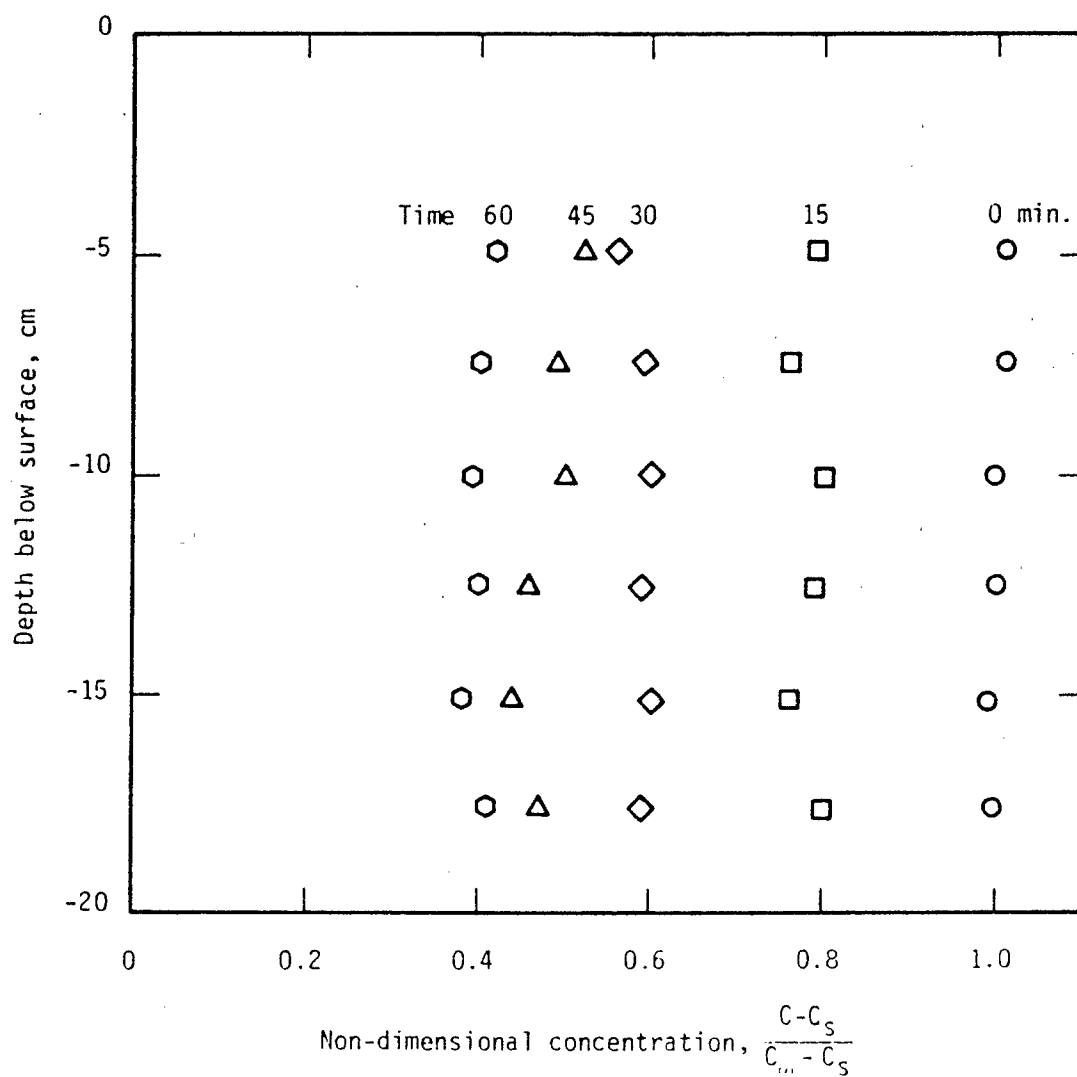


FIGURE IV.32 CONCENTRATION PROFILES OF HEXANOL IN WATER AT 7.5 m/s WIND SPEED WITH A WAVEMAKER

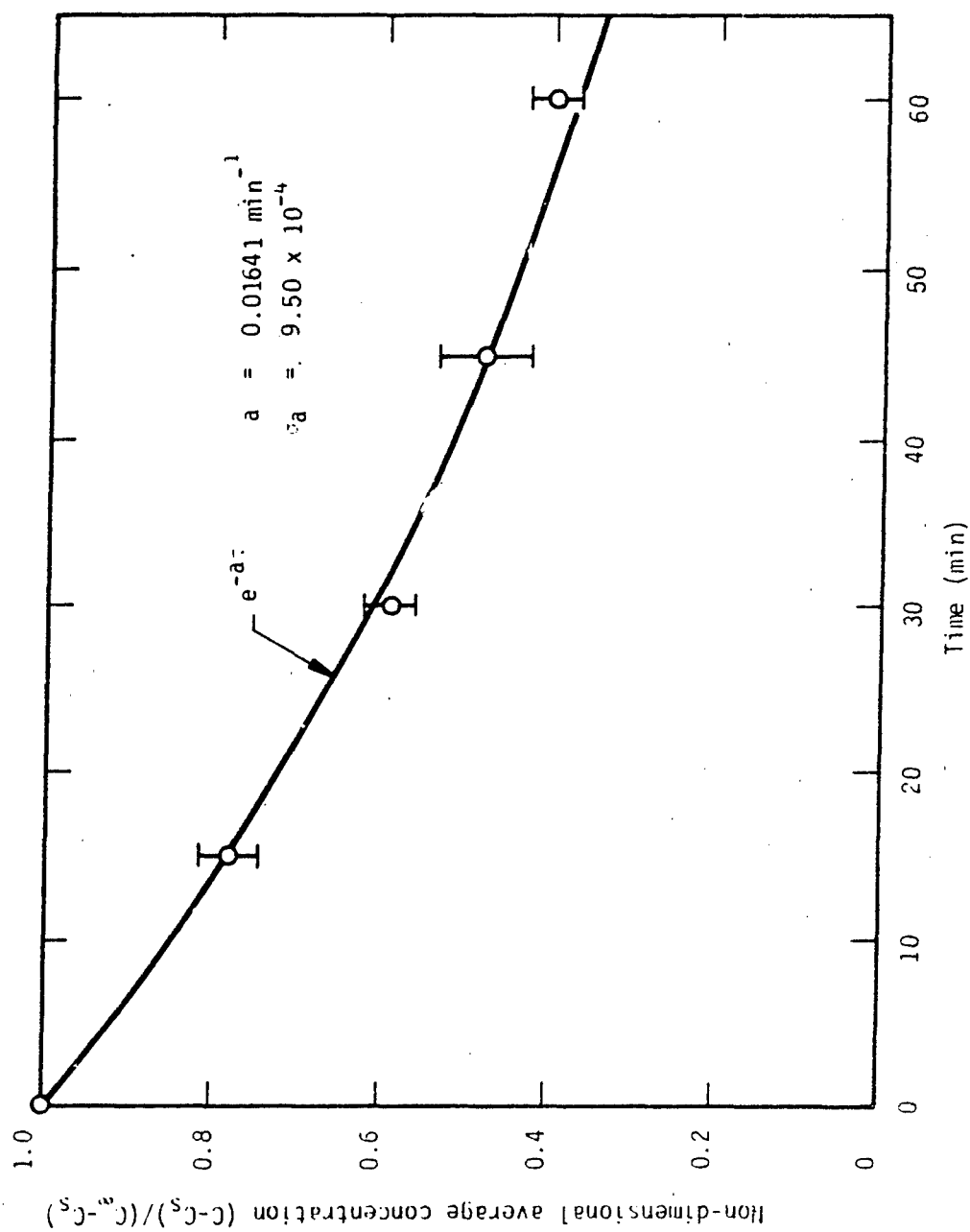


FIGURE IV.33 AVERAGE CONCENTRATION OF HEXANOL IN WATER TO A DEPTH OF 17.6 cm AT 7.5 m/s WIND SPEED WITH A WAVEMAKER

V. COMPARISON OF MODELS AND TESTS

V.1 Spreading Models

The tests described in Section IV.3.1 are sufficient to establish (1) the empirical constants K_{10} , K_{20} , K_{11} , and K_{21} in the spreading models for instantaneous and continuous spills in open water without a current, and (2) the empirical constants K_{12} and K_{22} in the spreading model of continuous spills in open water with a current. Although the empirical constants in the channel models cannot be established directly by any of the tests, their values can be inferred from the constants that can be established. According to the model derivation presented in Section III.2.4, for example, the lateral spreading of a slick formed by a continuous spill in a current is identical with the one-dimensional spreading of an instantaneous spill in a channel without a current; therefore, it is reasonable to assume that $C_{10} = K_{12}$ and $C_{20} = K_{22}$. In addition, as is shown below, there is little difference between the constants for instantaneous and continuous spills in open water without a current; it is reasonable to expect the same kind of relations for spills in a channel, so $C_{11} \approx C_{10}$ ($= K_{12}$) and $C_{22} \approx C_{20}$ ($= K_{22}$). Finally, if there is a current in a channel, the downstream spreading of the slick from a continuous spill is mostly due to the current; thus, there can be little error involved in assuming that $C_{12} = C_{10}$ and $C_{22} = C_{20}$. With these physically reasonable assumptions, all the empirical constants in the spreading models can be established by the test data.

After a portion of the test data is used to determine the empirical constants, the rest of the test data is used to verify the models.

Instantaneous Spill in Open Water (Negligible Evaporation). Typical data (from Test I.2.4) are shown in Figure V.1, in the form of the logarithm of the observed spill diameter plotted against the logarithm of the elapsed time. This form of plot is convenient to reveal a power-law type of dependency of the diameter on the time, as expected from Equations (III.3) and (III.5). It is evident that the data points do fall naturally on two straight lines, whose slopes are, to within the accuracy of the data measurements, equal to the theoretically-predicted values of 0.50 and 0.25 for gravity-inertial and gravity-viscous spreading. The fundamental assumptions



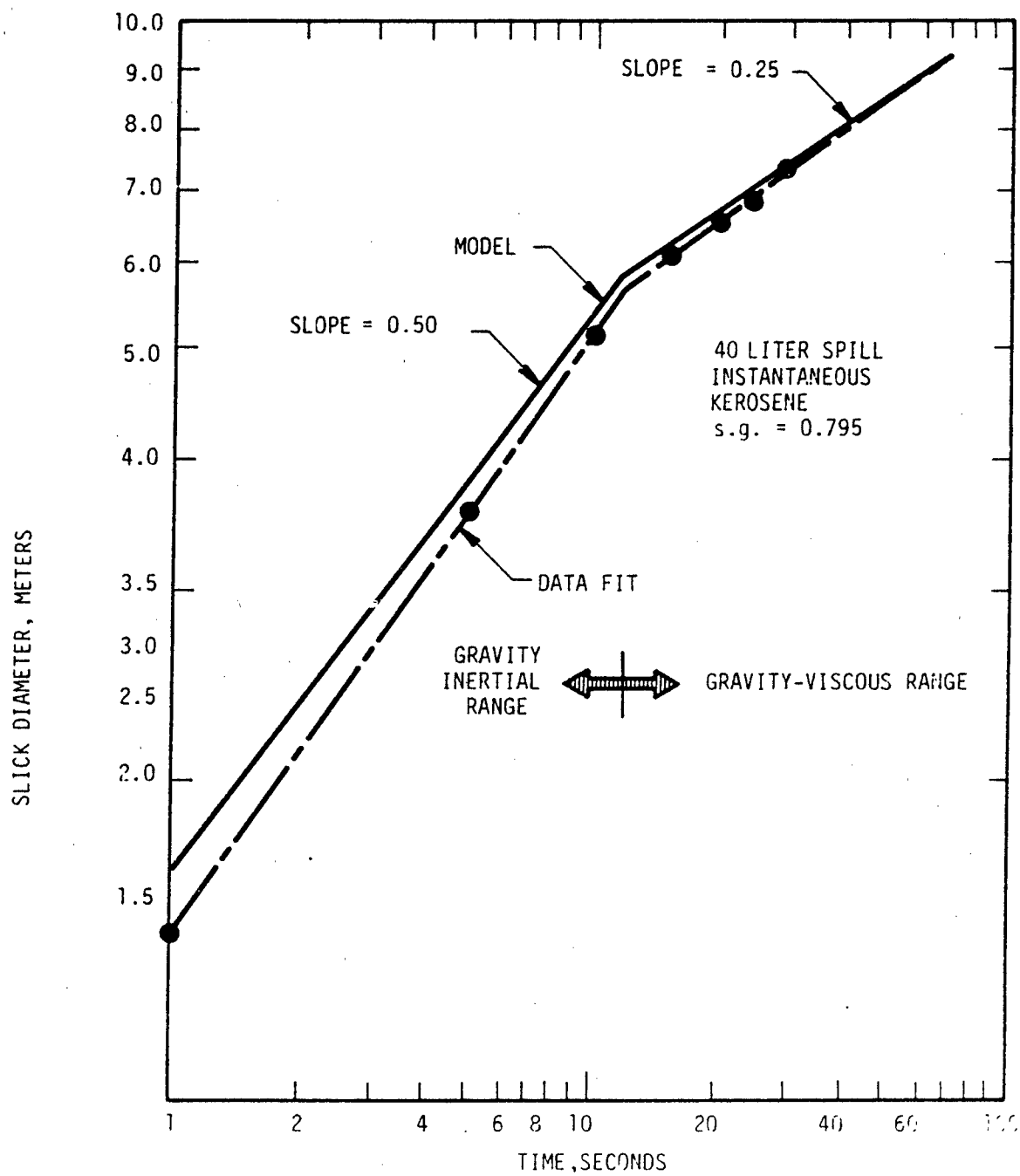


Figure V.1. Spreading Regimes for Instantaneous Spill Test I.2-4

of the model are therefore confirmed. (It ought to be noted that mass loss due to evaporation and dissolution is negligible for this chemical and test condition; hence, Equations (III.3) and (III.5) are applicable, rather than the more complicated version of the model given in Table III.2.) The time of transition from gravity-inertial to gravity-viscous spreading in Figure V.1 and the slick diameter at that time are used to compute the empirical constants; the result is that $K_{10} = 1.53$ and $K_{20} = 1.21$. Both constants are of order unity as expected. Previous semi-analytical estimates gave $K_{10} = 1.14$ and $K_{20} = 0.98$ [7]. The present values are slightly larger than the previous estimates but the ratio K_{20}/K_{11} is about the same for both.

Figures V.2 through V.4 compare predictions of the model with $K_{10} = 1.53$ and $K_{20} = 1.21$ to test results for a variety of spill sizes and chemical densities. (Again, the evaporative loss of mass from the slick is negligible, so Equations (III.3) and (III.5) can be applied directly.) The predictions match the data very well, especially for the larger spills where any influence of a lack of true "instantaneous" initial conditions is small.

Continuous Spill in Open Water Without a Current (Negligible Evaporation). The test data from a typical test (Test II.4.4) are plotted in log-log form in Figure V.5. Just as for the instantaneous spills, the data points fall on two straight lines whose slopes are in agreement with theory. (Mass loss from the slick is negligible, also as before.) From the observed transition time and diameter, the computed empirical constants are $K_{11} = 1.24$ and $K_{21} = 1.09$. There are no previous data or analyses to which these values can be compared.

Figures V.6 through V.9 show comparisons of the revised model to tests with a variety of discharge rates and chemical densities. The predictions overall match the data well, although the comparison for the hexanol spill shown in Figure V.8 is not good near the end of the discharge period. (In many of the tests, the behavior of hexanol was noticeably different from that of the other chemicals. Although the reasons for the differences could not be isolated, it is believed that the large spreading coefficient of hexanol

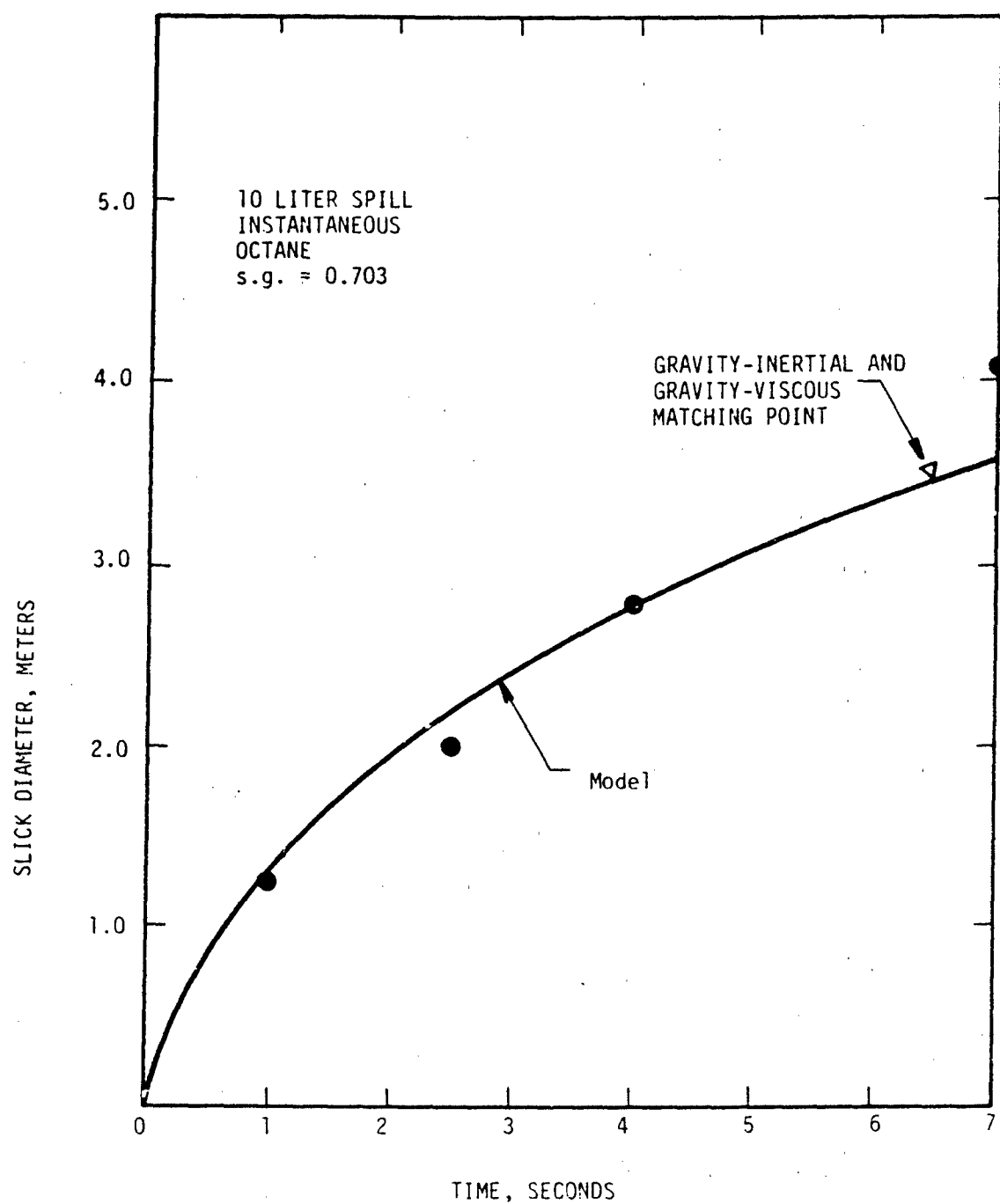


Figure V.2 Comparison of Model and Test for Instantaneous Spill Test 1.1-2

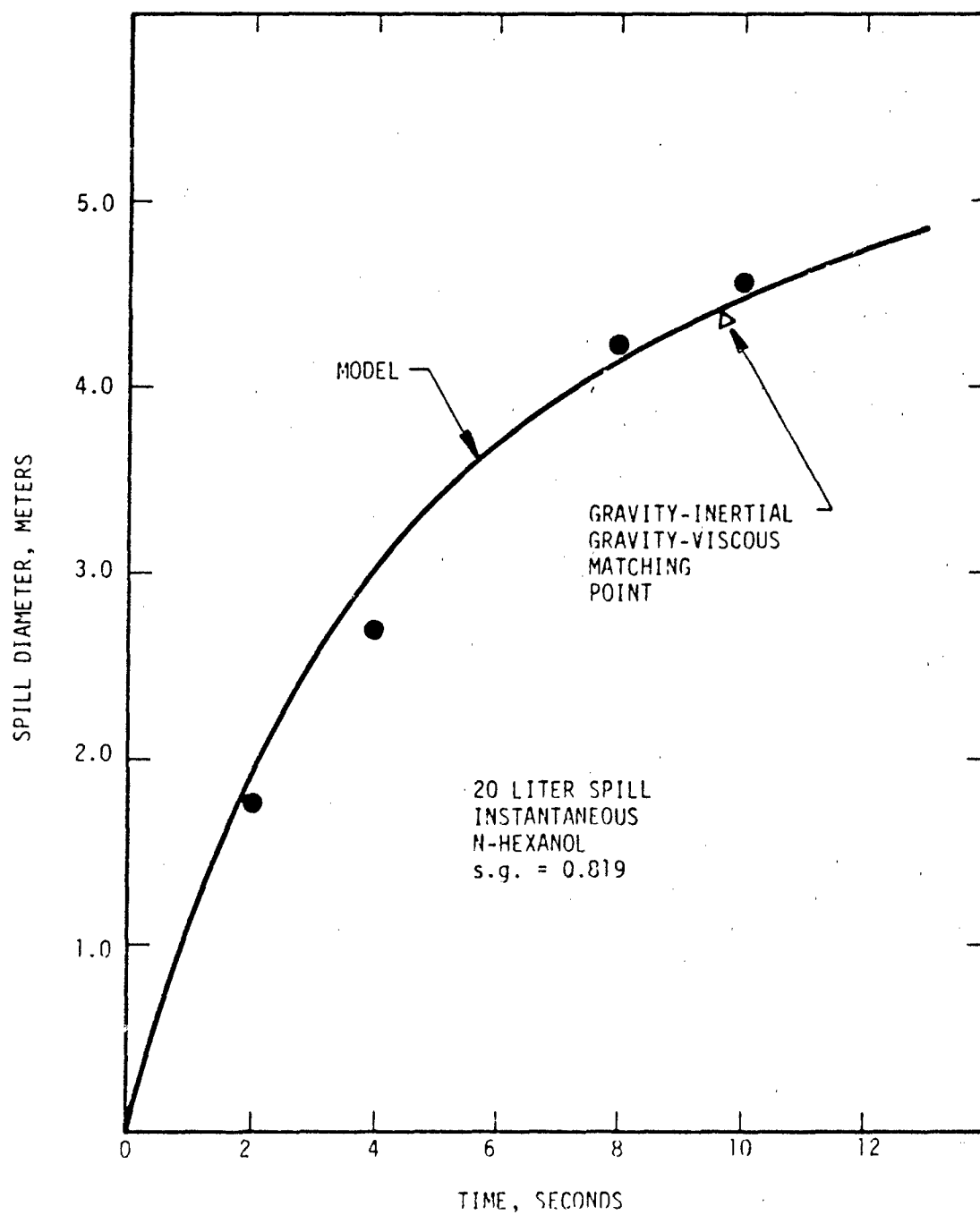


Figure V.3. Comparison of Model and Test for Instantaneous Spill Test 1.3-3

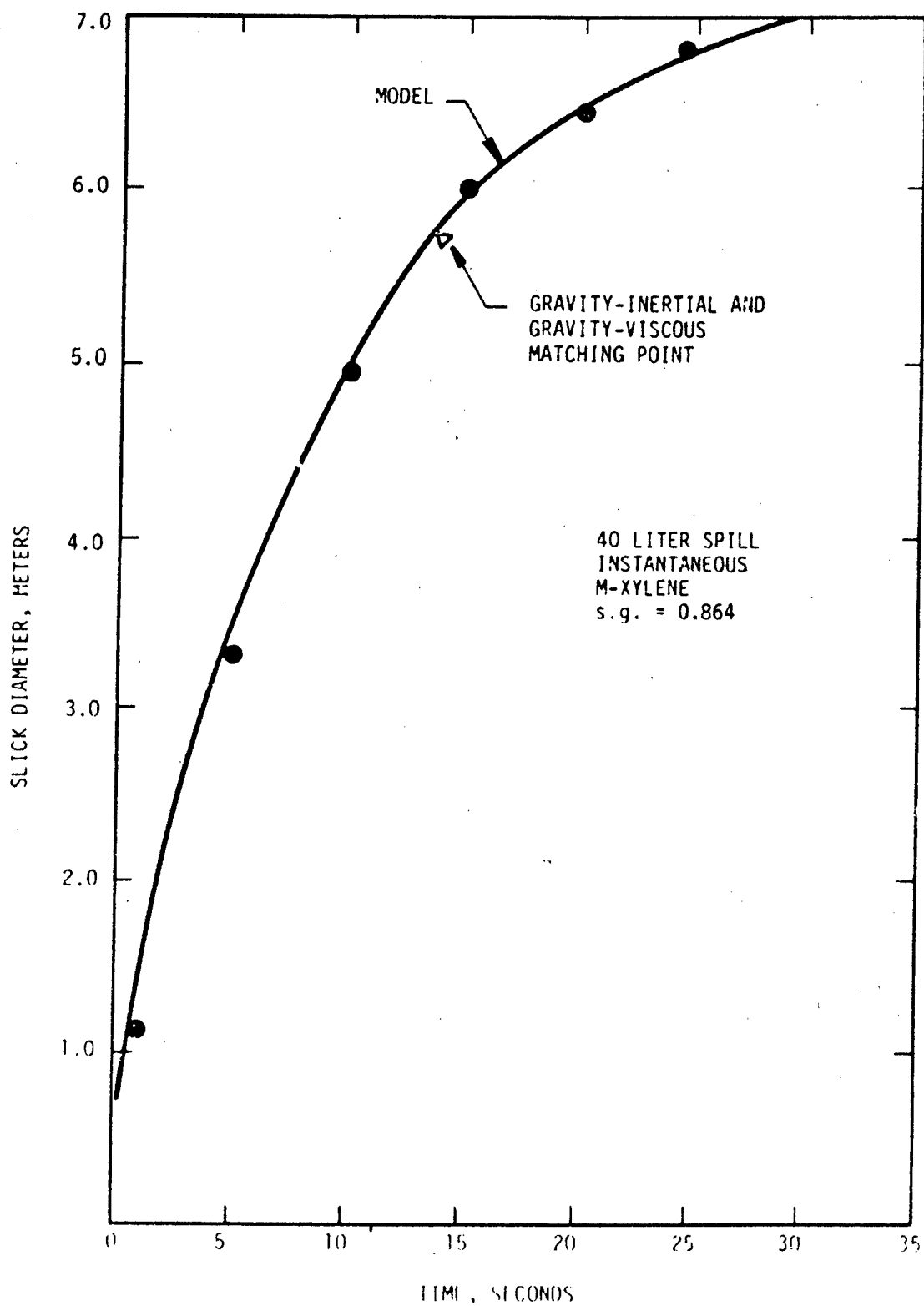


Figure V.4 Comparison of Model and Test for Instantaneous Spill Test I.5-4

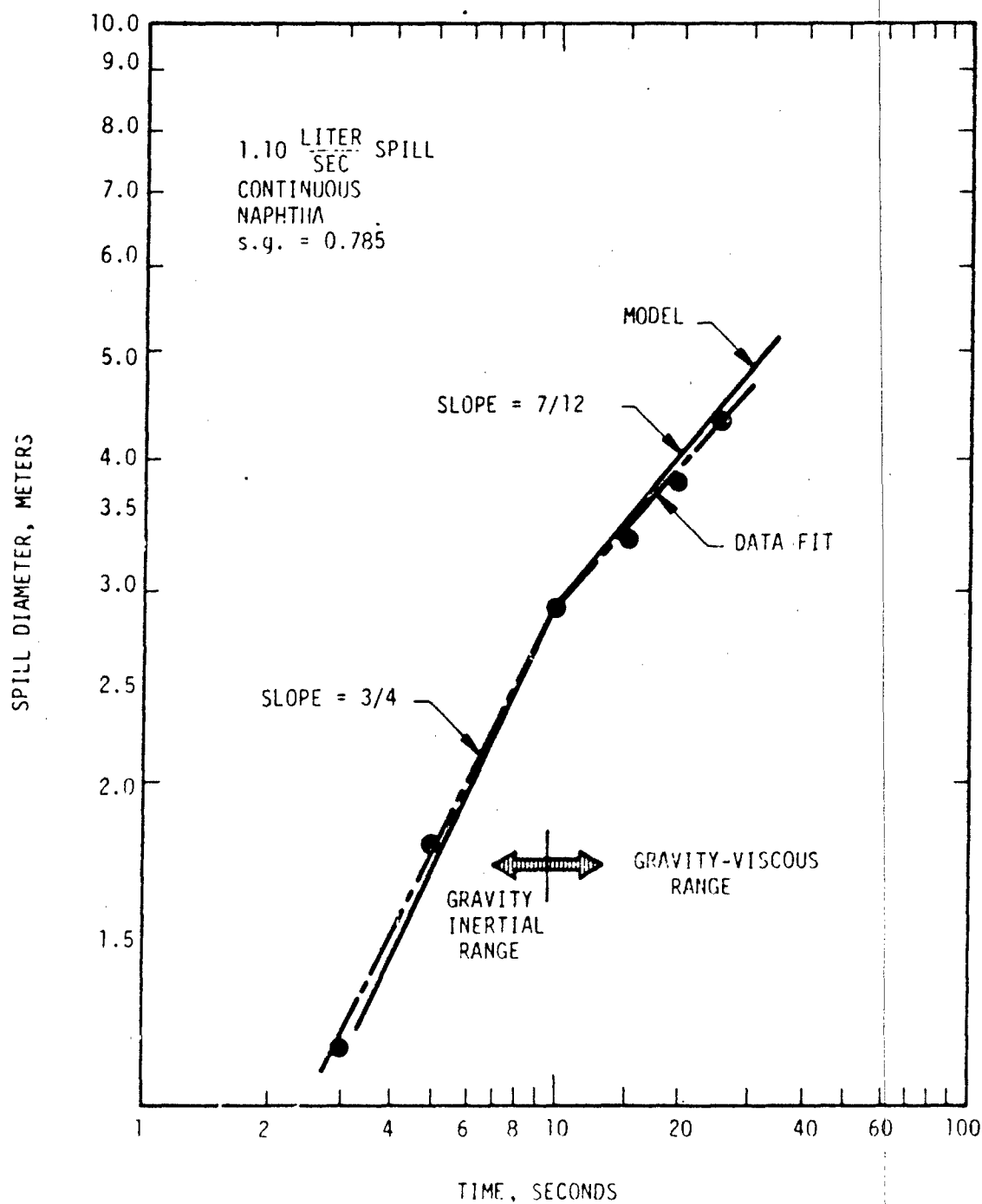


Figure V.5. Spreading Regimes for Continuous Spill Test II.4-4

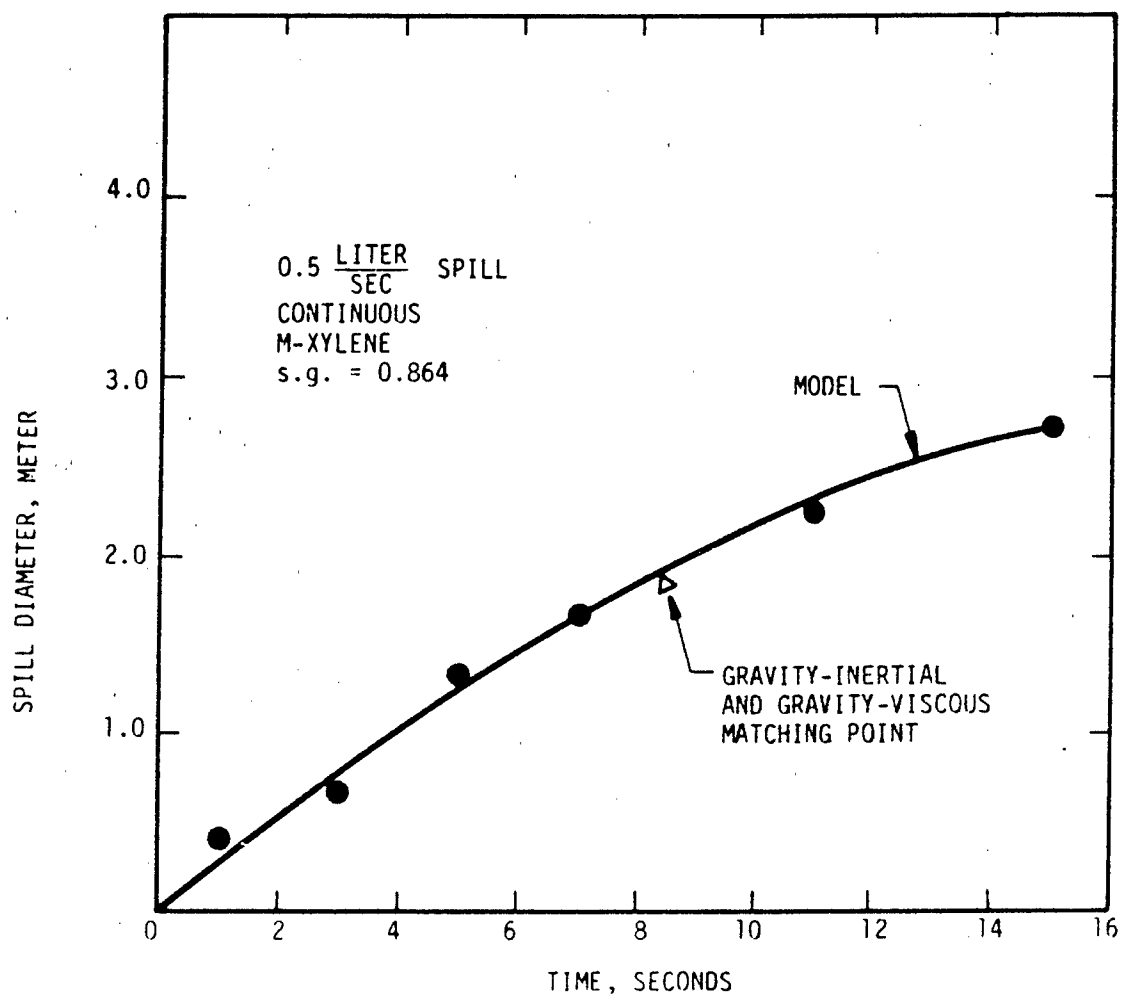


Figure V.6 Comparison of Model and Test for Continuous Spill Test II.5-1

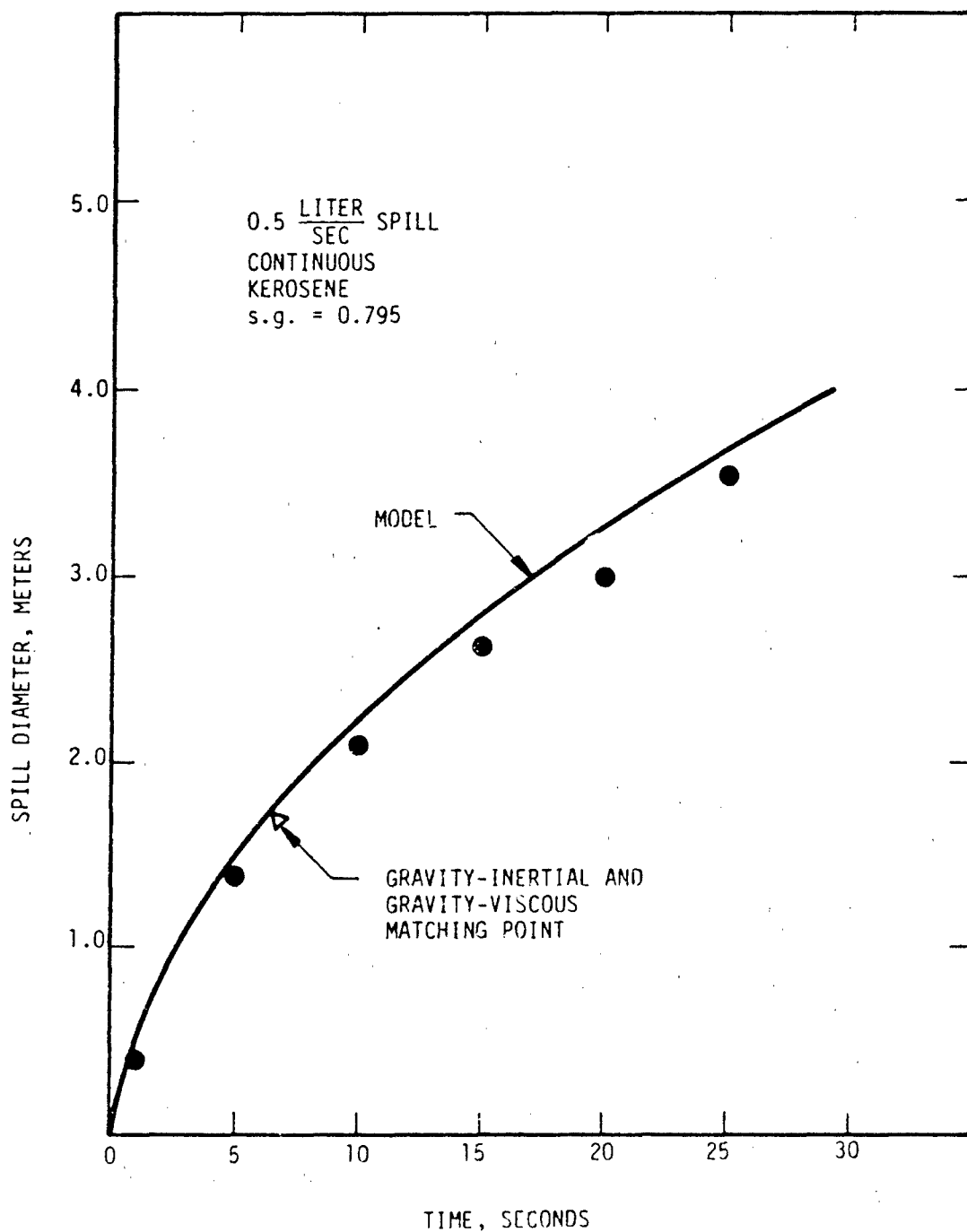


Figure V.7 Comparison of Model and Test for Continuous Spill Test 11.2-1

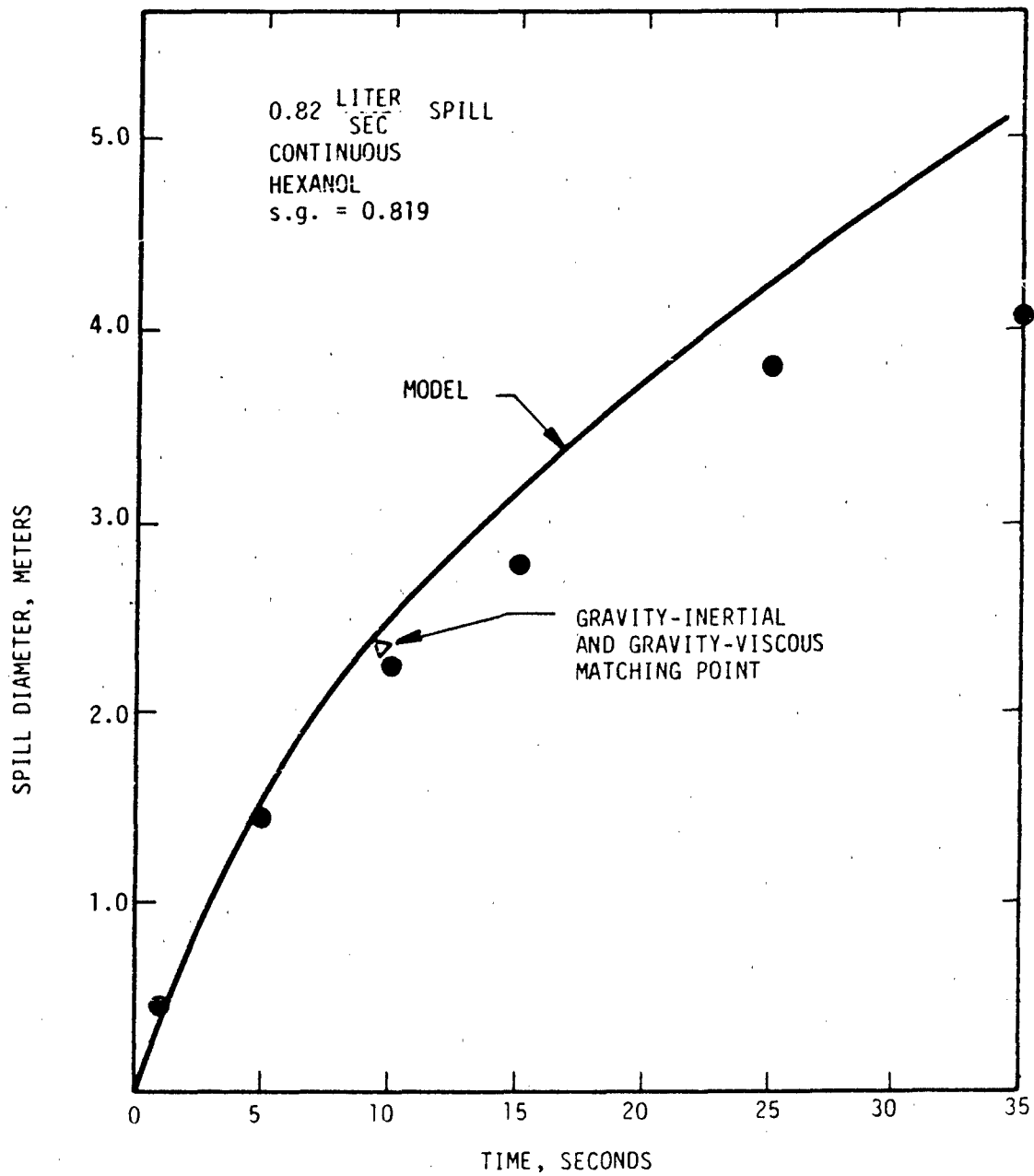


Figure V.8 Comparison of Model and Test for Continuous
Spill Test II.3-2

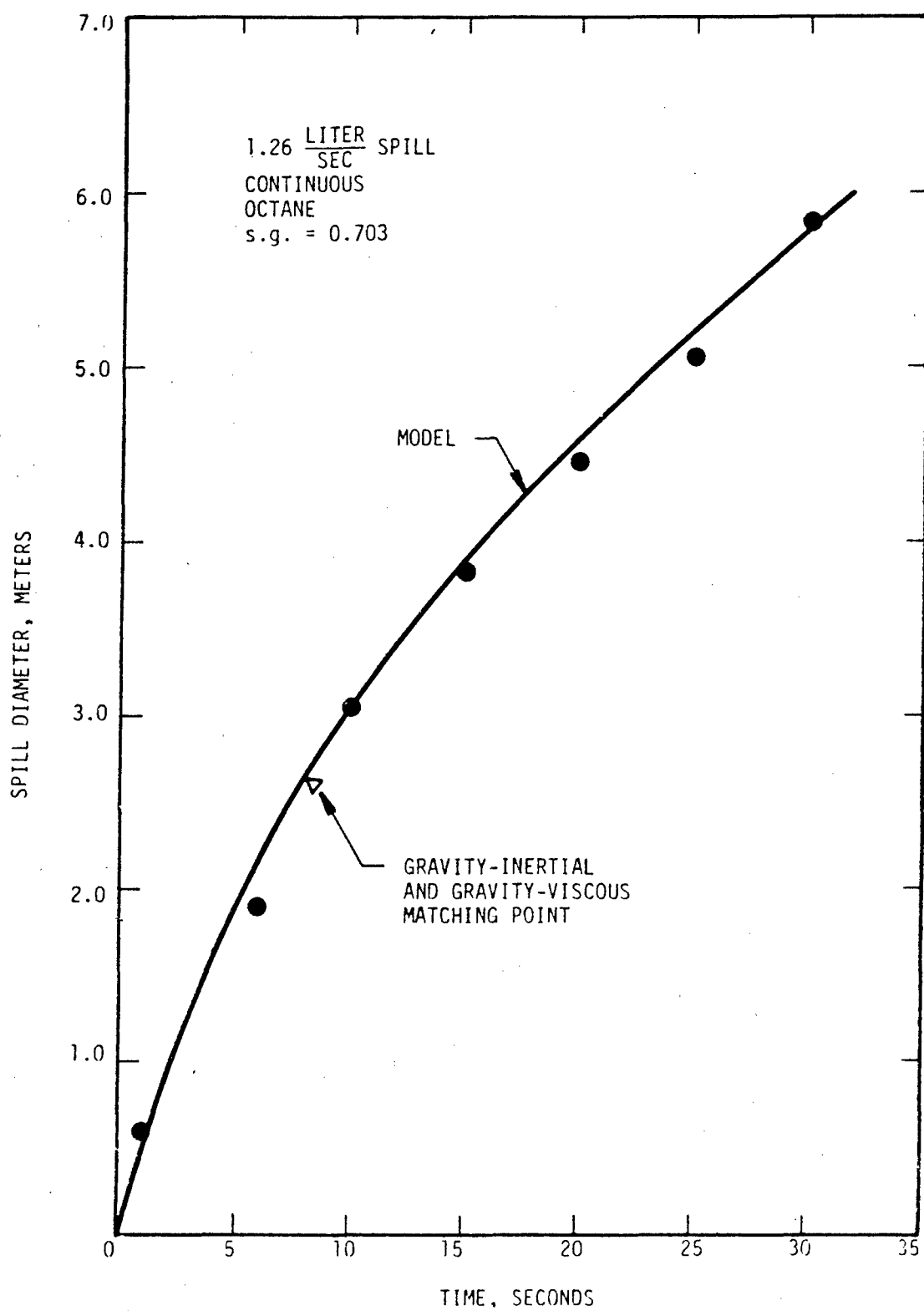


Figure V.9 Comparison of Model and Test for Continuous Spill Test II.1-4

caused a rapid growth of the thin slick and a subsequent change of the surface spreading properties in the water ahead of the thick slick. There was some tendency noted for hexanol to form lenses in the small-scale spreading tests.)

Continuous Spill in Open Water With a Current (Negligible Evaporation).

Although these tests were conducted in a channel, data were measured only during the time when the thick slick was still well away from the channel walls. The test data therefore correspond to a discharge in open water with a current.

The results of a typical test (Test V.1.4) are shown in log-log form in Figure V.10. Once again, the test data points fall on two straight lines having the theoretically-predicted slopes for gravity-inertial and gravity-viscous spreading when mass losses are negligible. Because there was somewhat more scatter in the data from test-to-test than for the open-water, zero-current tests, the data from two tests were used to establish the empirical constants in the spreading model. The best fit to the data gives $K_{12} = 2.37$ and $K_{22} = 3.65$. As mentioned previously, the empirical constants for the one-dimensional spreading of an instantaneous spill are theoretically identical to $K_{12} = K_{22}$. Previous estimates of the constants for one-dimensional spreading of instantaneous spills are $C_{10} = 1.39$ to 1.50 and $C_{20} = 1.39$ to 1.50 [7]. The present constants are thus about twice as large as the previous estimates, according to this idea of similarity between the two forms of spreading. The previous estimates, which are based on semi-analytical theories and small-scale test results, may be in error; on the other hand, the two types of spreading may be qualitatively similar but require different constants.

Figures V.11 through V.14 show comparisons of the revised model to test results for a variety of discharge rates, chemical densities, and currents. The comparisons are sufficiently close to verify the model, although not quite as close as for the tests conducted in the large basin. The slightly poorer correlation is perhaps not surprising considering the scatter in the data inherent in measuring slick widths from video recordings.

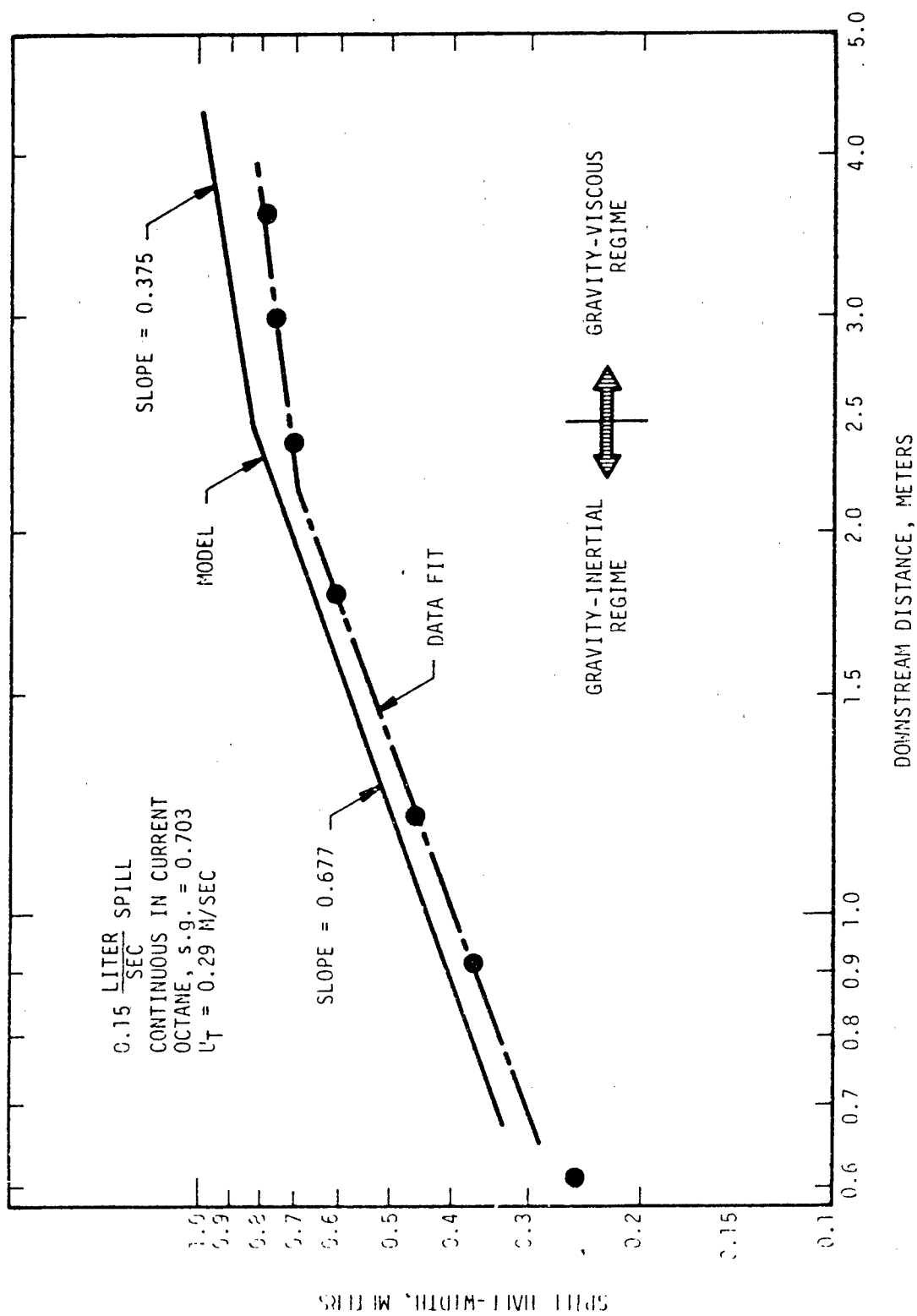


Figure V.10 Spreading Regimes for Continuous-Spill-In-A-Current Test V.1-4

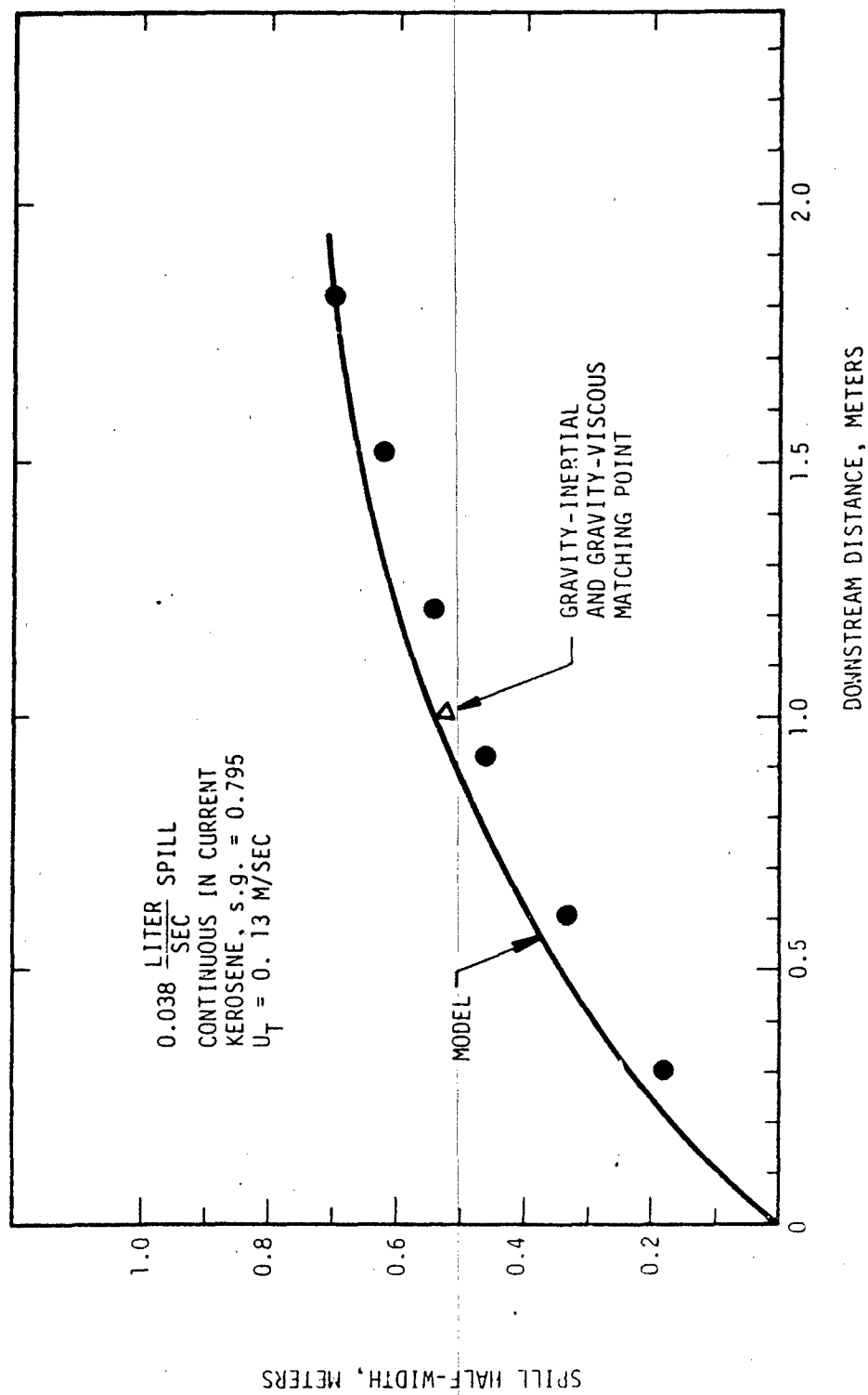


Figure V.11 Comparison of Model and Test for Continuous-Spill-in-a-Current Test V.2-1

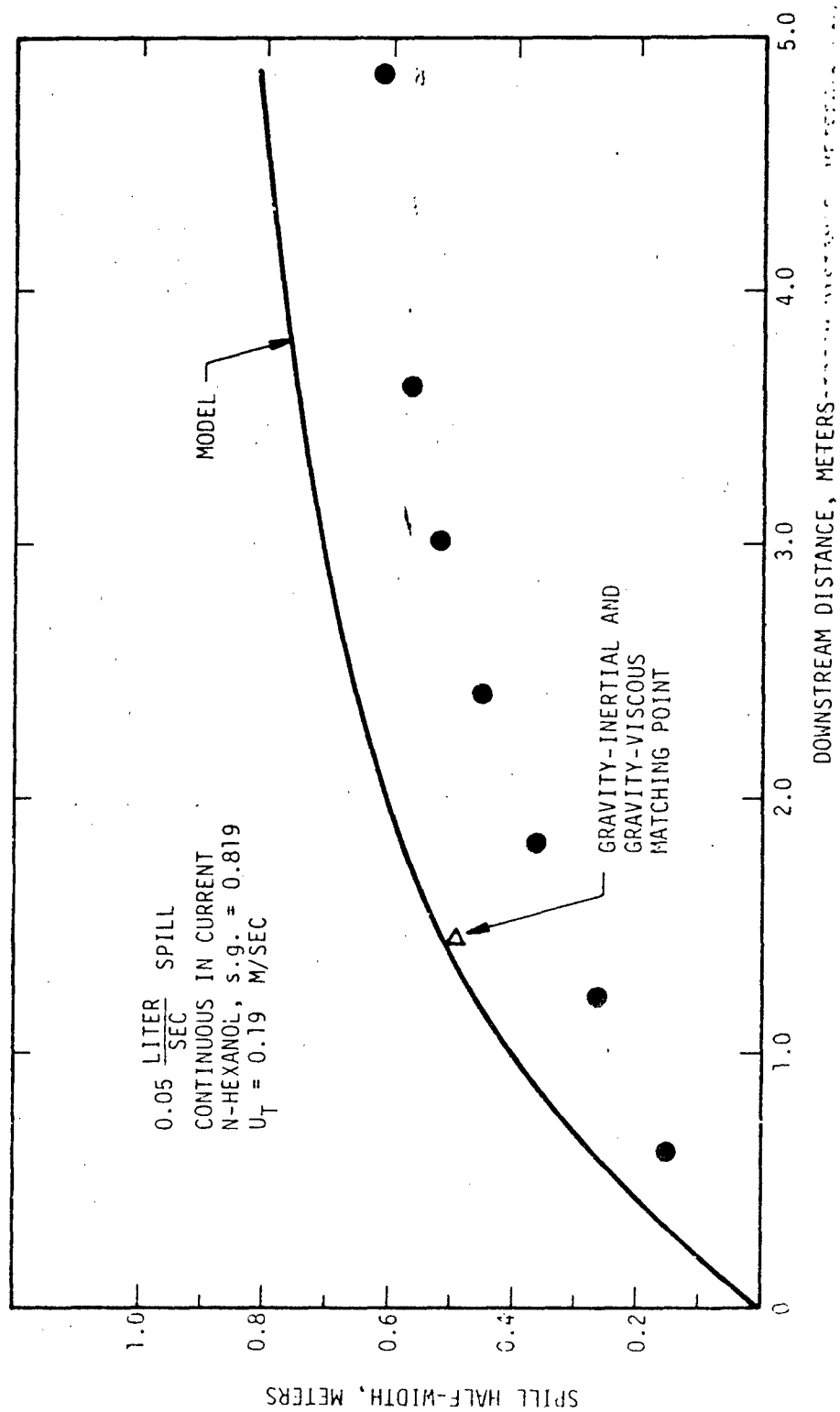


Figure V.12 Comparison of Model and Test for Continuous-Spill-in-a-Current Test V.3-2

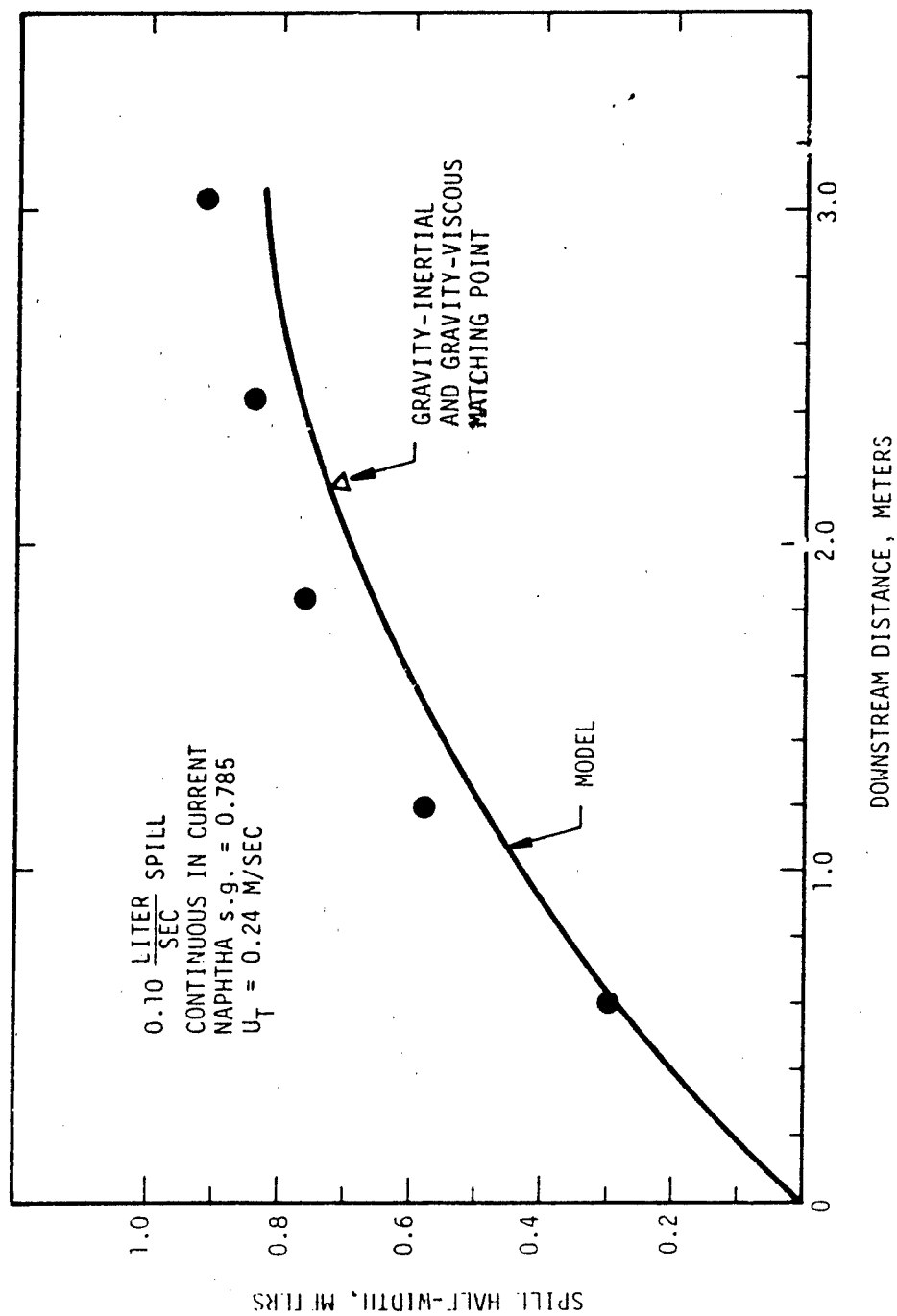


Figure V.13 Comparison of Model and Test for Continuous-Spill-in-a-Current Test V.4-3

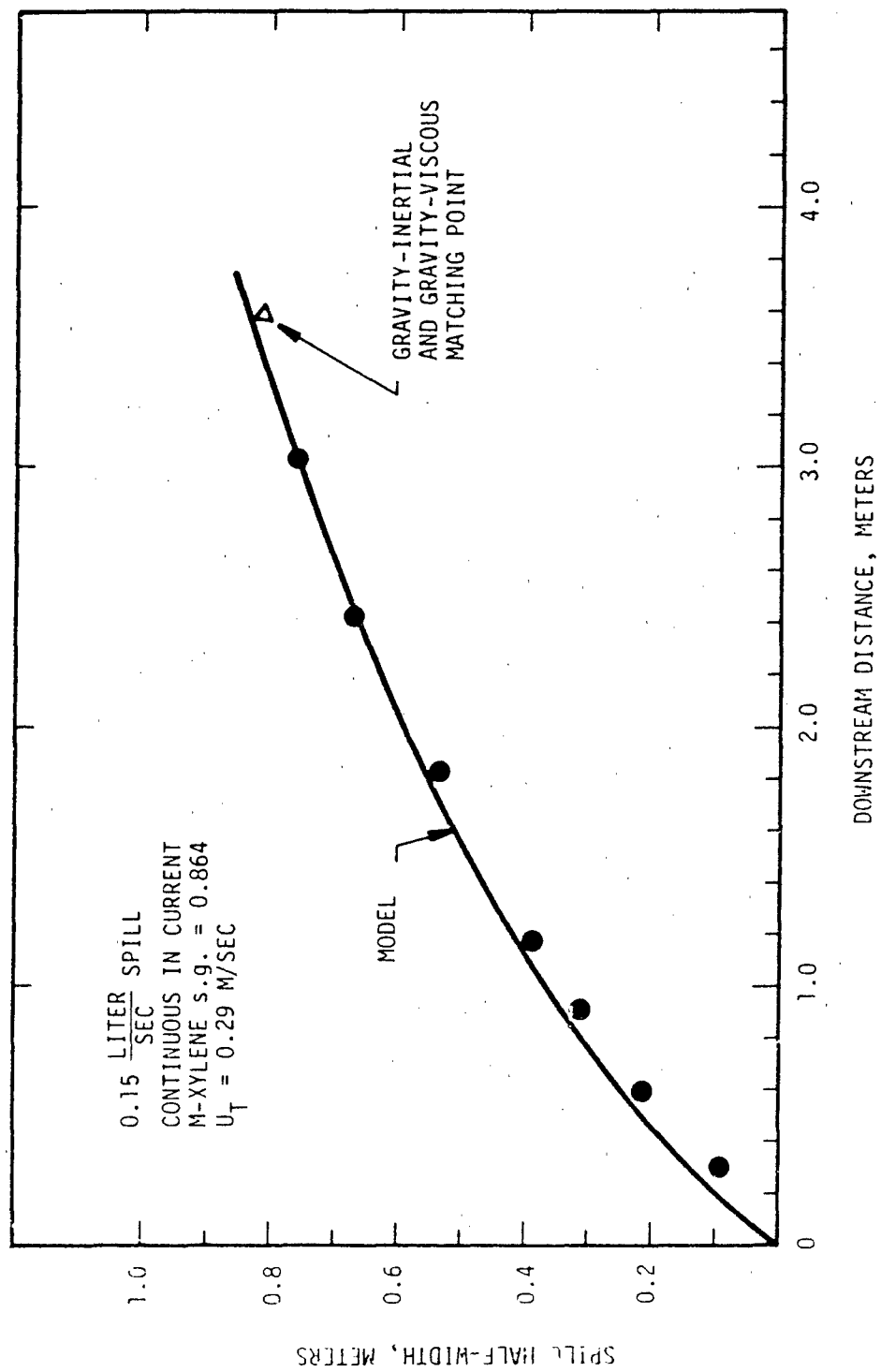


Figure V.14 Comparison of Model and Test for Continuous-Spill-in-a-Current Test V.5-4

V.2 Evaporation Rate Model

The proposed evaporation model appears to be adequate for the present application without any changes. These experiments are probably the first where mass transfer of a hydrocarbon is measured by the profile method. The differences between theory and experiment are likely within the uncertainties of the experimental methods. In future experiments, the inflow and outflow of chemical from the water surface should be measured, and the effects of slick thickness evaluated. Also, the influence of spreading coefficient on waves should be evaluated since such roughness effects are coupled with mass transfer.

V.3 Dissolution Rate Model

The boundary layer model suggested for dissolution may be adequate for certain classes of highly insoluble hydrocarbons such as hexane and octane. For other chemicals such as hexanol, droplet dispersion in the water may be the dominant mechanism for dissolution, and breaking waves are not required necessarily for droplet dispersion. No models are currently available which adequately describe such a mechanism. Probably the interfacial tension of the chemical with water is an important physical property.

V.4 Spreading Models With Evaporation

As discussed in Section V.1, spreading tests with non-volatile chemicals established the empirical constants in the spreading models, and the wind tunnel and wind-wave tunnel tests discussed in Section V.2 established the empirical constants in the evaporative mass-transfer coefficient correlation. In this section, the effects of spreading and evaporation are combined, and the model predictions are compared to tests of instantaneous and continuous spills of volatile chemicals in the large basin. Spreading tests that adequately demonstrate the effects of evaporation are difficult to conduct since the high wind needed to cause significant evaporation also tends to move the slick to the boundary of the basin rapidly. The wind also distorts the shape of the slick so that it is more difficult to determine the slick area and the average diameter than it is for tests with little or no wind.

Figure V.15 shows a comparison of the data for a large spill of pentane, the most volatile of the test chemicals, to the prediction of the model with evaporation included, as well as to predictions with the evaporation suppressed by setting the wind speed to zero. Although the model fits the data to within the scatter in the tests that were used to establish the empirical spreading coefficients, the comparison is not as close as the typical comparison with non-volatile chemicals. This lack of good comparison is not believed to be a deficiency in the model but, as mentioned above, due to the difficulty in computing an accurate average diameter for a slick that moved a significant distance away from the source during the test.

Figure V.16 shows a typical comparison of model and data for a continuous spill. The spreading model for these test conditions falls into the exceptional category discussed previously in Section III.2.4, namely, the case where U_T is small in comparison to the gravitationally-induced spreading velocity. The model assumes a triangular shape for the slick when $U_T > 0$ (no matter how small U_T is), although the observed slick was elliptical and surrounded the source rather than being totally downwind of it. Thus, a first estimate of the spill size as a function of time was made by setting the wind speed equal to zero in order to predict a radial spreading. Although the model then matches the observed shape very well, evaporative losses are not predicted since the assumed wind speed is zero. Thus, to estimate the mass lost by evaporation, the model of an instantaneous spill of the same total volume was exercised twice, once with the true wind speed and once with the wind speed set equal to zero. The difference in evaporative losses and slick diameters were then applied to the continuous spill results. The comparison to the data is not quite so close as was obtained in general with the non-volatile chemical tests, but in this case the model over-predicts the results.

Altogether, it is concluded that the models adequately predict the effects of evaporation on the spreading of instantaneous and continuous spills.

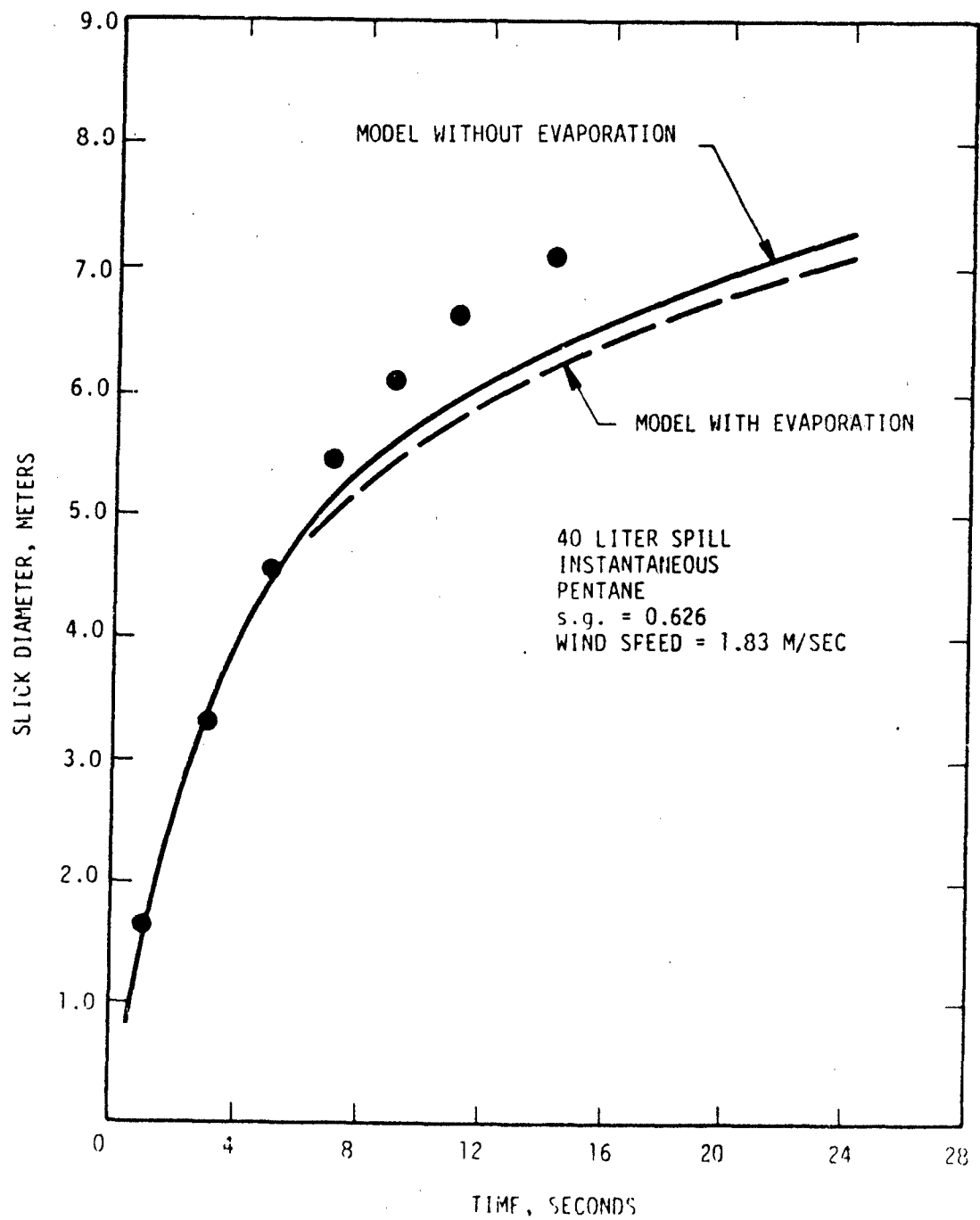


Figure V.15 Comparison of Model and Test for Instantaneous Volatile Spill Test III.1-3

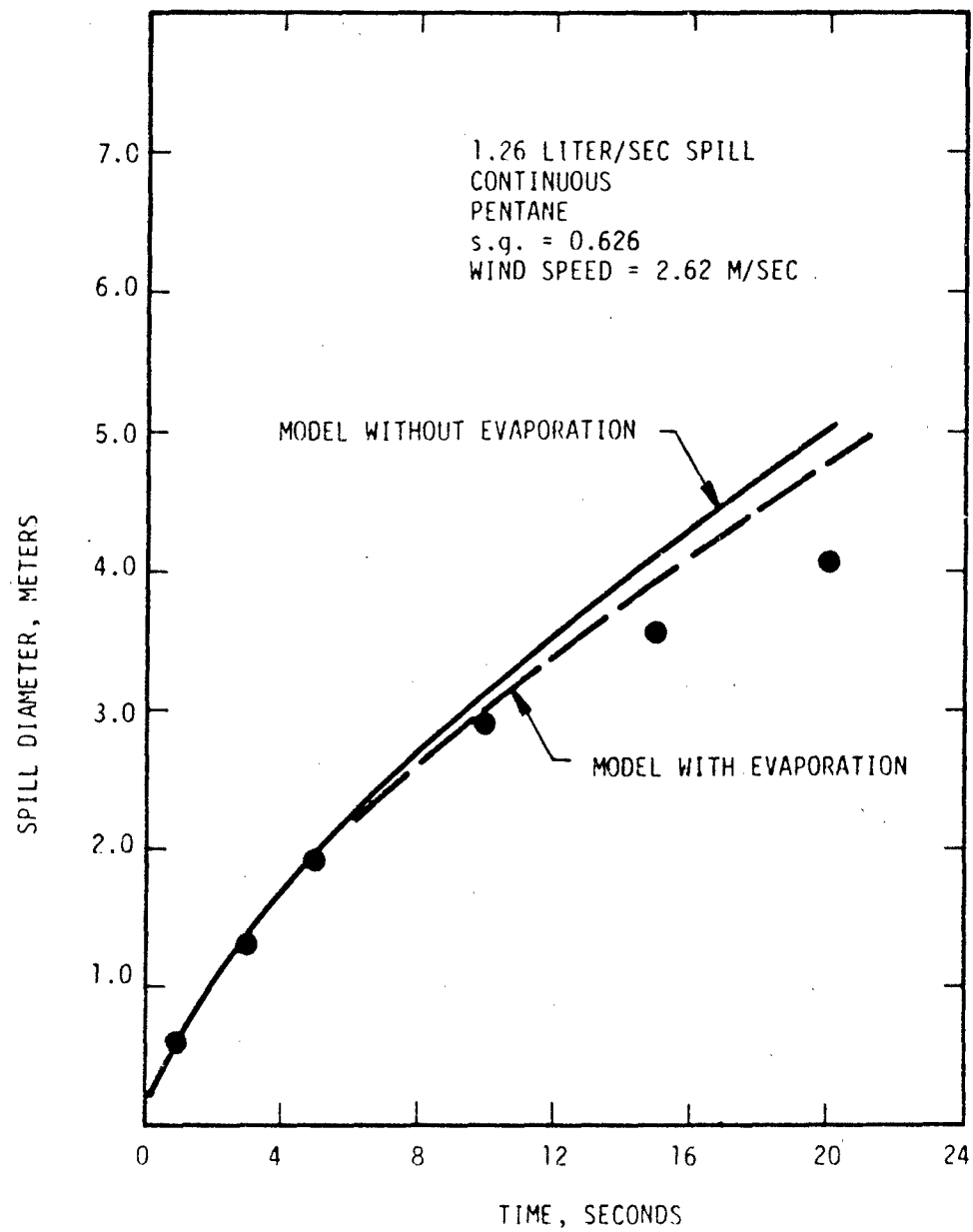


Figure V.16 Comparison of Model and Test for Continuous Volatile Spill Test IV.1-4

VI. DEMONSTRATION CASES

The input and output data for five different examples of the computerized models are presented in this section. Table VI.1 gives a brief description of each of the examples. They show most of the features of the models and were selected to highlight potential difficulties in interpreting the computed results.

Table VI.2a is an exact copy of the user "prompts", the input data, and the input printout of Demonstration Case No. 1 as they would appear on a terminal screen. The data following each ? are the input supplied by the user. Most of the required input is self-explanatory. The "time increment" requested at the fourth prompt is the integration time step; a value of 1.0 second is suggested and has been found to be satisfactory for spills of practical size and duration, but here the spill is quite small so a shorter time step is used. The "run time" requested at the fifth prompt is the maximum length of time that the slick motion will be followed; the computations will cease at this time unless one of the other termination criteria is met first. (The criteria are: slick has evaporated and/or dissolved to zero thickness; the thickness of the thick slick is less than the allowed value given as input; or the slick has reached a lake boundary or a coast.) The "minimum thickness of thick slick" requested at the sixth prompt is the user's estimate of the thickness below which the thick slick begins to spread predominantly in the surface tension-viscous mode (i.e., as a thin slick); computations cease when the thickness falls below the input value, and a notification is printed in the output. The present experiments indicate that 0.0001/meters is an appropriate value for this thickness. The "thickness of thin slick" requested is normally the same as the minimum allowed value of the thick slick thickness although the equality is not specifically required. Later in the input, the requested wind direction is referenced to the positive x-axis. The last input, the printout time step, is the time duration between printouts of the results; only forty printouts are allowed, so the user should make sure that the ratio of run time to printout time step is not larger than forty.



TABLE VI.1 DESCRIPTION OF DEMONSTRATION CASES

Chemical Name	Type of Spill	Waterbody Description	Wind and Waves
1. Pentane	Instantaneous $V_0 = 0.04 \text{ m}^3$	Circular Lake $R = 20 \text{ m}$; depth = 0.3 m $U_C = 0$	$V_W = 1.83 \text{ m/s}$ Wave height = 0.01 m
2. Pentane	Continuous $\dot{m}/\rho_0 = 0.001 \text{ m}^3/\text{s}$ for 60 sec.	Circular Lake $R = 20 \text{ m}$; depth = 0.3 m $U_C = 0$	$V_W = 1.94 \text{ m/s}$ Wave height = 0.01 m
3. Octane (but with $\rho_0 = 800$ kg/m^3)	Continuous $\dot{m}/\rho_0 = 0.0333 \text{ m}^3/\text{s}$ for 30 minutes	Circular Lake $R = 20,000 \text{ m}$; depth = 100 m $U_C = 0.51 \text{ m/s}$	$V_W = 3.0 \text{ m/s}$ at 19.7° ; Wave height = 0.5 m
4. Octane	Continuous $\dot{m}/\rho_0 = 0.1 \text{ m}^3/\text{s}$ for 60 minutes	Channel $W = 50 \text{ m}$; depth = 10 m $U_C = 1.0 \text{ m/s}$	$V_W = 3 \text{ m/s}$ at 135°
5. Octane	Continuous $\dot{m}/\rho_0 = 0.05 \text{ m}^3/\text{s}$ for 60 minutes	Irregularly-Shaped Lake Depth = 100 m U_C is a function of space and time.	$V_W = 2.0 \text{ m/s}$ at 15° ; Wave height = 0.5 m

TABLE VI.2a INTERACTIVE INPUT FOR
DEMONSTRATION CASE NO. 1

ENTER THE TITLE FOR THIS RUN..
? DEMO NO. 1
INPUT THE AMBIENT TEMPERATURE IN CELSIUS.
? 20
INPUT THE BAROMETRIC PRESSURE IN MILLIBARS
OR ZERO, 0, FOR THE STANDARD SEA LEVEL PRESSURE
OF 1013.25 MB.
? 0
INPUT THE TIME INCREMENT IN SECONDS. TRY 1.0.
? .1
INPUT THE DESIRED RUN TIME IN MINUTES
? 1.33333
INPUT MINIMUM ALLOWABLE THICKNESS OF THICK SLICK IN METERS.
? 1.E-4
INPUT THICKNESS OF THIN SLICK IN METERS.
? 1.E-4

* WATER BODY DESCRIPTION *

IS SPILL IN RIVER OR CHANNEL? Y/N
? N

IS IT A LAKE? Y/N
? Y

IS IT A CIRCULAR LAKE? Y/N
? Y

GIVE THE RADIUS AND DEPTH OF THE CIRCULAR LAKE
(UNIT : METER)
? 20,0.3

IS THERE CURRENT? Y/N
? N

IS THERE WIND IN THE AREA ? Y/N
? Y

IS WIND SPEED CONSTANT? Y/N
? Y

INPUT WIND SPEED (METER/SEC) AND DIRECTION
ANGLE (DEGREES)
? 1.83,0

INPUT MEAN WAVE HEIGHT.(METER)
DEFAULT VALUE (EQ.(III.32) OF REPORT) IS USED
BY INPUTTING -1.

? .01
GIVE SPILL COORDINATES X AND Y, IN METERS
? 0,0

* SPILL TYPE *

WE HAVE STANDARD PROPERTIES FOR THE FOLLOWING CHEMICALS

1. ALLYL CHLORIDE	2. BENZENE
3. BUTADIENE (1,2)	4. BUTYL ACETATE (ISO)
5. BUTYL MERCAPTAN (N)	6. CHLOROBUTA-1-3-DIENE
7. CYCLOHEXANE	8. CYCLOHEXENE
9. DIPROPYL ETHER (ISO)	10. ETHYL CHLORIDE

TABLE VI.2a (CONTD)

11. ETHYL MERCAPTAN	12. HEPTANE (N)
13. HEXANE (N)	14. METHYL CYCLOHEXANE
15. NONANE (N)	16. OCTANE (N)
17. PENTANE	18. TOLUENE
19. TRIMETHYLBENZENE	20. XYLENE (M)

ENTER THE NO. YOU WANT OR
 NEGATIVE VALUE - IF YOU WANT TO INPUT THE PROPERTIES
 99 - IF THE CHEMICAL IS NOT ON THE LIST

? 17

BAROMETRIC PRESSURE : 1013.250 MILLIBAR

TEMPERATURE : 20.000 DEGREES C

CHEMICAL NAME IS: PENTANE

CHEMICAL DENSITY = 626.00 KG/CU.M.

MOLECULAR WEIGHT = 72.151 KG/KG-MOLE

DIFFUSION COEFF (AIR) = .75000E-05 SQ.M./SEC

DIFFUSION COEFF (WATER) = .84000E-09 SQ.M./SEC

CHEMICAL VAPOR PRESSURE = 58772.29 NEWTON/SQ.M.

SOLUBILITY IN WATER = .36 KG/CU.M.

THE INTERFACE TENSION WRT AIR IS .16046E-01 NEWTON/M.

THE INTERFACE TENSION WRT WATER IS .50200E-01 NEWTON/M.

THE SPREADING COEFFICIENT IS .65142E-02 NEWTON/M.

IS SPILL 1. INSTANTANEOUS OR 2. CONTINUOUS?

? 1

INPUT THE TOTAL SPILLED VOLUME (CUBIC METER)

? .04

INPUT THE PRINTOUT TIME STEP IN MINUTES.

? .066667

Table VI.2b shows some of the computed results for Demonstration Case No. 1. (The printout of the input conditions is not given in the table, only the computed results. The actual printout includes the input.) First, the results at the end of the gravity-inertial phase (0.14445 minutes, or 8.7 seconds in this case) are printed. Then the regular printout routine begins at about 12 seconds, which is the first printout time greater than the gravity-inertial spreading time that is an integral multiple of the requested printout time step. (The printout occurs at 12.073 seconds rather than exactly 12 seconds because the time step of the numerical integration scheme rarely coincides with the requested printout time step.) The printout gives information about the thick slick size, thickness, and mass, the position of the center of the slick, and the mass of evaporated and dissolved chemical. Similar printout is given every four seconds (although the results between 16 seconds and 80 seconds are not included here, for brevity) until the requested run time is exceeded. None of the other termination criteria is met.

Table VI.3a shows the input for a continuous spill that is otherwise similar to Demonstration Case No. 1. The computed results are shown in Table VI.3b. Again, the results at the end of the gravity-inertial spreading phase are given first. Note that for a continuous spill, the output includes data about the thin slick. Because there is no current, the transport velocity is due only to the wind and is thus very small. As a result, the triangular slick is much wider (17.0 meters) than it is long (3.55 meters). In reality, the slick formed under such small transport velocity conditions would be roughly elliptical and would enclose the spill source, rather than being entirely downstream of it; this was discussed earlier in Section III. After the discharge stops at 1 minute, a switch is made to an instantaneous model and the form of the printout changes to indicate it. Because of the difference in shape of the slick assumed in the two models, there is a small discrepancy in the predicted slick position at the time of the switch. Moreover, only the location of the center of the slick is printed out for the instantaneous model. In this case, the triangular slick is so wide compared to its length that the instantaneous slick is allowed to spread one-dimensionally (as if it were in a channel) until the shape becomes more "squarish". At that time (which would occur here for a time longer than

TABLE VI.2b SAMPLE COMPUTED OUTPUT FOR
DEMONSTRATION CASE NO. 1

.....
* SPREADING MODEL OUTPUT *
.....

THICK SLICK HAS SPREAD OVER A CIRCULAR AREA OF .24393E+02 SQUARE METERS,
WITH A RADIUS OF .27865E+01 METERS AFTER THE FIRST .14454E+00 MINUTES

TIME = 0.00 MINUTES 12.073 SECONDS
THICK SLICK AREA = .28605E+02 SQ.M. THICK SLICK THICKNESS = .13857E-02 METERS
THICK SLICK RADIUS = .30175E+01 METERS

TOTAL MASS OF THICK SLICK = .24813E+02 KG.
TOTAL EVAPORATED MASS = .22663E+00 KG.
RATE OF EVAPORATION = .25091E-02 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .46835E-04 KG.
RATE OF DISSOLUTION = .51853E-06 KG/(SEC-SQ.M.)

TOTAL MASS = .25040E+02 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .77325E+00 METERS AND Y = 0. METERS

TIME = 0.00 MINUTES 16.073 SECONDS
THICK SLICK AREA = .32732E+02 SQ.M. THICK SLICK THICKNESS = .11959E-02 METERS
THICK SLICK RADIUS = .32278E+01 METERS

TOTAL MASS OF THICK SLICK = .24505E+02 KG.
TOTAL EVAPORATED MASS = .53504E+00 KG.
RATE OF EVAPORATION = .25091E-02 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .11057E-03 KG.
RATE OF DISSOLUTION = .51853E-06 KG/(SEC-SQ.M.)

TOTAL MASS = .25040E+02 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .46295E+01 METERS AND Y = 0. METERS

TIME = 1.00 MINUTES 20.073 SECONDS
THICK SLICK AREA = .56427E+02 SQ.M. THICK SLICK THICKNESS = .47049E-03 METERS
THICK SLICK RADIUS = .42381E+01 METERS

TOTAL MASS OF THICK SLICK = .16633E+02 KG.
TOTAL EVAPORATED MASS = .84049E+01 KG.
RATE OF EVAPORATION = .25091E-02 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .17370E-02 KG.
RATE OF DISSOLUTION = .51853E-06 KG/(SEC-SQ.M.)

TOTAL MASS = .25040E+02 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .51287E+01 METERS AND Y = 0. METERS

TABLE VI.3a INTERACTIVE INPUT FOR
DEMONSTRATION CASE NO. 2

ENTER THE TITLE FOR THIS RUN..
? DEMO NO. 2
INPUT THE AMBIENT TEMPERATURE IN CELSIUS.
? 20
INPUT THE BAROMETRIC PRESSURE IN MILLIBARS
OR ZERO, 0, FOR THE STANDARD SEA LEVEL PRESSURE
OF 1013.25 MB.
? 0
INPUT THE TIME INCREMENT IN SECONDS. TRY 1.0.
? .1
INPUT THE DESIRED RUN TIME IN MINUTES
? 1.33333
INPUT MINIMUM ALLOWABLE THICKNESS OF THICK SLICK IN METERS.
? 1.E-4
INPUT THICKNESS OF THIN SLICK IN METERS.
? 1.E-4

* WATER BODY DESCRIPTION *

IS SPILL IN RIVER OR CHANNEL? Y/N
? N

IS IT A LAKE? Y/N
? Y

IS IT A CIRCULAR LAKE? Y/N
? Y

GIVE THE RADIUS AND DEPTH OF THE CIRCULAR LAKE
(UNIT : METER)
? 20,0.3

IS THERE CURRENT? Y/N
? N

IS THERE WIND IN THE AREA ? Y/N
? Y

IS WIND SPEED CONSTANT? Y/N
? Y

INPUT WIND SPEED (METER/SEC) AND DIRECTION
ANGLE (DEGREES)
? 1.94,0

INPUT MEAN WAVE HEIGHT.(METER)
DEFAULT VALUE (EQ.(III.32) OF REPORT) IS USED
BY INPUTTING -1.

? .01
GIVE SPILL COORDINATES X AND Y, IN METERS
? 0,0

* SPILL TYPE *

WE HAVE STANDARD PROPERTIES FOR THE FOLLOWING CHEMICALS

1. ALLYL CHLORIDE	2. BENZENE
3. BUTADIENE (1,2)	4. BUTYL ACETATE (ISO)
5. BUTYL MERCAPTAN (N)	6. CHLOROBUTA-1-3-DIENE
7. CYCLOHEXANE	8. CYCLOHEXENE
9. DIPROPYL ETHER (ISO)	10. ETHYL CHLORIDE

TABLE VI.3a (CONTD)

11. ETHYL MERCAPTAN	12. HEPTANE (N)
13. HEXANE (N)	14. METHYL CYCLOHEXANE
15. NONANE (N)	16. OCTANE (N)
17. PENTANE	18. TOLUENE
19. TRIMETHYLBENZENE	20. XYLENE (N)

ENTER THE NO. YOU WANT OR
 NEGATIVE VALUE - IF YOU WANT TO INPUT THE PROPERTIES
 99 - IF THE CHEMICAL IS NOT ON THE LIST

? 17

BAROMETRIC PRESSURE : 1013.250 MILLIBAR

TEMPERATURE : 20.000 DEGREES C

CHEMICAL NAME IS: PENTANE

CHEMICAL DENSITY = 626.00 KG/CU.M.

MOLECULAR WEIGHT = 72.151 KG/KG-MOLE

DIFFUSION COEFF (AIR) = .75000E-05 SQ.M./SEC

DIFFUSION COEFF (WATER) = .84000E-09 SQ.M./SEC

CHEMICAL VAPOR PRESSURE = 58772.29 NEWTON/SQ.M.

SOLUBILITY IN WATER = .36 KG/CU.M.

THE INTERFACE TENSION WRT AIR IS .16046E-01 NEWTON/M.
 THE INTERFACE TENSION WRT WATER IS .50200E-01 NEWTON/M.

THE SPREADING COEFFICIENT IS .65142E-02 NEWTON/M.

IS SPILL 1. INSTANTANEOUS OR 2. CONTINUOUS?

? 2

INPUT THE RATE OF DISCHARGE (CU.M./SEC)

? .001

INPUT THE TOTAL DURATION OF SPILL IN MINUTES

? 1.

INPUT THE PRINTOUT TIME STEP IN MINUTES.

? .066667

TABLE VI.3b SAMPLE COMPUTED OUTPUT FOR
DEMONSTRATION CASE NO. 2

.....
* SPREADING MODEL OUTPUT *
.....

THICK SLICK HAS SPREAD OVER AN ELONGATED TRIANGULAR AREA OF .3016E+02
SQUARE METERS AFTER A TIME OF .8711E+00 MINUTES.
THE THICK SLICK LEADING EDGE IS .17000E+02 METERS WIDE AND IS .3549E+01 METERS
DOWNSTREAM.

THE THIN SLICK AREA IS EQUAL TO .24135E+03 SQUARE METERS.

TIME = 0.00 MINUTES 56.070 SECONDS
THICK SLICK AREA = .3344E+02 SQ.M. THICK SLICK THICKNESS = .92715E-03 METERS
THICK SLICK DOWNSTREAM WIDTH = .1756E+02 METERS
THIN SLICK AREA = .24556E+03 SQ.M.
THIN SLICK DOWNSTREAM WIDTH = .1290E+03 METERS

TOTAL MASS OF THICK SLICK = .19409E+02 KG.
TOTAL EVAPORATED MASS = .31867E+00 KG.
RATE OF EVAPORATION = .26372E-02 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .66037E-04 KG.
RATE OF DISSOLUTION = .54650E-06 KG/(SEC-SQ.M.)
TOTAL MASS OF THIN SLICK = .15372E+02 KG.

TOTAL MASS = .35100E+02 KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = .38672E+01 METERS AND
Y = 0. METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT THE SPILL ORIGIN

TIME = 1.00 MINUTES .070 SECONDS
THICK SLICK AREA = .36957E+02 SQ.M. THICK SLICK THICKNESS = .91905E-03 METERS
THICK SLICK DOWNSTREAM WIDTH = .18122E+02 METERS
THIN SLICK AREA = .25002E+03 SQ.M.
THIN SLICK DOWNSTREAM WIDTH = .1226E+03 METERS

TOTAL MASS OF THICK SLICK = .21262E+02 KG.
TOTAL EVAPORATED MASS = .68992E+00 KG.
RATE OF EVAPORATION = .26372E-02 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .14297E-03 KG.
RATE OF DISSOLUTION = .54650E-06 KG/(SEC-SQ.M.)
TOTAL MASS OF THIN SLICK = .15651E+02 KG.

TOTAL MASS = .37604E+02 KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = .4079E+01 METERS AND
Y = 0. METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT THE SPILL ORIGIN

TIME = 1.00 MINUTES 4.070 SECONDS
THICK SLICK AREA = .36618E+02 SQ.M. THICK SLICK THICKNESS = .91062E-03 METERS

TOTAL MASS OF THICK SLICK = .20874E+02 KG.
TOTAL EVAPORATED MASS = .10780E+01 KG.
RATE OF EVAPORATION = .26372E-02 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .22339E-03 KG.
RATE OF DISSOLUTION = .54650E-06 KG/(SEC-SQ.M.)

TOTAL MASS = .21952E+02 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .2590E+01 METERS AND Y = 0. METERS

TABLE VI.3b (CONTO)

TIME = 1.00 MINUTES 11.070 SECONDS
THICK SLICK AREA = $.16279E+02$ SQ.M. THICK SLICK THICKNESS = $.40220E-03$ METERS

TOTAL MASS OF THICK SLICK = $.20490E+02$ KG.
TOTAL EVAPORATED MASS = $.14625E+01$ KG.
RATE OF EVAPORATION = $.26372E-02$ KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = $.30306E-03$ KG.
RATE OF DISSOLUTION = $.54650E-06$ KG/(SEC-SQ.M.)

TOTAL MASS = $.21952E+02$ KG.

THE CENTER OF THE SLICK IS LOCATED AT X = $.32624E+01$ METERS AND Y = 0. METER

TIME = 1.00 MINUTES 12.070 SECONDS
THICK SLICK AREA = $.35940E+02$ SQ.M. THICK SLICK THICKNESS = $.49377E-03$ METERS

TOTAL MASS OF THICK SLICK = $.20109E+02$ KG.
TOTAL EVAPORATED MASS = $.18434E+01$ KG.
RATE OF EVAPORATION = $.26372E-02$ KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = $.38200E-03$ KG.
RATE OF DISSOLUTION = $.54650E-06$ KG/(SEC-SQ.M.)

TOTAL MASS = $.21952E+02$ KG.

THE CENTER OF THE SLICK IS LOCATED AT X = $.35340E+01$ METERS AND Y = 0. METER

TIME = 1.00 MINUTES 16.070 SECONDS
THICK SLICK AREA = $.35602E+02$ SQ.M. THICK SLICK THICKNESS = $.88534E-03$ METERS

TOTAL MASS OF THICK SLICK = $.19731E+02$ KG.
TOTAL EVAPORATED MASS = $.22207E+01$ KG.

RATE OF EVAPORATION = $.26372E-02$ KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = $.46019E-03$ KG.
RATE OF DISSOLUTION = $.54650E-06$ KG/(SEC-SQ.M.)

TOTAL MASS = $.21952E+02$ KG.

THE CENTER OF THE SLICK IS LOCATED AT X = $.38056E+01$ METERS AND Y = 0. METER

TIME = 1.00 MINUTES 20.070 SECONDS
THICK SLICK AREA = $.35263E+02$ SQ.M. THICK SLICK THICKNESS = $.47692E-03$ METERS

TOTAL MASS OF THICK SLICK = $.19357E+02$ KG.
TOTAL EVAPORATED MASS = $.25945E+01$ KG.
RATE OF EVAPORATION = $.26372E-02$ KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = $.53765E-03$ KG.
RATE OF DISSOLUTION = $.54650E-06$ KG/(SEC-SQ.M.)

TOTAL MASS = $.21952E+02$ KG.

THE CENTER OF THE SLICK IS LOCATED AT X = $.40772E+01$ METERS AND Y = 0. METER

the run time), the instantaneous model is changed to the open-water case, and the slick is assumed to be circular subsequently.

Input for Demonstration Case No. 3 is shown in Table VI.4a. For this case, the current is non-zero and its x and y components are input at the fourteenth prompt. Also, the chemical properties are input separately, rather than taken from the data for the twenty chemicals included as samples in the model. Sample output is shown in Table VI.4b. The change in the form of the output should again be noted when the discharge stops after 30 minutes. In this example, the shape of the slick is such that the instantaneous model is immediately assumed to be the open water case; the slick spreads symmetrically, and the radius of the thick slick is printed out.

Input for Demonstration Case No. 4 is shown in Table VI.5a. The width and depth of the channel are input at the eighth prompt. The bottom roughness is input at the ninth prompt; the computed results are practically independent of bottom roughness for realistic values of channel depth, so the default value can be used with little or no loss of accuracy when the actual bottom roughness is unknown. The wind direction for a channel is referred to the downstream channel direction (the fifteenth prompt). Sample output is given in Table VI.5b. The initial printout for this case is data about the slick at the time it has just spread across the entire channel. During this first 2.09 minutes, the slick is triangular and the leading edge moves downstream at a speed equal to U_T ; see Equation (III.17). After the slick extends across the entire channel, the spreading is one-dimensional, and the leading edge is transported downstream at a speed equal to a combination of U_T and the gravitational spreading velocity. Further, at the time the models are switched, the area of the triangular slick is assumed to be instantaneously spread uniformly across the channel width. For these reasons, there is a small discrepancy at the switch-over time in the position of the leading edge of the slick. (The discrepancy is not apparent in the printout because of the long time between the first 2.09 minutes and the first of the regular printouts at 15 minutes.) Note that after the discharge stops at 60 minutes, the printout form changes and the slick moves bodily downstream.

TABLE VI.4a INTERACTIVE INPUT FOR
DEMONSTRATION CASE NO. 3

ENTER THE TITLE FOR THIS RUN..
 ? DEMO NO. 3
 INPUT THE AMBIENT TEMPERATURE IN CELSIUS.
 ? 20
 INPUT THE BAROMETRIC PRESSURE IN MILLIBARS
 OR ZERO, 0, FOR THE STANDARD SEA LEVEL PRESSURE
 OF 1013.25 MB.
 ? 0
 INPUT THE TIME INCREMENT IN SECONDS. TRY 1.0.
 ? 1.
 INPUT THE DESIRED RUN TIME IN MINUTES
 ? 60.
 INPUT MINIMUM ALLOWABLE THICKNESS OF THICK SLICK IN METERS.
 ? 1.E-4
 INPUT THICKNESS OF THIN SLICK IN METERS.
 ? 1.E-4

 * WATER BODY DESCRIPTION *

IS SPILL IN RIVER OR CHANNEL? Y/N
 ? N

IS IT A LAKE? Y/N
 ? Y

IS IT A CIRCULAR LAKE? Y/N
 ? Y

GIVE THE RADIUS AND DEPTH OF THE CIRCULAR LAKE
 (UNIT : METER)
 ? 20000,100

IS THERE CURRENT? Y/N
 ? Y

IS CURRENT CONSTANT? Y/N
 ? Y

INPUT CONSTANT CURRENT SPEED UCX AND UCY
 (UNIT : METER/SEC)
 ? 0.5,0.1

IS THERE WIND IN THE AREA ? Y/N
 ? Y

IS WIND SPEED CONSTANT? Y/N
 ? Y

INPUT WIND SPEED (METER/SEC) AND DIRECTION
 ANGLE (DEGREES)
 ? 3.,30

INPUT MEAN WAVE HEIGHT.(METER)
 DEFAULT VALUE (EQ.(III.32) OF REPORT) IS USED
 BY INPUTTING -1.

? .5
 GIVE SPILL COORDINATES X AND Y, IN METERS
 ? 0,0

 * SPILL TYPE *

WE HAVE STANDARD PROPERTIES FOR THE FOLLOWING CHEMICALS

1. ALLYL CHLORIDE	2. BENZENE
3. BUTADIENE (1,2)	4. BUTYL ACETATE (ISO)
5. BUTYL MERCAPTAN (N)	6. CHLOROBUTA-1-3-DIENE
7. CYCLOHEXANE	8. CYCLOHEXENE

TABLE VI.4a (CONTD)

9. DIPROPYL ETHER (ISO)	10. ETHYL CHLORIDE
11. ETHYL MERCAPTAN	12. HEPTANE (N)
13. HEXANE (N)	14. METHYL CYCLOHEXANE
15. NONANE (N)	16. OCTANE (N)
17. PENTANE	18. TOLUENE
19. TRIMETHYLBENZENE	20. XYLENE (M)

ENTER THE NO. YOU WANT OR
 NEGATIVE VALUE - IF YOU WANT TO INPUT THE PROPERTIES
 99 - IF THE CHEMICAL IS NOT ON THE LIST

? -1

ENTER ITS DENSITY IN KG/CU M.

? 800.

INPUT ITS MOLECULAR WEIGHT IN KG/KG-MOLE.

? 114.32

ENTER DIFFUSION COEFFICIENT OF VAPOR IN AIR IN SQ M/SEC.

? 5.8E-6

ENTER DIFFUSION COEFFICIENT OF LIQUID IN WATER IN SQ M/SEC.

? 6.38E-9

IS PU (VAPOR) 1. A NUMBER OR 2. A FORMULA?

? 1

ENTER CONSTANT PU

? 1391.74

INPUT THE SOLUBILITY LIMIT OF CHEMICAL IN WATER (KG/CU.M.)

? .02

INPUT (1) CHEMICAL/AIR INTERFACE TENSION AND

(2) WATER/CHEMICAL INTERFACE TENSION

UNIT : NEWTON/M.

? 2.1618E-2

? 5.08E-2

BAROMETRIC PRESSURE : 1013.250 MILLIBAR

TEMPERATURE : 20.000 DEGREES C

CHEMICAL NAME IS:

:::

CHEMICAL DENSITY = 800.00 KG/CU.M.

MOLECULAR WEIGHT = 114.320 KG/KG-MOLE

DIFFUSION COEFF (AIR) = .58000E-05 SQ.M./SEC

DIFFUSION COEFF (WATER) = .63800E-08 SQ.M./SEC

CHEMICAL VAPOR PRESSURE = 1391.74 NEWTON/SQ.M.

SOLUBILITY IN WATER = .02 KG/CU.M.

THE INTERFACE TENSION WRT AIR IS .21618E-01 NEWTON/M.

THE INTERFACE TENSION WRT WATER IS .50000E-01 NEWTON/M.

THE SPREADING COEFFICIENT IS .34200E-03 NEWTON/M.

IS SPILL 1. INSTANTANEOUS OR 2. CONTINUOUS?

? 2

TABLE VI.4a (CONTD)

INPUT THE RATE OF DISCHARGE (CU.M./SEC)

? .0333

INPUT THE TOTAL DURATION OF SPILL IN MINUTES

? 30.

INPUT THE PRINTOUT TIME STEP IN MINUTES.

? 10.

TABLE VI.4b SAMPLE COMPUTED OUTPUT FOR
DEMONSTRATION CASE NO. 3

* SPREADING MODEL OUTPUT *

THICK SLICK HAS SPREAD OVER AN ELONGATED TRIANGULAR AREA OF .21905E+04
SQUARE METERS AFTER A TIME OF .25361E+01 MINUTES.
THE THICK SLICK LEADING EDGE IS .47175E+02 METERS WIDE AND IS .92867E+02 METERS
DOWNSTREAM.

THE THIN SLICK AREA IS EQUAL TO .17524E+05 SQUARE METERS.

TIME = 10.00 MINUTES .168 SECONDS
THICK SLICK AREA = .15298E+05 SQ.M. THICK SLICK THICKNESS = .11258E-02 METERS
THICK SLICK DOWNSTREAM WIDTH = .83532E+02 METERS
THIN SLICK AREA = .22478E+05 SQ.M.
THIN SLICK DOWNSTREAM WIDTH = .12274E+03 METERS

TOTAL MASS OF THICK SLICK = .13774E+05 KG.
TOTAL EVAPORATED MASS = .41207E+03 KG.
RATE OF EVAPORATION = .11161E-03 KG/(SEC-SQ.P.)
TOTAL DISSOLVED MASS = .53931E+00 KG.
RATE OF DISSOLUTION = .14608E-06 KG/(SEC-SQ.P.)
TOTAL MASS OF THIN SLICK = .17982E+04 KG.

TOTAL MASS = .15988E+05 KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = .35466E+03 METERS AND
Y = .41526E+02 METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT THE SPILL ORIGIN

TIME = 20.00 MINUTES .168 SECONDS
THICK SLICK AREA = .34133E+05 SQ.M. THICK SLICK THICKNESS = .47421E-03 METERS
THICK SLICK DOWNSTREAM WIDTH = .10886E+03 METERS
THIN SLICK AREA = .24922E+05 SQ.M.
THIN SLICK DOWNSTREAM WIDTH = .81705E+02 METERS

TOTAL MASS OF THICK SLICK = .27369E+05 KG.
TOTAL EVAPORATED MASS = .22073E+04 KG.
RATE OF EVAPORATION = .11161E-03 KG/(SEC-SQ.P.)
TOTAL DISSOLVED MASS = .28889E+01 KG.
RATE OF DISSOLUTION = .14608E-06 KG/(SEC-SQ.P.)

TOTAL MASS OF THIN SLICK = .23934E+04 KG.

TOTAL MASS = .31972E+05 KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = .70922E+03 METERS AND
Y = .18303E+03 METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT THE SPILL ORIGIN

TABLE VI.4b (CONTD)

TIME = 30.00 MINUTES .168 SECONDS
 THICK SLICK AREA = .66465E+05 SQ.M. THICK SLICK THICKNESS = .73644E-03 METERS
 THICK SLICK DOWNSTREAM WIDTH = .1210CE+03 METERS
 THIN SLICK AREA = .38261E+05 SQ.M.
 THIN SLICK DOWNSTREAM WIDTH = .69652E+02 METERS

TOTAL MASS OF THICK SLICK = .39158E+C5 KG.
 TOTAL EVAPORATED MASS = .57302E+C4 KG.
 RATE OF EVAPORATION = .11161E-C3 KG/(SEC-SQ.P.)
 TOTAL DISSOLVED MASS = .74996E+01 KG.
 RATE OF DISSOLUTION = .14608E-C6 KG/(SEC-SQ.P.)
 TOTAL MASS OF THIN SLICK = .3C609E+C4 KG.

TOTAL MASS = .47956E+C5 KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = .1C638E+04 METERS AND
 Y = .27453E+03 METERS
 THE TRAILING EDGE OF THE SLICK IS LOCATED AT THE SPILL ORIGIN

TIME = 40.00 MINUTES .168 SECONDS
 THICK SLICK AREA = .63835E+C5 SQ.M. THICK SLICK THICKNESS = .68118E-03 METERS
 THICK SLICK RADIUS = .14255E+C3 METERS

TOTAL MASS OF THICK SLICK = .34787E+C5 KG.
 TOTAL EVAPORATED MASS = .10096E+C5 KG.
 RATE OF EVAPORATION = .11161E-03 KG/(SEC-SQ.P.)
 TOTAL DISSOLVED MASS = .13213E+C2 KG.
 RATE OF DISSOLUTION = .14608E-C6 KG/(SEC-SQ.P.)

TOTAL MASS = .44896E+C5 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .1C637E+C4 METERS AND Y = .27452E+03 METERS

TIME = 50.00 MINUTES .168 SECONDS
 THICK SLICK AREA = .60749E+C5 SQ.M. THICK SLICK THICKNESS = .62979E-03 METERS
 THICK SLICK RADIUS = .13906E+C3 METERS

TOTAL MASS OF THICK SLICK = .30607E+C5 KG.
 TOTAL EVAPORATED MASS = .14270E+C5 KG.
 RATE OF EVAPORATION = .11161E-C3 KG/(SEC-SQ.P.)

TOTAL DISSOLVED MASS = .18676E+C2 KG.
 RATE OF DISSOLUTION = .14608E-C6 KG/(SEC-SQ.P.)

TOTAL MASS = .44896E+C5 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .14183E+C4 METERS AND Y = .36602E+03 METERS

TIME = 60.00 MINUTES .168 SECONDS
 THICK SLICK AREA = .57271E+C5 SQ.M. THICK SLICK THICKNESS = .58163E-03 METERS
 THICK SLICK RADIUS = .13502E+C3 METERS

TOTAL MASS OF THICK SLICK = .26648E+C5 KG.
 TOTAL EVAPORATED MASS = .18223E+C5 KG.
 RATE OF EVAPORATION = .11161E-C3 KG/(SEC-SQ.P.)
 TOTAL DISSOLVED MASS = .23851E+C2 KG.
 RATE OF DISSOLUTION = .14608E-C6 KG/(SEC-SQ.P.)

TOTAL MASS = .44896E+C5 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .17729E+C4 METERS AND Y = .45752E+03 METERS

TABLE VI.5a INTERACTIVE INPUT FOR
DEMONSTRATION CASE NO. 4

ENTER THE TITLE FOR THIS RUN..
? DEMO NO. 4
INPUT THE AMBIENT TEMPERATURE IN CELSIUS.
? 20
INPUT THE BAROMETRIC PRESSURE IN MILLIBARS
OR ZERO, 0, FOR THE STANDARD SEA LEVEL PRESSURE
OF 1013.25 MB.
? 0
INPUT THE TIME INCREMENT IN SECONDS. TRY 1.0.
? 1.
INPUT THE DESIRED RUN TIME IN MINUTES
? 120.
INPUT MINIMUM ALLOWABLE THICKNESS OF THICK SLICK IN METERS.
? 1.E-4
INPUT THICKNESS OF THIN SLICK IN METERS.
? 1.E-4

* WATER BODY DESCRIPTION *

IS SPILL IN RIVER OR CHANNEL? Y/N
? Y

GIVE THE WIDTH AND DEPTH OF THE CHANNEL (IN METERS)
? 50,10

INPUT THE BOTTOM ROUGHNESS(METERS) OF THE CHANNEL.
INPUT ZERO, 0 IF YOU WANT TO USE THE DEFAULT VALUE.
? 0

IS THERE CURRENT IN THE CHANNEL? Y/N
? Y

IS IT TIDAL CURRENT? Y/N
?

CURRENT SPEED MUST BE CONSTANT.
INPUT CURRENT SPEED METER/SEC
? 1.

IS THERE WIND IN THE AREA ? Y/N
? Y

IS WIND SPEED CONSTANT? Y/N
? Y

INPUT WIND SPEED (METER/SEC) AND DIRECTION
ANGLE (DEGREES)
? 3.,135.

* SPILL TYPE *

WE HAVE STANDARD PROPERTIES FOR THE FOLLOWING CHEMICALS

1. ALLYL CHLORIDE	2. BENZENE
3. BUTADIENE (1,2)	4. BUTYL ACETATE (ISO)
5. BUTYL MERCAPTAN (N)	6. CHLOROBUTA-1-3-DIENE
7. CYCLOHEXANE	8. CYCLOHEXENE
9. DIPROPYL ETHER (ISO)	10. ETHYL CHLORIDE
11. ETHYL MERCAPTAN	12. HEPTANE (N)
13. HEXANE (N)	14. METHYL CYCLOHEXANE
15. NONANE (N)	16. OCTANE (N)
17. PENTANE	18. TOLUENE
19. TRIMETHYLBENZENE	20. XYLENE (M)

ENTER THE NO. YOU WANT OR
NEGATIVE VALUE - IF YOU WANT TO INPUT THE PROPERTIES
99 - IF THE CHEMICAL IS NOT ON THE LIST

TABLE VI.5a (CONTD)

BAROMETRIC PRESSURE : 1013.250 MILLIBAR

TEMPERATURE : 20.000 DEGREES C

CHEMICAL NAME IS: OCTANE (N)

CHEMICAL DENSITY = 703.00 KG/CU.M.

MOLECULAR WEIGHT = 114.232 KG/KG-MOLE

DIFFUSION COEFF (AIR) = .58000E-05 SQ.M./SEC

DIFFUSION COEFF (WATER) = .63800E-09 SQ.M./SEC

CHEMICAL VAPOR PRESSURE = 1391.74 NEWTON/SQ.M.

SOLUBILITY IN WATER = .02 KG/CU.M.

THE INTERFACE TENSION WRT AIR IS .21618E-01 NEWTON/M.

THE INTERFACE TENSION WRT WATER IS .50800E-01 NEWTON/M.

THE SPREADING COEFFICIENT IS .34180E-03 NEWTON/M.

IS SPILL 1. INSTANTANEOUS OR 2. CONTINUOUS?
? 2

INPUT THE RATE OF DISCHARGE (CU.M./SEC)
? .1

INPUT THE TOTAL DURATION OF SPILL IN MINUTES
? 60.

INPUT THE PRINTOUT TIME STEP IN MINUTES.
? 15.

TABLE VI.5b SAMPLE COMPUTED OUTPUT FOR
DEMONSTRATION CASE NO. 4

* SPREADING MODEL OUTPUT *

THICK SLICK HAS SPREAD ACROSS THE CHANNEL WIDTH AND COVERS AN AREA OF .29075E+04
SQUARE METERS AFTER A TIME OF .20938E+01 MINUTES.
THE SLICK LEADING EDGE IS .11E30E+03 METERS DOWNSTREAM.

TIME = 15.00 MINUTES .626 SECONDS
THICK SLICK AREA = .62949E+05 SQ.M. THICK SLICK THICKNESS = .13165E-02 METERS
THIN SLICK AREA = .23265E+05 SQ.M.

TOTAL MASS OF THICK SLICK = .58259E+05 KG.
TOTAL EVAPORATED MASS = .34025E+04 KG.
RATE OF EVAPORATION = .13604E-03 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .16499E+02 KG.
RATE OF DISSOLUTION = .67966E-06 KG/(SEC-SQ.M.)
TOTAL MASS OF THIN SLICK = .16355E+04 KG.

TOTAL MASS = .63314E+05 KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = .12590E+04 METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT X = 0. METERS

TIME = 30.00 MINUTES .626 SECONDS
THICK SLICK AREA = .13481E+06 SQ.M. THICK SLICK THICKNESS = .11538E-02 METERS
THIN SLICK AREA = .23271E+05 SQ.M.

TOTAL MASS OF THICK SLICK = .10935E+06 KG.
TOTAL EVAPORATED MASS = .15524E+05 KG.
RATE OF EVAPORATION = .13604E-03 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .77562E+02 KG.
RATE OF DISSOLUTION = .67966E-06 KG/(SEC-SQ.M.)
TOTAL MASS OF THIN SLICK = .16359E+04 KG.

TOTAL MASS = .12658E+06 KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = .26962E+04 METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT X = 0. METERS

TIME = 60.00 MINUTES .626 SECONDS
THICK SLICK AREA = .26992E+06 SQ.M. THICK SLICK THICKNESS = .97912E-03 METERS
THIN SLICK AREA = .23282E+05 SQ.M.

TOTAL MASS OF THICK SLICK = .18574E+06 KG.
TOTAL EVAPORATED MASS = .65367E+05 KG.
RATE OF EVAPORATION = .13604E-03 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .12660E+03 KG.
RATE OF DISSOLUTION = .67966E-06 KG/(SEC-SQ.M.)
TOTAL MASS OF THIN SLICK = .16367E+04 KG.

TOTAL MASS = .25312E+06 KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = .53986E+04 METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT X = 0. METERS

TABLE VI.5b (CONTD)

TIME = 75.00 MINUTES .626 SECONDS
THICK SLICK AREA = .24905E+06 SQ.M. THICK SLICK THICKNESS = .47874E-03 METERS

TOTAL MASS OF THICK SLICK = .15385E+06 KG.
TOTAL EVAPORATED MASS = .57150E+05 KG.
RATE OF EVAPORATION = .13604E-03 KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = .48538E+03 KG.
RATE OF DISSOLUTION = .67966E-06 KG/(SEC-SQ.M.)

TOTAL MASS = .25149E+06 KG.

THE WHOLE SLICK HAS MOVED .35324E+04 METERS
THE DOWNSTREAM EDGE OF THE SLICK IS AT = .60229E+04 METERS AND THE UPSTREAM EDGE IS AT =
.10419E+04 METERS

Input for Case No. 5, a continuous spill in an irregularly-shaped lake with a current that is a function of both position and time, is shown in Table VI.6a. Figure VI.1 shows the lake graphically as well as the currents in the 3x3 grid at the instant the spill occurs. As shown in Table VI.6a, the shape of the lake is specified (beginning at the twelfth prompt) by ten pairs of x,y coordinates. The coordinates should be input in counterclockwise order, starting with the point having the smallest x-coordinate. (An arbitrarily-shaped coast should also be input starting with the smallest x-coordinate.) The x-coordinates of the current grids are input as a group, starting with the smallest value (which must equal the smallest x-coordinate of the lake) and ending with the largest value (which must equal the largest x-coordinate of the lake). Likewise, the y-coordinates of the grid are input as a group, and the largest and smallest coordinates must satisfy similar conditions. Next, the x and y components of the current in each of the nine boxes of the grid are input. Since the current has been specified as a function of time in the input, the x and y components must be input ten times, one for each of the ten instants of time that are input after the currents are given. The smallest time value must be zero, and the largest must be at least as large as the run time. Sample output is shown in Table VI.6b. When the leading edge of the slick moves from grid to grid, the transport velocity varies and the slick will be predicted to bend and kink. (In this example, the continuous spill ends before the leading edge moves out of the original grid.) Although the correct value of U_T is used to compute the incremental change in the position of the leading edge during the next integration time step (Equation (III.38)), the shape of the entire slick behind the leading edge is not adjusted to account for the new value of the time-varying current; that is, when the current varies in time, the position of the entire slick is not updated, only the leading edge is. Otherwise, the calculations are similar to a case when the current is constant.

TABLE VI.6a INTERACTIVE INPUT FOR
DEMONSTRATION CASE NO. 5

ENTER THE TITLE FOR THIS RUN..
 ? DEMO NO. 5
 INPUT THE AMBIENT TEMPERATURE IN CELSIUS.
 ? 20
 INPUT THE BAROMETRIC PRESSURE IN MILLIBARS
 OR ZERO, 0, FOR THE STANDARD SEA LEVEL PRESSURE
 OF 1013.25 MB.
 ? 0
 INPUT THE TIME INCREMENT IN SECONDS. TRY 1.0.
 ? 1.
 INPUT THE DESIRED RUN TIME IN MINUTES
 ? 240.
 INPUT MINIMUM ALLOWABLE THICKNESS OF THICK SLICK IN METERS.
 ? 1.E-4
 INPUT THICKNESS OF THIN SLICK IN METERS.
 ? 1.E-4

 * WATER BODY DESCRIPTION *

IS SPILL IN RIVER OR CHANNEL? Y/N
 ? N

IS IT A LAKE? Y/N
 ? Y

IS IT A CIRCULAR LAKE? Y/N
 ? N

IS IT A RECTANGULAR LAKE? Y/N
 ? N

THE SPILL IS IN A LAKE WITH ARBITRARY SHAPE.
 DESCRIBE THE SHAPE WITH 10 PAIRS OF X,Y COORDINATES (METERS). (0,0) SHOULD
 BE NEAR THE SPILL SITE.

? -4500.,0.
 ? -3500.,-3000.
 ? -1000.,-4000.
 ? 0.,-5000.
 ? 2000.,-4000.
 ? 4000.,-2000.
 ? 5000.,500.
 ? 4000.,2000.
 ? 1000.,3500.
 ? -3000.,3000.

	X	Y
1	-.45000E+04	0.
2	-.35000E+04	-.30000E+04
3	-.10000E+04	-.40000E+04
4	0.	-.50000E+04
5	.20000E+04	-.40000E+04
6	.40000E+04	-.20000E+04
7	.50000E+04	.50000E+03
8	.40000E+04	.20000E+04
9	.10000E+04	.35000E+04
10	-.30000E+04	.30000E+04

INPUT WATER DEPTH
 ? 100

TABLE VI.6a (CONTD)

IS THERE CURRENT? Y/N

? Y

IS CURRENT CONSTANT? Y/N

? N

IS CURRENT A FUNCTION OF TIME ? Y/N

? Y

IS CURRENT A FUNCTION OF TIME ONLY ? Y/N

? N

IF A LAKE, THE X,Y CURRENT MUST BE GIVEN AT CENTER
OF 9 RECTANGULAR BOXES (3X3 GRID) THAT COVER LAKE.

IF A COAST, THE X,Y CURRENT MUST BE GIVEN FOR THE
9 Y-SLICES THAT EXTEND OUT FROM THE 10 X,Y POINTS DESCRIBING THE COAS

T.

GIVE THE 4 X-COORDINATES (METERS) THAT SPECIFY
THE HORIZONTAL GRID. THE FIRST AND LAST MUST
COINCIDE WITH THE LENGTH OF THE LAKE.

? -4500.

? -2000.

? 2000.

? 5000.

NOW GIVE THE 4 Y-COORDINATES (METERS).

THE FIRST AND LAST MUST COINCIDE WITH THE WIDTH OF THE LAKE.

? -5000.

? -2500.

? 1000.

? 3500.

INPUT UX AND UY CURRENTS(M/SEC) FOR EACH OF THE 9
BOXES OR SLICES. BOXES ARE NUMBERED LEFT-TO-RIGHT
1,2,3 IN BOTTOM ROW, 4,5,6 IN MIDDLE ROW, AND 7,8,9
IN TOP ROW. SLICES FOR A COAST ARE NUMBERED 1 TO 9,
LEFT-TO-RIGHT. IF THE CURRENTS ALSO DEPEND ON TIME,
YOU WILL BE ASKED FOR 10 SUCH SETS OF CURRENTS.

CURRENTS FOR NUMBER 1 TIME.

? 0.1,-0.1

? 0.2,0.

? 0.1,0.1

? 0.05,-0.15

? 0.05,0.

? 0.05,0.15

? -0.1,-0.1

? -0.2,0.

? -0.1,0.1

CURRENTS FOR NUMBER 2 TIME.

? 0.15,-0.15

? 0.3,0.

? 0.15,0.15

? 0.075,-0.225

? 0.075,0.

? 0.075,0.225

? -0.15,-0.15

? -0.3,0.

? -0.15,0.15

CURRENTS FOR NUMBER 3 TIME.

? 0.2,-0.2

? 0.4,0.

? 0.2,0.2

? 0.1,-0.3

? 0.1,0.

? 0.1,0.3

? -0.2,-0.2

? -0.4,0.

? -0.2,0.2

TABLE VI.6a (CONTD)

CURRENTS FOR NUMBER 4 TIME.

? 0.15,-0.15
 ? 0.3,0.
 ? 0.15,0.15
 ? 0.075,-0.225
 ? 0.075,0.
 ? 0.075,0.225
 ? -0.15,-0.15
 ? -0.3,0.
 ? -0.15,0.15

CURRENTS FOR NUMBER 5 TIME.

? 0.1,-0.1
 ? 0.2,0.
 ? 0.1,0.1
 ? 0.05,-0.15
 ? 0.05,0.
 ? 0.05,0.15
 ? -0.1,-0.1
 ? -0.2,0.
 ? -0.1,0.1

CURRENTS FOR NUMBER 6 TIME.

? 0.1,-0.1
 ? 0.2,0.
 ? 0.1,0.1
 ? 0.05,-0.15
 ? 0.05,0.
 ? 0.05,0.15
 ? -0.1,-0.1
 ? -0.2,0.
 ? -0.1,0.1

CURRENTS FOR NUMBER 7 TIME.

? 0.1,-0.1
 ? 0.2,0.
 ? 0.1,0.1
 ? 0.05,-0.15
 ? 0.05,0.
 ? 0.05,0.15
 ? -0.1,-0.1
 ? -0.2,0.
 ? -0.1,0.1

CURRENTS FOR NUMBER 8 TIME.

? 0.1,-0.1
 ? 0.2,0.
 ? 0.1,0.1
 ? 0.05,-0.15
 ? 0.05,0.
 ? 0.05,0.15
 ? -0.1,-0.1
 ? -0.2,0.
 ? -0.1,0.1

CURRENTS FOR NUMBER 9 TIME.

? 0.1,-0.1
 ? 0.2,0.
 ? 0.1,0.1
 ? 0.05,-0.15
 ? 0.05,0.
 ? 0.05,0.15
 ? -0.1,-0.1
 ? -0.2,0.
 ? -0.1,0.1

CURRENTS FOR NUMBER 10 TIME.

? 0.1,-0.1
 ? 0.2,0.
 ? 0.1,0.1
 ? 0.05,-0.15
 ? 0.05,0.
 ? 0.05,0.15
 ? -0.1,-0.1
 ? -0.2,0.
 ? -0.1,0.1

TABLE VI.6a (CONTD)

NOW GIVE THE TEN TIME INSTANTS IN MINUTES.

? 0.
 ? 30.
 ? 60.
 ? 90.
 ? 120.
 ? 140.
 ? 160.
 ? 200.
 ? 240.

TIME= 0. MINUTES

UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.

	1	2	3	4	5	6	7	8
9 UX	.10	.20	.10	.05	.05	.05	-.10	-.20
.10 UY	-.10	0.00	.10	-.15	0.00	.15	-.10	0.00

TIME= .30000E+02 MINUTES

UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.

	1	2	3	4	5	6	7	8
9 UX	.15	.30	.15	.00	.00	.00	-.15	-.30
.15 UY	-.15	0.00	.15	-.23	0.00	.23	-.15	0.00

TIME= .60000E+02 MINUTES

UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.

	1	2	3	4	5	6	7	8
9 UX	.20	.40	.20	.10	.10	.10	-.20	-.40
.20 UY	-.20	0.00	.20	-.30	0.00	.30	-.20	0.00

TIME= .90000E+02 MINUTES

UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.

	1	2	3	4	5	6	7	8
9 UX	.15	.30	.15	.00	.00	.00	-.15	-.30
.15 UY	-.15	0.00	.15	-.23	0.00	.23	-.15	0.00

TIME= .10000E+03 MINUTES

UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.

	1	2	3	4	5	6	7	8
9 UX	.10	.20	.10	.05	.05	.05	-.10	-.20
.10 UY	-.10	0.00	.10	-.15	0.00	.15	-.10	0.00

TIME= .12000E+03 MINUTES

UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.

	1	2	3	4	5	6	7	8
9 UX	.10	.20	.10	.05	.05	.05	-.10	-.20
.10 UY	-.10	0.00	.10	-.15	0.00	.15	-.10	0.00

TABLE VI.6a (CONTD)

TIME= .14000E+03 MINUTES

		UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.							
		1	2	3	4	5	6	7	8
9	UX	.10	.20	.10	.05	.05	.05	-.10	-.20
.10	UY	-.10	0.00	.10	-.15	0.00	.15	-.10	0.00
.10									

TIME= .16000E+03 MINUTES

		UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.							
		1	2	3	4	5	6	7	8
9	UX	.10	.20	.10	.05	.05	.05	-.10	-.20
.10	UY	-.10	0.00	.10	-.15	0.00	.15	-.10	0.00
.10									

TIME= .20000E+03 MINUTES

		UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.							
		1	2	3	4	5	6	7	8
9	UX	.10	.20	.10	.05	.05	.05	-.10	-.20
.10	UY	-.10	0.00	.10	-.15	0.00	.15	-.10	0.00
.10									

TIME= .24000E+03 MINUTES

		UX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SLICES.							
		1	2	3	4	5	6	7	8
9	UX	.10	.20	.10	.05	.05	.05	-.10	-.20
.10	UY	-.10	0.00	.10	-.15	0.00	.15	-.10	0.00
.10									

IS THERE WIND IN THE AREA ? Y/N

? Y

IS WIND SPEED CONSTANT? Y/N

? Y

INPUT WIND SPEED (METER/SEC) AND DIRECTION
ANGLE (DEGREES)

? 2.0,15

INPUT MEAN WAVE HEIGHT.(METER)

DEFAULT VALUE (EQ.(III.32) OF REPORT) IS USED
BY INPUTTING -1.

? .5

GIVE SPILL COORDINATES X AND Y, IN METERS

? 0,0

WHAT BOX (LAKE) OR SLICE (COAST) DOES THE SPILL ORIGIN LIE IN?

? 5

1

* SPILL TYPE *

WE HAVE STANDARD PROPERTIES FOR THE FOLLOWING CHEMICALS

1. ALLYL CHLORIDE	2. BENZENE
3. BUTADIENE (1,2)	4. BUTYL ACETATE (ISO)
5. BUTYL MERCAPTAN (N)	6. CHLOROBUTA-1-3-DIENE
7. CYCLOHEXANE	8. CYCLOHEXENE
9. DIPROPYL ETHER (ISO)	10. ETHYL CHLORIDE
11. ETHYL MERCAPTAN	12. HEPTANE (N)

TABLE VI.6a (CONTD)

13. HEXANE (N)	14. METHYL CYCLOHEXANE
15. NONANE (N)	16. OCTANE (N)
17. PENTANE	18. TOLUENE
19. TRIMETHYLBENZENE	20. XYLENE (N)

ENTER THE NO. YOU WANT OR
 NEGATIVE VALUE - IF YOU WANT TO INPUT THE PROPERTIES
 99 - IF THE CHEMICAL IS NOT ON THE LIST

? 16

BAROMETRIC PRESSURE : 1013.250 MILLIBAR

TEMPERATURE : 20.000 DEGREES C

CHEMICAL NAME IS: OCTANE (N)

CHEMICAL DENSITY = 703.00 KG/CU.M.

MOLECULAR WEIGHT = 114.232 KG/KG-MOLE

DIFFUSION COEFF (AIR) = .58000E-05 SQ.M./SEC

DIFFUSION COEFF (WATER) = .63800E-09 SQ.M./SEC

CHEMICAL VAPOR PRESSURE = 1391.74 NEWTON/SQ.M.

SOLUBILITY IN WATER = .02 KG/CU.M.

THE INTERFACE TENSION WRT AIR IS .21618E-01 NEWTON/M.

THE INTERFACE TENSION WRT WATER IS .50000E-01 NEWTON/M.

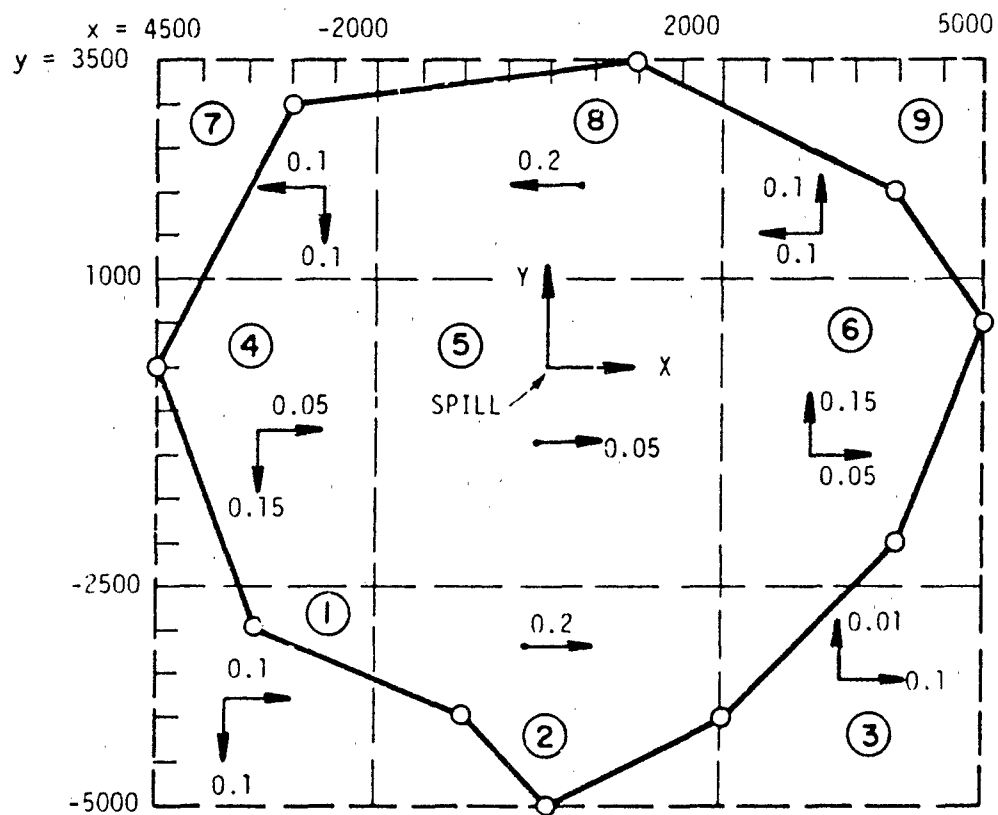
THE SPREADING COEFFICIENT IS .34180E-03 NEWTON/M.

IS SPILL 1. INSTANTANEOUS OR 2. CONTINUOUS?
 ? 2

INPUT THE RATE OF DISCHARGE (CU.M./SEC)
 ? 0.95

INPUT THE TOTAL DURATION OF SPILL IN MINUTES
 ? 60

INPUT THE PRINTOUT TIME STEP IN MINUTES.
 ? 15



NOTE: Currents are given in Meter/Second

Figure VI.1 Irregularly-Shaped Lake and Current Grid at $t = 0$

TABLE VI.6b SAMPLE COMPUTED OUTPUT FOR
DEMONSTRATION CASE NO. 5

* SPREADING MODEL OUTPUT *

THICK SLICK HAS SPREAD OVER AN ELONGATED TRIANGULAR AREA OF $.44671E+04$
SQUARE METERS AFTER A TIME OF $.40541E+01$ MINUTES.
THE THICK SLICK LEADING EDGE IS $.17097E+03$ METERS WIDE AND IS $.92255E+02$ METERS
DOWNSTREAM.

THE THIN SLICK AREA IS EQUAL TO $.15736E+05$ SQUARE METERS.

TIME = 15.00 MINUTES .485 SECONDS
THICK SLICK AREA = $.17095E+05$ SQ.M. THICK SLICK THICKNESS = $.23630E-02$ METERS
THICK SLICK DOWNSTREAM WIDTH = $.26411E+03$ METERS

THIN SLICK AREA = $.34141E+05$ SQ.M.
THIN SLICK DOWNSTREAM WIDTH = $.60470E+03$ METERS

TOTAL MASS OF THICK SLICK = $.28399E+05$ KG.
TOTAL EVAPORATED MASS = $.50152E+03$ KG.
RATE OF EVAPORATION = $.89460E-04$ KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = $.14169E+00$ KG.
RATE OF DISSOLUTION = $.25273E-07$ KG/(SEC-SQ.M.)
TOTAL MASS OF THIN SLICK = $.27516E+04$ KG.

TOTAL MASS = $.31692E+05$ KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = $.11062E+03$ METERS AND
Y = $.16314E+02$ METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT THE SPILL ORIGIN

TIME = 60.00 MINUTES .485 SECONDS
THICK SLICK AREA = $.11369E+06$ SQ.M. THICK SLICK THICKNESS = $.13392E-02$ METERS
THICK SLICK DOWNSTREAM WIDTH = $.43928E+03$ METERS
THIN SLICK AREA = $.59225E+05$ SQ.M.
THIN SLICK DOWNSTREAM WIDTH = $.22498E+03$ METERS

TOTAL MASS OF THICK SLICK = $.10703E+06$ KG.
TOTAL EVAPORATED MASS = $.15431E+09$ KG.
RATE OF EVAPORATION = $.87978E-04$ KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = $.43571E+01$ KG.
RATE OF DISSOLUTION = $.24833E-07$ KG/(SEC-SQ.M.)
TOTAL MASS OF THIN SLICK = $.40932E+04$ KG.

TOTAL MASS = $.12656E+06$ KG.

THE LEADING EDGE OF THE SLICK IS LOCATED AT X = $.51255E+03$ METERS AND
Y = $.65231E+02$ METERS
THE TRAILING EDGE OF THE SLICK IS LOCATED AT THE SPILL ORIGIN

TIME = 75.00 MINUTES .485 SECONDS
THICK SLICK AREA = $.10889E+06$ SQ.M. THICK SLICK THICKNESS = $.12827E-02$ METERS

TOTAL MASS OF THICK SLICK = $.98190E+05$ KG.
TOTAL EVAPORATED MASS = $.24267E+09$ KG.
RATE OF EVAPORATION = $.88470E-04$ KG/(SEC-SQ.M.)
TOTAL DISSOLVED MASS = $.68517E+01$ KG.
RATE OF DISSOLUTION = $.24979E-07$ KG/(SEC-SQ.M.)

TOTAL MASS = $.12246E+06$ KG.

THE CENTER OF THE SLICK IS LOCATED AT X = $.48691E+03$ METERS AND Y = $.59793E+02$ METERS

TABLE VI.6b (CONTD)

TIME = 225.00 MINUTES .485 SECONDS
 THICK SLICK AREA = .60080E+05 SQ.M. THICK SLICK THICKNESS = .70771E-03 METERS
 TOTAL MASS OF THICK SLICK = .29891E+05 KG.
 TOTAL EVAPORATED MASS = .92547E+05 KG.
 RATE OF EVAPORATION = .89954E-04 KG/(SEC-SQ.P.)
 TOTAL DISSOLVED MASS = .26144E+02 KG.
 RATE OF DISSOLUTION = .25419E-07 KG/(SEC-SQ.P.)

TOTAL MASS = .12246E+06 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .15811E+04 METERS AND Y = .22285E+03 METERS

TIME = 240.00 MINUTES .485 SECONDS
 THICK SLICK AREA = .55191E+05 SQ.M. THICK SLICK THICKNESS = .65011E-03 METERS
 TOTAL MASS OF THICK SLICK = .25224E+05 KG.
 TOTAL EVAPORATED MASS = .97213E+05 KG.
 RATE OF EVAPORATION = .89954E-04 KG/(SEC-SQ.P.)
 TOTAL DISSOLVED MASS = .27462E+02 KG.
 RATE OF DISSOLUTION = .25419E-07 KG/(SEC-SQ.P.)

TOTAL MASS = .12246E+06 KG.

THE CENTER OF THE SLICK IS LOCATED AT X = .16869E+04 METERS AND Y = .23915E+03 METERS

VII. CONCLUSIONS AND RECOMMENDATIONS

The models of spreading, evaporation, dissolution, and movement for spills of buoyant, insoluble chemicals have been completely reformulated and now cover nearly every practical combination of chemical thermophysical properties, discharge rate, total volume spilled, and type of waterway. Eight experimentally-verified models are now available that can be used to assess the hazards of a floating chemical slick from an accidental tank rupture: (1) continuous or (2) instantaneous spills in a steady river; (3) continuous or (4) instantaneous spills in a tidal river; (5) continuous or (6) instantaneous spills in a circular, rectangular, or irregularly-shaped (user-specified) lake; and (7) continuous or (8) instantaneous spills near a straight or irregularly-shaped (user-specified) coast. The wind can be specified as constant or time-varying for all the models, and the currents for the lake and coastal models can be specified as a function of position as well as of time.

The spreading and movement models were adapted from the best state-of-the-art models available. None of the spreading models in the literature accounted for a loss of mass, as would be caused by evaporation of dissolution, and so, the available models had to be modified to include this effect in a realistic way. The final form of the models concentrate on predicting the dynamics of the "gravity-viscous" or "thick slick" phase of the spreading since that phase represents the greatest and most prolonged hazard. The initial, short-duration "gravity-inertial" phase of spreading is included primarily to provide the initial conditions for the gravity-viscous phase. Likewise, the surface tension-viscous or "thin slick" phase of the spreading is included primarily as a small loss-of-mass term in the thick slick equations; evaporation and dissolution from the thin slick are neglected as being very small.

The models for the rate of mass-transfer due to evaporation and dissolution were developed from boundary layer theory and realistically account for the effects of winds and currents. It is recognized that a boundary layer model may not predict all the dissolution processes of floating insoluble chemicals when significant waves are present, but better models are not yet available.

Large scale instantaneous and continuous spills of a variety of chemicals were used to establish the empirical constants in the spreading models. The spills, organized in accordance with the Test Plan approved by the USCG, were conducted in two facilities—a large outdoor basin, in which spreading could be investigated in water without a current, and an indoor channel, in which spreading in a current could be investigated. Some of the outdoor spills employed volatile chemicals in order to assess the effects of evaporation on spreading. An environmental wind tunnel and a wind-wave tunnel were used to investigate evaporation and dissolution in detail. A variety of different volatile chemicals were employed, and the tests were conducted for many wind speeds and wave characteristics. The predictions of the spreading, evaporation, and dissolution models were then compared to results of tests covering a wide range of conditions of discharge rate, volume spilled, winds, currents, and chemical properties. In all cases, a generally close comparison was found with the test results.

Although the revised models for the spreading, evaporation, dissolution, and movement of floating, insoluble chemicals are now suitable for the Hazard Assessment Computer System, the models could still be extended in several ways. Chemicals of moderate (but low) solubility could be included by further development of the dissolution model to incorporate such mass transfer processes as droplet entrainment by waves; this extension would require additional wind-wave tunnel experiments to acquire the necessary physical insight and data. The continuous-discharge spreading model could be improved by further analysis and testing to make it applicable to conditions of very low transport velocity (e.g., wind without current). All the spreading models could be modified to incorporate the anomalous behavior (e.g., lens formation and slick breakup) observed for some chemicals for some spill conditions. Finally, the long-term movement and potential breakup of the slick in open water could also be included in the model by further research.

REFERENCES

1. Phani P. K. Raj and Ashok S. Kalelkar, "Assessment Models in Support of the Hazard Assessment Handbook," Arthur D. Little, Inc., Cambridge, Mass., AD-776617 (1974).
2. Phani P. K. Raj and Peter M. O'Farrel, "Development of Additional Hazard Assessment Models," Arthur D. Little, Inc., Cambridge, Mass., Contract DOT-CG-24655A-Mod 16, AD-A042365 (March 1977).
3. N. A. Eisenberg, C. J. Lynch, R. M. Kumar, R. J. Breedina, and M. N. Durrani, "A Critical Technical Review of Six Hazard Assessment Models," Enviro Control, Inc., Rockville, Maryland, AD-A035399 (December 1975).
4. A. H. Rausch, R. M. Kumar, and C. J. Lynch, "A Critical Technical Review of Six Additional Hazard Assessment Models," Enviro Control, Inc., Rockville, Maryland, AD-A044198 (1977).
5. F. T. Dodge, E. B. Bowles, J. E. Mann, and R. E. White, "Experimental Verification and Revision of the Venting Rate Model of the Hazard Assessment Computer System and the Vulnerability Model," Southwest Research Institute, San Antonio, Texas, Final Report, Contract DOT-CG-73623-A, AD-A095413 (July 1980).
6. F. T. Dodge and E. B. Bowles, "Draining of Tanks with Submerged Outlets or Without Vacuum-Relief," Trans. ASME, J. Fluids Engineering, 104, pp. 67-71, (1982).
7. G. A. Waldman, R. A. Johnson, and P. C. Smith, "The Spreading and Transport of Oil Slicks on the Open Ocean in the Presence of Wind, Waves, and Currents," AVCO Corporation, Wilmington, Mass., AD-765926 (July 1973).
8. Keith D. Stolzenbach, Ole S. Madsen, E. Eric Adams, Andrew M. Pollack, and Cortis K. Cooper, "A Review and Evaluation of Basic Techniques for Predicting the Behavior of Surface Oil Slicks," Massachusetts Institute of Technology Report No. MIT SG77-8, PB-268-220 (1977).
9. R. C. Kollmeyer and M. E. Thompson, "New York Harbor Oil Drift Prediction Model," in Proceedings, 1977 Joint Conference on Prevention and Control of Oil Spills, (American Petroleum Institute, Washington, 1977) pp. 441-445.
10. S. P. Murray, "Turbulent Diffusion of Oil in the Ocean," Limnology and Oceanography, 27: 651-660 (1972).
11. F. Krogh, "OILSIM, Oil Spill Simulation Model," Report 77-189, Det norske Veritas, Oslo, Norway (1977).
12. H. Wang, J. R. Campbell, and J. D. Ditmars, "Computer Modeling of Oil Drift and Spreading in Delaware Bay," Report CMS-RANN-1-76, Department of Civil Engineering and College of Marine Studies, University of Delaware, Newark, Delaware (March 1976).

13. J. A. Fay, "The Spread of Oil Slicks on a Calm Sea," Oil on the Sea, edited by D. P. Hoult, (Plenum Publishing Corp., London, 1969) pp. 53-63.
14. T. K. Fannelop and G. D. Waldman, "Dynamics of Oil Slicks," AIAA Journal, 10: 506-510 (1972).
15. T. R. Sundaram, "Spread of Oil Slicks on a Natural Body of Water," Journal of Hydronautics, 14: 124-126 (1980).
16. P. C. Blokker, "Spreading and Evaporation of Petroleum Products on Water," Proceedings Fourth International Harbour Conference (Antwerp, Belgium, 1964), pp. 911-919.
17. D. Mackay, I. Buist, R. Mascarenhas, and S. Paterson, "Oil-Spill Processes and Models," Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, Canada (1978).
18. J. Buckmaster, "Viscous-Gravity Spreading of an Oil Slick," Journal of Fluid Mechanics, 59: 481-491 (1973).
19. P. R. Pujado and L. E. Scriven, "Sessile Lenticular Configurations: Translationally and Rotationally Symmetric Lenses," Journal of Colloid and Interface Science, 40: 82-98 (1972).
20. M. F. Coantic, "Coupled Energy Transfer and Transformation Mechanisms Across the Ocean-Atmosphere Interface," 6th International Heat Transfer Conference, Volume 5, (Hemisphere Publishing Corp., Washington, 1978) pp. 73-87.
21. A. Favre and Klaus Hasselmann, Turbulent Fluxes Through the Sea Surface, Wave Dynamics, and Prediction, (Plenum Publishing Corp., London, 1978).
22. F. J. Resch and J. P. Selva, "Turbulent Air-Water Mass Transfer Under Varied Stratification Conditions," Journal of Geophysical Research, 84C: 3205-3217 (1979).
23. Herman Schlichting, Boundary Layer Theory, Fourth Edition (McGraw-Hill Book Company, New York, 1960).
24. E. R. G. Eckert and Robert M. Drake, Jr., Heat and Mass Transfer, Second edition (McGraw Hill, New York, 1959) p. 215.
25. Jin Wu, "Wind-Stress Coefficients Over Sea Surface Near Neutral Conditions - A Revisit," Journal of Physical Oceanography, 10: 727-740 (1980).
26. B. A. Kader and A. M. Yaglom, "Heat and Mass Transfer Laws for Fully Turbulent Wall Flows," International Journal of Heat and Mass Transfer, 15: 2329-2351 (1972).
27. B. A. Kader and A. M. Yaglom, "The Universal Law of Turbulent Heat and Mass Transfer from the Wall at Large Reynolds and Peclet Number," Soviet Physics-Doklady, 15: 16-19 (1970).

28. A. M. Yaglom and B. A. Kader, "Heat and Mass Transfer Between a Rough Wall and Turbulent Fluid Flow at High Reynolds and Peclet Numbers," Journal of Fluid Mechanics, 62: 601-623 (1974).
29. Robert L. Street, "Turbulent Heat and Mass Transfer Across a Rough, Air-Water Interface: A Simple Theory," International Journal of Heat and Mass Transfer, 22: 885-899 (1979).
30. J. T. Park and F. T. Dodge, "Revision and Experimental Verification of the HACS Model for Spreading, Movement, Dissolution, and Dissipation of Insoluble Chemicals Spilled Onto Water," Task 1 Interim Report, Contract DTCG23-80-C-20026, Southwest Research Institute.
31. P. A. Mangarella, A. J. Chambers, R. L. Street, and E. Y. Hsu, "Laboratory Studies of Evaporation and Energy Transfer Through a Wavy Air-Water Interface," Journal of Physical Oceanography, 3: 93-101 (1973).
32. Stuart D. Smith, "Comment on A New Evaluation of the Wind Stress Coefficient Over Water Surfaces," Journal of Geophysical Research, 86C: 4307 (1981).
33. J. Amorochio and J. J. DeVries, "Reply," Journal of Geophysical Research, 86C: 4308 (1981).
34. William G. Van Dorn, Oceanography and Seamanship, (Dodd, Mead and Company, New York, 1974) pp. 187-227.
35. G. E. Fortescue and J. R. A. Pearson, "On Gas Absorption Into a Turbulent Liquid," Chemical Engineering Science, 22: 1163-1175 (1967).
36. Dudley A. Shaw and Thomas J. Hanratty, "Turbulent Mass Transfer Rates to a Wall for Large Schmidt Number," AIChE Journal, 23: 28-37 (1977).
37. Hiromasa Ueda, Reinhardt Moller, Satoru Komori, and Tokuro Mizushima, "Eddy Diffusivity Near the Free Surface of Open Channel Flow," International Journal of Heat and Mass Transfer, 20: 1127-1136 (1977).
38. Hugo B. Fischer, E. John List, Robert C. Y. Koh, Jorg Imberger, and Norman H. Brooks, Mixing in Inland and Coastal Waters (Academic Press, New York, 1979) pp. 104-472.
39. Hugo B. Fischer, "Longitudinal Dispersion and Turbulent Mixing in Open-Channel Flow," in Annual Review of Fluid Mechanics, Volume 5, edited by Milton Van Dyke, Walter G. Vincenti, and J. V. Wehausen, (Annual Reviews, Inc., Palo Alto, California, 1973) pp. 59-78.
40. N. Yotsukura and W. W. Sayre, "Transverse Mixing in Natural Channels," Water Resource Research, 12: 695-704 (1976).
41. L. E. Webb, R. Taranto, and E. Hashimoto, "Operational Oil Spill Drive Forecasting," 7th U. S. Navy Symposium of Military Oceanography (May 1970).

42. R. L. Reisbig, "Oil Spill Drift Caused by the Coupled Effects of Wind and Waves," University of Missouri, Rolla, Missouri, AD-777702 (October 1973).
43. F. Pasquill, "Evaporation from a Plane, Free-Liquid Surface Into a Turbulent Air Stream," Proceedings of the Royal Society (London) A182: 75-94 (1943).
44. R. Reijnhart and R. Rose, "Vapour Cloud Dispersion and the Evaporation of Volatile Liquids in Atmospheric Wind Fields - II. Wind Tunnel Experiments," Atmospheric Environment, 14: 759-762 (1980).
45. J. T. Lin, M. Gad-el-Hak, and H. T. Liu, "A Study to Conduct Experiments Concerning Turbulent Dispersion of Oil Slicks," Flow Research Company, Kent, Washington, AD-A058802 (1978).
46. R. L. Street, C. S. Wang, D. A. McIntosh, and A. W. Miller, Jr., "Fluxes Through the Boundary Layers at an Air-Water Interface: Laboratory Studies," in Turbulent Fluxes Through the Sea Surface, Wave Dynamics, and Prediction, edited by A. Favre and Klaus Hasselmann (Plenum Publishing Corp., London, 1978) pp. 99-120.
47. R. J. Moffatt, "Contributions to the Theory of Uncertainty Analysis for Single-Sample Experiments," in The 1980-81 AFOSR-HTTM - Stanford Conference on Complex Turbulent Flows: Comparison of Computation and Experiment, edited by S. J. Kline, B. J. Cantwell, and G. M. Lilley (Stanford Univ., 1981) pp. 40-56.
48. Donald Mackay and Wan Ying Shiu, "A Critical Review of Henry's Law Constants for Chemicals of Environmental Interest," J. Phys. Chem. Ref. Data, 10: 1175-1199 (1981).
49. A. S. Monin and A. M. Yaglom, Statistical Fluid Mechanics: Mechanics of Turbulence, Volume 1, (The MIT Press, Cambridge, Massachusetts, 1971) pp. 270-295.
50. J. O. Hinze, Turbulence, (McGraw-Hill Book Company, Inc., New York, 1959) pp. 465-487.

APPENDIX A
Physical Properties of Chemicals

Appendix A

PHYSICAL PROPERTIES OF CHEMICALS

A.1 Introduction

Some of the chemical properties for spills on water of slightly soluble chemicals with a specific gravity of less than one were included in the revised HACS computer model. Several of these properties, molecular diffusivity for example, were not in the previous HACS model. This appendix describes the models of these physical properties. Tables A.1 through A.4 contain numerical values of various physical properties and their relevant constants for twenty chemicals of interest. The list was expanded to include the seven chemicals in Tables A.5 through A.7; however, this latter list has not been added to the computer code. The physical properties of air and water have also been modeled, but they are not listed in the tables.

Five of the chemicals in Table A.1, butadiene (1,2), chlorobutane-1, 3-diene (2), cyclohexene, methyl cyclohexane, and trimethylbenzene (1,2,3), are not in HACS. Two of these chemicals have boiling points less than 20°C. Butadiene (1,2) and ethyl chloride have boiling points of 10.3 and 12.2°C, respectively. Butadiene (1,2) should not be confused with butadiene (1,3), HACS code BDI, which has the same atomic weight but a boiling point of -4.4°C.

A.2 Density

The density of the chemicals in HACS is a linear function of temperature from Potts [A.1]

$$\rho = a_0 + a_1 t \quad \text{A.(1)}$$

where ρ is the density in gm/cm³, t is the temperature in °C, and a_0 and a_1 are constants. Since all chemicals are not in HACS, another model for density was selected. Reid, et al. [A.2] recommend the following formula from Yamada and Gunn [A.3].

$$\rho = \rho_0 z^\phi \quad \text{A.(2a)}$$

$$\phi = (1 - T_0/T_c)^{2/7} - (1 - T/T_c)^{2/7} \quad \text{A.(2b)}$$

$$z = 0.29056 - 0.08775 w \quad \text{A.(2c)}$$

where ρ_0 is the reference density at temperature T_0 in °K, T_c is the critical temperature in °K, and w is the Pitzer acentric factor. The necessary constants for the calculation of density are tabulated in Tables A.1 and A.5. From [A.2], the Pitzer acentric factor is defined as

$$w = -\log(p_v/p_c) - 1 \quad \text{A.(3)}$$

where p_c is the critical pressure and p_v is the vapor pressure at $T = 0.7 T_c$. Values of w have been compiled by Reid, et al., but those that are not available can be estimated from Eq. A.(3). Critical temperature and pressure are tabulated by Dean [A.4] and Reid, et al. [A.2].

Equations A.(2) are valid over a wider temperature range than the linear approximation of Eq. A.(1). A detailed analysis of the density data has not been done, but spot checks indicate that Eq. A.(1) is accurate within the range of temperatures likely to be encountered in the environment. For example, the difference in density for benzene for Eqs. A.(1) and A.(2) is less than 0.2% between 0 and 40°C. Equations A.(2) appear to be in agreement with the density plots for hydrocarbons from Gallant [A.5; A.6].

The reference values in Tables A.1 and A.5 are all at 20°C although two of the chemicals will vaporize at that temperature. The properties in this table were extrapolated to 20°C by the appropriate formulas for convenience.

A.3 Vapor Pressure and Density

Vapor pressure is required in the calculation of w in Eq. A.(3) and the vapor density. From [A.4] and [A.1], vapor pressure is related to temperature by

$$\log p_v = A - B/(t+C) \quad \text{A.(4)}$$

where A, B, and C are constants. The constants from HACS and Dean [A.4] are compared in Table A.2. For the present, the constants from [A.4] are being used in the computer program. Some differences exist, but these may be attributable to the temperature ranges of validity for the constants. Changes in units only affect the constant A which is

$$A = \log K + A' \quad \text{A.(5)}$$

where K is the conversion constant. For example, if A' is for p_v in Torr, then K must be 1333.2279 for p_v in dynes/cm². Values of A, B, and C are also tabulated by Reid, et al. [A.2] for p_v , but no comparisons have been made since their results must be converted to base 10 logarithm, log. The conversion formulas are

$$A = A_0 \log e \quad \text{A.(6a)}$$

$$B = B_0 \log e \quad \text{A.(6b)}$$

where A_0 and B_0 are the constants for the natural logarithm, ln, version of Eq. A.(4).

The mass transfer equation for evaporation from Eq.(III.19) is

$$J_0 = Da_s \rho_s u_{s,s} (C_s - C_\infty) \quad \text{A.(7)}$$

where J_0 is the mass transfer per unit area, Da_* is the Dalton number, ρ_a is the air density, u_{*a} is the friction velocity of the air, and C_s and C_∞ are the vapor concentrations at the surface and freestream, respectively. Normally, C_∞ is zero. The quantity $\rho_a C_s$ is the vapor density which is given by the perfect gas law

$$\rho_v = M p_v / R_* T_s \quad A.(8)$$

where M is the molecular weight of the chemical from Table A.1, p_v is the vapor pressure from Eq. A.(4), T_s is the absolute surface temperature, and R_* is the universal gas constant whose value is 8.31432×10^7 dyne-cm/mole-°K from the U.S. Standard Atmosphere, 1976. [A.7].

A.4 Diffusivity in Air and Water

Diffusivity is required in the calculation of Dalton number for the mass transfer. The diffusivities in water and air are respectively

$$D_w = (D_{ow} \mu_{ow}/T_o) (T/\mu_w) \quad A.(9)$$

$$D_a = (D_{oa} p_o/T_o^{3/2}) (T^{3/2}/p) \quad A.(10)$$

where the subscript o is for the reference value. The reference temperature, T_o , and pressure, p_o , are 293.15°K (20°C) and 1.01325×10^6 dynes/cm², respectively. The reference values of the diffusivities are listed in Table A.1. The experimental diffusivities of benzene, cyclohexane, pentane, and toluene in water, D_{ow} , are taken from Witherspoon and Bonoli [A.8] and those of benzene, octane, and toluene in air, D_{oa} , are from Gray [A.9]. The remaining diffusivities were estimated by methods described by Park and Dodge [A.30]. Data on the diffusivities in sea water are not available.

A.5 Surface and Interfacial Tensions

The surface tension and the interfacial tension with water for the various chemicals are required in the spreading model. The surface tension of a liquid as a function of temperature is according to [A.4]

$$\sigma_{oa} = a_0 - a_1 t \quad A.(11)$$

where a_0 and a_1 are constants and t is the temperature in °C. Values of the constants from [A.4] are tabulated in Table A.3. Similar information of the interfacial tensions in water as a function of temperature is not available. The surface and interfacial tensions at a specific temperature are also listed in Davies and Rideal [A.10], and Weast and Astle [A.11].

An important parameter in spreading is the net spreading coefficient which is

$$\sigma = \sigma_{wa} - \sigma_{ow} - \sigma_{oa} \quad A.(12)$$

where σ_{wa} is the surface tension of water or the interfacial tension of water and air, σ_{oa} is the surface tension of the chemical, and σ_{ow} is the interfacial tension of the chemical with water. Estimates of the net spreading coefficient are listed in Tables A.3 and A.7.

The mass transfer equation for dissolution is similar to that of evaporation except that the friction velocity and density are in water. From Eq. A.(7), the mass transfer for dissolution is

$$J_o = Da_* \rho_w u_{*w} (C_s - C_\infty) \quad A.(13)$$

The available data on solubility or water concentration at the surface, C_s , are contained in Tables A.4 and A.7. The units on solubility are grams of chemical per 100 grams of water. The only data on solubility as a function of temperature are from Guseva and Parnov [A.12] for benzene, toluene, and xylene(m). The best curve fit for benzene and toluene seems to be

$$\log C_s = a_0 + a_1 t \quad A.(14)$$

whereas the solubility of xylene(m) is nearly constant between 25 and 100°C. The deviation of experimental data is less than 2% in the temperature range of $0 \leq t \leq 50^\circ\text{C}$ for benzene and $-10 \leq t \leq 50^\circ\text{C}$ for toluene. The remaining data in Tables A.4 and A.7 are compiled from [A.4] and [A.13].

A.6 Properties of Air

The necessary physical properties of air are taken from the U.S. Standard Atmosphere, 1976. In particular, air density and viscosity are required in the Reynolds number. The density is computed from the perfect gas law, Eq. A.(8), where the pressure and temperature are the ambient values. The molecular weight of air is 28.9644 while standard pressure and temperature are, respectively, 1.01325×10^6 dynes/cm² (1013.25 mb) and temperature 288.15 °K (15°C). Viscosity is computed from Sutherland's formula

$$\mu = \beta T^{3/2} / (T + S) \quad A.(15)$$

where β is a constant equal to 1.458×10^{-5} , S is Sutherland's constant equal to 110.4 °K, and μ is the absolute viscosity in Poise.

A.7 Properties of Water

The density, viscosity, and surface tension of water are required in the spreading model. These quantities are very accurately known for pure water. The density of water from Gildseth, et al. [A.14] is

$$\rho = 1 - [(\tau - 3.9863)^2 (\tau + 288.9414)] / [508929.2 (\tau + 68.12967)] + 0.011445 \exp (-374.3/\tau) \quad A.(16)$$

where ρ is in g/ml. Equation A.(16) fits experimental data with a mean absolute deviation of 0.7×10^{-6} g/ml for $5 < t < 80^\circ\text{C}$.

The viscosity of water has been correlated with temperature within a $\pm 0.05\%$ average deviation by Korosi and Fabus [A.15] with their measurements as

$$\log \mu_{20}/\mu = [A(t-20) + B(t-20)^2]/(C+t) \quad \text{A.(17)}$$

for $20 \leq t \leq 150^\circ\text{C}$ where $A = 1.37023$, $B = 0.000836$, and $C = 109$. The viscosity at 20°C , μ_{20} , has been measured as 0.010019 ± 0.000003 Poise by Swindells, et al. [A.16], and the National Bureau of Standards (NBS) has adopted 0.01002 as the standard value. Hardy and Cottingham [A.17] proposed the following interpolation formula for their measurements for $0 \leq t \leq 40^\circ\text{C}$

$$\log \mu = 1301./[998.333 + 8.1855 (t-20) + 0.00585 (t-20)^2] - 3.30233 \quad \text{A.(18)}$$

which has been altered to give the newer value of viscosity at 20°C .

Similar formulas for the density and viscosity of sea water have not been discovered although tabulated values are available. Cox [A.18] has tabulated the specific gravity anomaly of sea water as a function of temperature and salinity. The viscosity of sea water as a function of temperature for a salinity of 35 o/oo has been compiled by King [A.19]. Cox [A.17] has given the surface tension of sea water as

$$\sigma_{wa} = 75.64 - 0.144 t + 0.0399 C_2 \quad \text{A.(19)}$$

where C_2 is chlorinity in o/oo and chlorinity and salinity are related by

$$S_2 = 1.805 C_2 + 0.030 \quad \text{A.(20)}$$

APPENDIX A. REFERENCES

- A.1 Richard G. Potts, "Hazard Assessment Computer System HACS/UIM Users' Operation Manual Volume I," Report No. CG-D-76-81, AD-A110375 (1981).
- A.2 Robert C. Reid, John M. Prausnitz, and Thomas K. Sherwood, The Properties of Gases and Liquids, Third Edition (McGraw-Hill Book Company, New York, 1977) pp. 566-588.
- A.3 Tomoyoshi Yamada and Robert D. Gunn, "Saturated Liquid Molar Volumes, The Rackett Equation," Journal of Chemical and Engineering Data, 18:234-236 (1973).
- A.4 John A. Dean, Lange's Handbook of Chemistry, 12th Edition (McGraw-Hill Book Company, New York, 1979).
- A.5 R. W. Gallant, Physical Properties of Hydrocarbons, Volume 1 (Gulf Publishing Company, Houston, 1968).
- A.6 Robert W. Gallant, Physical Properties of Hydrocarbons, Volume 2 (Gulf Publishing Company, Houston, 1970).
- A.7 U. S. Standard Atmosphere, 1976, NOAA-S/T 76-1562 (U.S. Government Printing Office, Washington, 1976).
- A.8 F. A. Witherspoon and Luciano Bonoli, "Correlation of Diffusion Coefficients for Paraffin, Aromatic, and Cycloparaffin Hydrocarbons in Water," I and EC Fundamentals, 8:589-591 (1969).
- A.9 Douglas C. Gray, "Solvent Evaporation Rates," American Industrial Hygiene Association Journal, 35:695-710 (1974).
- A.10 J. T. Davies and E. K. Rideal, Interfacial Phenomena, Second Edition (Academic Press, New York, 1979).
- A.11 Robert C. Weast and Melvin J. Astle, CRC Handbook of Chemistry and Physics, 61st Edition (CRC Press, Inc., Boca Raton, Florida, 1980).
- A.12 A. N. Guseva and Ye. I. Parnov, "The Solubility of Several Aromatic Hydrocarbons in Water," Vestnik Moskovskogo Universiteta, 18:76-78 (1963). U. S. Army Medical Intelligence and Information Agency, Translation USAMIIA-K-6467, AD-A029649 (1976).
- A.13 Frank W. Mackison, R. Scott Stricoff, and Lawrence J. Partridge, Jr., NIOSH/OSHA Pocket Guide to Chemical Hazards, DHEW (NIOSH) Publication No. 78-210 (U.S. Government Printing Office, Washington, 1980).
- A.14 Wayne Gildseth, Anton Habenschuss, and Frank H. Spedding, "Precision Measurements of Densities and Thermal Dilation of Water Between 5° and 80°C," Journal of Chemical and Engineering Data, 17:402-409 (1972).

- A.15 Alexander Korosi and Bela M. Fabuss, "Viscosity of Liquid Water From 25° to 150°C Measurements in Pressurized Glass Capillary Viscometer," Analytical Chemistry, 40:157-162 (1968).
- A.16 J. F. Swindells, J. R. Coe, Jr., and T. B. Godfrey, "Absolute Viscosity of Water at 20°C," Journal of Research of the National Bureau of Standards, 48:1-31 (1952).
- A.17 Robert C. Hardy and Robert L. Cottingham, "Viscosity of Deuterium Oxide and Water in the Range 5° to 125°C," Journal of Research of the National Bureau of Standards, 42:573-578 (1949).
- A.18 R. A. Cox, "The Physical Properties of Sea Water," in Chemical Oceanography edited by J. P. Riley and G. Skirrow (Academic Press, London, 1965).
- A.19 D. A. King, "Basic Hydrodynamics" in Handbook of Ocean and Underwater Engineering, edited by J. J. Myers, C. H. Holm, and R. F. McAllister (McGraw-Hill Book Company, New York, 1969) pp. 2-6.

TABLE A.1 Properties of Relevant Chemicals at 20°C and 1013.25 mb

Chemical Name	HACS [1]	Dean No. [2]	Reid No. [3]	Molecular Weight M	Reference Density ρ_0 (gm/cm ³)	Pitzer Acentric Factor ω	Critical Temperature T_c (°K)	Diffusivity in Air D_{0a} (cm ² /s)	Diffusivity in Water $10^5 D_{0w}$ (cm ² /s)
Allyl Chloride	ALC	202	116	76.526	0.938	0.13	514.15	0.097	1.019
Benzene	BNZ	656	242	78.114	0.879	0.212	562.09	0.087	1.02
Butadiene (1,2)		1018	152	54.092	0.652	0.255	443.75		1.062
Butyl Acetate (iso)	IBA	1031	267	116.160	0.871	0.479	561.15	0.064	0.712
Butyl Mercaptan (n)	BTM	1103		90.19	0.841	0.300	562.95		
Chlorobuta-1,3-diene (2)	CRP	1345		88.54	0.956				
Cyclohexane	CHX	1601	249	84.162	0.779	0.213	553.45	0.081	0.84
Cyclohexene		1609	247	82.146	0.810	0.210	560.41	0.085	0.870
Dipropyl Ether (iso)	IPE	2784	278	102.177	0.725	0.34	500.05	0.063	0.744
Ethyl Chloride	ECL	3015	97	64.515	0.896	0.190	460.35	0.0913	1.128
Ethyl Mercaptan	EMC	3083	104	62.134	0.839	0.190	499.15	0.0983	1.533
Heptane (n)	HPT	3512	308	100.205	0.684	0.351	540.15	0.064	0.700
Hexane (n)	HXA	3603	271	86.178	0.659	0.296	507.35	0.070	0.764
Methyl Cyclohexane		4199	305	98.189	0.769	0.233	572.25	0.072	0.799
Nonane (n)	NAN	4917	389	128.259	0.718	0.444	594.56	0.058	0.597
Octane (n)	OAN	4944	354	114.232	0.703	0.394	568.76	0.058	0.638
Pentane	PTA	5083	223	72.151	0.626	0.251	469.65	0.075	0.84
Toluene	TOL	5960	286	92.141	0.867	0.257	591.72	0.083	0.85
Trimethylbenzene (1,2,3)		6253	383	120.195	0.894	0.39	664.45	0.065	0.695
Xylene (m)	XLM	6457	323	106.168	0.864	0.331	616.97	0.072	0.756

References:

1. Hazard Assessment Computer System (HACS) Property File Printout in CGS Units (April 1981).
2. John A. Dean, Lange's Handbook of Chemistry, 12th Edition (McGraw-Hill Book Company, New York, 1979) Table 7-4.
3. Robert C. Reid, John M. Prausnitz, and Thomas K. Sherwood, The Properties of Gases and Liquids, 3rd Edition (McGraw-Hill Book Company, New York, 1977) pp. 629-677.

TABLE A.2 Comparison of Constants in Vapor Pressure Equation^a

Chemical Name	HACS Code	A		B		C		Vapor Pressure, P_v (mb) @ 20°C	Vapor Density, ρ_v ($\mu\text{g}/\text{cm}^3$) @ 20°C
		[1]	[2]	[1]	[2]	[1]	[2]		
Allyl Chloride	ALC	10.84		1540.		273.2		386.91	1214.79
Benzene	BNZ	10.03	10.03055	1211.	1211.033	220.8	220.790	100.26	321.32
Butadiene (1,2)			10.11873		1041.117		242.274	1409.78	3128.73
Butyl Acetate (iso)	IBA	10.15		1343.		207.0		17.13	81.64
Butyl Mercaptan (n)	BTM	11.06		1877.		273.0		45.07	166.77
Chlorobuta-1,3-diene (2)	CRP		9.28640		783.45		179.7	230.82	838.49
Cyclohexane	CHX	10.87	9.96620	1720.	1201.53	273.2	222.65	103.40	357.04
Cyclohexene			10.01107		1229.973		224.10	93.81	316.17
Dipropyl Ether (iso)	IPE	10.81	9.9744	1644.	1139.34	273.0	218.7	158.96	666.38
Ethyl Chloride	ECL	10.82		1375.		273.2		1350.11	3573.66
Ethyl Mercaptan	EMC	10.75		1461.		273.0		580.30	1479.33
Heptane (n)	HPT	10.03	10.02167	1268.	1264.90	216.9	216.54	47.22	194.13
Hexane (n)	HXA	10.00	10.00091	1172.	1171.17	224.4	224.41	161.84	572.22
Methyl Cyclohexane			9.94790		1270.763		221.42	48.33	194.70
Nonane (n)	NAN	11.27	10.06383	2234.	1431.82	273.0	202.01	4.12	21.68
Octane (n)	OAN	11.09	10.04358	2028.	1351.99	273.0	209.15	13.92	65.24
Pentane	PTA	9.977	9.97786	1065.	1064.84	232.0	233.01	587.72	1739.79
Toluene	TOL	10.08	10.07954	1345.	1344.800	219.5	219.48	29.11	110.05
Trimethylbenzene (1,2,3)			10.16572		1593.958		207.08	1.40	6.90
Xylene (m)	XLM	10.13	10.13398	1462.	1462.266	215.1	215.11	8.21	35.76

^a $\log P_v = A - B/(t+C)$ - where P_v is the vapor pressure in dynes/cm², and t is the temperature in °C.

References:

1. Hazard Assessment Computer System (HACS) Property File Printout in CGS Units (April 1981).
2. John A. Dean, Lange's Handbook of Chemistry, 12th Edition (McGraw-Hill Book Company, New York, 1979) Table 10-8.

TABLE A.3 Surface and Interfacial Tensions of Relevant Chemicals

Chemical Name	IACS Code	Constants ^a		Surface Tension, σ_{oa} (dynes/cm)	Temperature t (°C)	Interfacial Tension, σ_{ow} (dynes/cm)	Temperature t (°C)	Spreading Coefficient σ (dynes/cm)
		σ_o (dynes/cm)	σ_1 (dynes/cm °C)					
Allyl Chloride	AIC			28.90	15.0	57.10	22.75	-13.24
Benzene	BNZ	31.54	0.1330	28.90 28.88 28.85	20.0	35.0	20.0	8.9
Butadiene (1,2)								
Butyl Acetate (iso)	IBA			23.70	20.0	40.0	19.85	9.1
Butyl Mercaptan (n)	BTM			26.10	20.0	30.0	20.0	16.7
Chlorobuta-1,3-diene(2)	CRP							
Cyclohexane	CHX	27.62	0.1188	24.60 25.5	20.0	50.0	24.85	-2.5
Cyclohexene		29.23	0.1223	26.78	20.0			
Dipropyl Ether (iso)	IPE	19.89	0.1048	17.10	25.05	17.10	25.05	37.7
Ethyl Chloride	ECL			19.50	20.0	40.0	-0.15	13.3
Ethyl Mercaptan	EMC			23.50		25.0		
Heptane (n)	HPT	22.10	0.0980	22.50 19.30	20.0		20.0	24.3
Hexane (n)	HXA	20.44	0.1022	18.40	20.0	51.0 51.1	19.85	1.6
Methyl Cyclohexane		26.11	0.1130	18.43	20.0	51.0	20.0	3.4
Nonane (n)	NAN	24.72	0.09347	23.85	20.0			
Octane (n)	OAN	23.52	0.09509	22.90 21.70	20.0	35.0	20.0	14.9
Pentane (n)	PTA	18.25	0.11021	21.8	20.0	50.8	20.0	0.3
Toluene	TOL	30.90	0.1189	16.0 29.0 28.43 28.5	20.0	50.2 36.10 36.53	19.85 25.0 20.0	6.5
Trimethylbenzene(1,2,3)		30.91	0.1040	28.83	20.0			6.7
Xylene (m)	XLN	31.23	0.1104	28.60 28.9			29.85	
Water		75.64	0.144	72.76	20.0	36.40	29.85	7.0

^a $\sigma_{oa} = \sigma_o - \sigma_1 t$ where t is temperature in °C.

^b $\sigma = \sigma_{oa} - \sigma_{ow}$

TABLE A.4 Solubility of Relevant Chemicals

Chemical Name	HACS Code	Constants ^a		Solubility C _s (%)	Temperature t (°C)
		a ₀	a ₁		
Allyl Chloride	ALC			0.330	25.0
Benzene	BNZ	-0.82130	0.00337	0.175	20.0
Butadiene (1,2)					
Butyl Acetate (iso)	IBA			0.600	20.0
Butyl Mercaptan (n)	BTM			0.06	
Chlorobuta-1,2-diene(2)	CRP				
Cyclohexane	CHX			0.015	28.34
Cyclohexene					
Dipropyl Ether (iso)	IPE			0.2	20.0
Ethyl Chloride	ECL			0.45 0.600	0.0 20.0
Ethyl Mercaptan	EMC			1.500	20.0
Heptane (n)	HPT			0.00027	18.0
Hexane (n)	HXA			0.00125	
Methyl Cyclohexane					
Nonane (n)	NAN			0.000015	
Octane (n)	OAN			0.000066	16.0
Pentane	PTA			0.0041	16.0
Toluene	TOL	-1.57767	0.01140	0.045	20.0
Trimethylbenzene (1,2,3)					
Xylene (m)	XLM			0.0196	25.0

$$^a \log C_s = a_0 + a_1 t$$

where C_s is solubility in g/100g of H₂O, and t is temperature in °C

TABLE A.5 Properties of Chemicals with High Spreading Coefficients

Chemical Name	HACS [1]	Dean No. [2]	Reid No. [3]	Molecular Weight M	Reference Density ρ_0 (gm/cm ³)	Pitzer Acentric Factor ω	Critical Temperature T_c (°K)	Diffusivity in Air D_{oa} (cm ² /s)	Diffusivity in Water $10^5 D_{ow}$ (cm ² /s)
Amyl Alcohol (n)	AAN	404	226	88.150	0.815	0.58	586.15	0.075	0.827
Butyl Alcohol (n)	BAN	1034	183	74.123	0.810	0.590	562.93	0.085	0.923
Ether	EET	2911	187	74.123	0.713	0.281	466.70	0.088	0.910
Ethyl Acetate	ETA	2935	172	88.107	0.901	0.303	523.25	0.083	0.898
Hexyl Alcohol (n)	HKN	3624	276	102.177	0.819	0.56	610.15	0.069	0.750
Octyl Alcohol (n)	OTA	4961	371	130.231	0.826	0.53	658.15	0.060	0.640
Undecylenic Acid		6376		184.27	0.910				

References:

1. Hazard Assessment Computer System (HACS) Property File Printout in CGS Units (April 1981).
2. John A. Dean, Lange's Handbook of Chemistry, 12th Edition (McGraw-Hill Book Company, New York, 1979) Table 7-4.
3. Robert C. Reid, John M. Prausnitz, and Thomas K. Sherwood, The Properties of Gases and Liquids, 3rd Edition (McGraw-Hill Book Company, New York, 1977) pp. 629-677.

TABLE A.6 Vapor Properties of Chemicals with High Spreading Coefficients

Chemical Name	A	B	C	Vapor Pressure, P_v @ 20°C (mb)	Vapor Density, ρ_v @ 20°C ($\mu\text{g}/\text{cm}^3$)
Amyl Alcohol (n)	10.30248	1314.56	168.11	2.062	7.457
Butyl Alcohol (n)	10.60170	1362.39	178.77	5.592	17.007
Ether	10.04522	1064.07	228.80	586.700	1784.235
Ethyl Acetate	10.22669	1244.95	217.88	98.440	355.850
Hexyl Alcohol (n)	10.98535	1761.26	196.66	0.718	3.011
Octyl Alcohol (n)	15.19500	4506.8	319.9	0.086	0.461
Undecylenic Acid					

$\log P_v = A - B/(t + c)$ where P_v is the vapor pressure in dynes/cm² and t is the temperature in °C

Reference:

John A. Dean, Lange's Handbook of Chemistry, 12th Edition (McGraw-Hill Book Company, New York, 1979) Table 10-8.

TABLE A.7 Surface and Interfacial Tensions and Solubilities of Chemicals with High Spreading Coefficients

Chemical Name	Constants		Surface Tension, σ_{oa} @ 20°C (dynes/cm)	Interfacial Tension, σ_{ow} (dynes/cm)	Temperature for σ_{ow} , t (°C)	Spreading Coefficient σ (dynes/cm)	Solubility c_s (o/o)	Temperature for c_s , t (°C)
	a_o (dynes/cm)	a_1 (dynes/cm-°C)						
Amyl Alcohol (n)	27.54	0.0874	25.79	4.4	25	42.57	2.7	22
Butyl Alcohol (n)	27.18	0.08983	25.38	1.6	20	45.78	7.7	20
Ether	18.92	0.0908	17.01	10.7	20	44.96	7.5	20
Ethyl Acetate	26.29	0.1161	23.97	2.9	30	45.89	8.7	20
Hexyl Alcohol (n)	27.81	0.0801	26.21	6.8	25	39.75	0.6	20
Octyl Alcohol (n)	29.09	0.0795	27.53	8.5	20	36.73	0.054	20
Undecylenic Acid						32.0	0	

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References:

1. John A. Dean, Lange's Handbook of Chemistry, 12th Edition (McGraw-Hill Book Company, New York, 1979) 10-35.
2. J. T. Davies and E. K. Rideal, Interfacial Phenomena, 2nd Edition (Academic Press, New York, 1963) Table 1.1 p. 2, Table 1-IV p. 17, and Table 1-VI p. 22.

APPENDIX B

Subroutines, Symbols, and Flow Charts
for Program DMODEL

TABLE B.1 LIST OF SUBROUTINES AND CALLS

1. DMODEL
Calls: AIR, SPLOC, SPREAD, SPTYPE, WATER, WB
Called by: ---
2. AIR
Calls: ---
Called by: DMODEL
3. CHEKMS
Calls: ---
Called by: INTE
4. CHEMCL
Calls: ---
Called by: SPTYPE
5. CURRT
Calls: ---
Called by: SPREAD
6. DISS
Calls: ---
Called by: INTE
7. EVAP
Calls: ---
Called by: INTE
8. FCN11, FCN12, FCN21, FCN22, FCN41, FCN42
Calls: ---
Called by: RUNKUT (through INTE)

TABLE B.1 (CONTD)

9. GROUND
Calls: ---
Called by: SPREAD
10. INIT
Calls: INT12A, INT12B, INIT4A, INIT4B
Called: SPREAD
11. INT12A
Calls: INTE, MOVE, PRINTO, TRANSP
Called by: INIT
12. INT12B
Calls: ---
Called by: INIT
13. INIT4A
Calls: INTE, MOVE, PRINTO, TRANSP
Called by: INIT
14. INIT4B
Calls: ---
Called by: INIT
15. INTE
Calls: CHEKMS, DISS, EVAP, RUNKUT
Called by: INT12A, INIT4A, SPREAD, SWITCH
16. MOVE
Calls: ---
Called by: INT12A, INIT4A, SPREAD, SWITCH

TABLE B.1 (CONTD)

17. PRINTO
Calls: ---
Called by: INT12A, INIT4A, SPREAD, SWITCH
18. RUNKUT
Calls: FCN11, FCN12, FCN21, FCN22, FCN41, FCN42, UERTST
Called by: INTE
19. SPLOC
Calls: ---
Called by: DMODEL
20. SPREAD
Calls: CURRT, GROUND, INIT, INTE, MOVE, PRINTO, SWITCH,
TRANSP, UTPEAK
Called by: DMODEL
21. SPTYPE
Calls: CHEMCL
Called by: DMODEL
22. SWITCH
Calls: INTE, MOVE, PRINTO, TRANSP
Called by: SPREAD
23. TRANSP
Calls: ---
Called by: INT12A, INIT4A, SPREAD, SWITCH
24. UERTST
Calls: UGETIO
Called by: RUNKUT

TABLE B.1 (CONTD)

- 25. UGETIO
Calls: ---
Called by: UERTST
- 26. UTPEAK
Calls: ---
Called by: SPREAD
- 27. WATER
Calls: ---
Called by: DMODEL
- 28. WBS
Calls: WIND
Called by: DMODEL
- 29. WIND
Calls: ---
Called by: WBS

TABLE B.2 INPUT VARIABLES

General

TITLE	Name of run (up to 30 characters)
TDC	Ambient temperature, °C
PB	Barometric pressure, millibars
DELT	Integration time step, seconds
TSTOP	Total run time, minutes
HMIN	Minimum allowed thickness of thick slick, meters
HTN	Thin slick thickness, meters (usually equal to HMIN)
TPT	Time interval between printout of results, minutes

Chemical Properties

DENO	Density, kg/m ³
CMW	Molecular weight
DCA	Diffusion coefficient in air, m ² /sec
DCW	Diffusion coefficient in water, m ² /sec
PV	Vapor pressure, newton/m ²
CS	Solubility limit in water, kg/m ³
SIGOA	Chemical-air interfacial tension, newton/meter
SIGOW	Chemical-water interfacial tension, newton/meter

Discharge Parameters

ITYPE	Descriptor for instantaneous or continuous spills
TEM	Total spilled volume, m ³ , for an instantaneous spill; discharge rate, m ³ /sec, for a continuous spill.
TSPILL	Total discharge time for a continuous spill, minutes.

TABLE B.2 (CONTD)

Water Body (not all are needed, depending on water body)

X0,Y0	Coordinates of spill source, meters (open water only)
W	Width of river, meters
D	Depth of river, lake, or coastal water, meters
RO	Roughness of river bottom, meters
UC	Current in river, meter/sec
U0,U1,WT,ALPH	For a tidal river: average current, m/sec; amplitude of sinusoidal current, m/sec; tidal period, minutes; phase of tide with respect to time of spill, minutes
R	Radius of circular lake, meters
L1,L2	Width and breadth of rectangular lake, meters
X(I),Y(I)	Ten x,y coordinates describing irregularly- shaped lake or coast, meters
X(1),Y(1); X(2),Y(2)	Two x,y coordinates describing a straight coast line, meters
UX(1,1),UY(1,1)	Components of a constant current in open water, meter/sec
UX(I,J),UY(I,J)	Components of a time- or spatial-varying current in open water, meter/sec; I = spatial position; J = time.
TI(I)	Ten specified time instants for a time-varying current in open water, minutes
XU(I), YU(I)	Four x,y coordinates (lake) or 10 x,y coordinates (coastal water) that describe space grid for a spatially-varying current in open water, meters
VW	Constant wind speed, meter/second
THETA1	Direction of constant wind with respect to channel axis or x-axis (open water), degrees
VWX(I)	Magnitude of time-varying wind at time I, meter/second
THETA(I)	Direction of time-varying wind with respect to channel axis or x-axis (open water), degrees
TT(I)	Ten specified time instants for a time-varying wind, minutes

TABLE B.3 COMPUTED OUTPUT VARIABLES

Initial Conditions (not all used for any case)

ATK	Thick slick area, m ²
TIIT	Time required for thick slick to spread across channel, minutes
HTK	Thick slick thickness, meters
Z	Downstream location of leading edge of thick slick (continuous spill), meters
DMASS	Mass lost from thick slick, kg
WTK	Downstream width of triangular slick, meters
RADIUS	Radius of thick slick, meters

Regular Printout. (not all used for any case)

TEMP,DIFFT	Time of printout, minutes and seconds
YY(1)	Thick slick area, m ²
YY(3)	Thick slick thickness, meters
RAD1	Thick slick radius, meters
YY(2)	Thin slick area, m ²
RAD2	Thin slick radius, m ²
TOTALM	Mass of thick slick, kg
TOTALE	Evaporated mass, kg
TOTALD	Dissolved mass, kg
EVAPM	Rate of evaporation, kg/second
DISSOM	Rate of dissolution, kg/second
TMASS	Mass of thin slick, kg
TOTS	Mass of thin and thick slicks added to evaporated and dissolved masses, kg
XW	Downstream width of triangular slick, meters

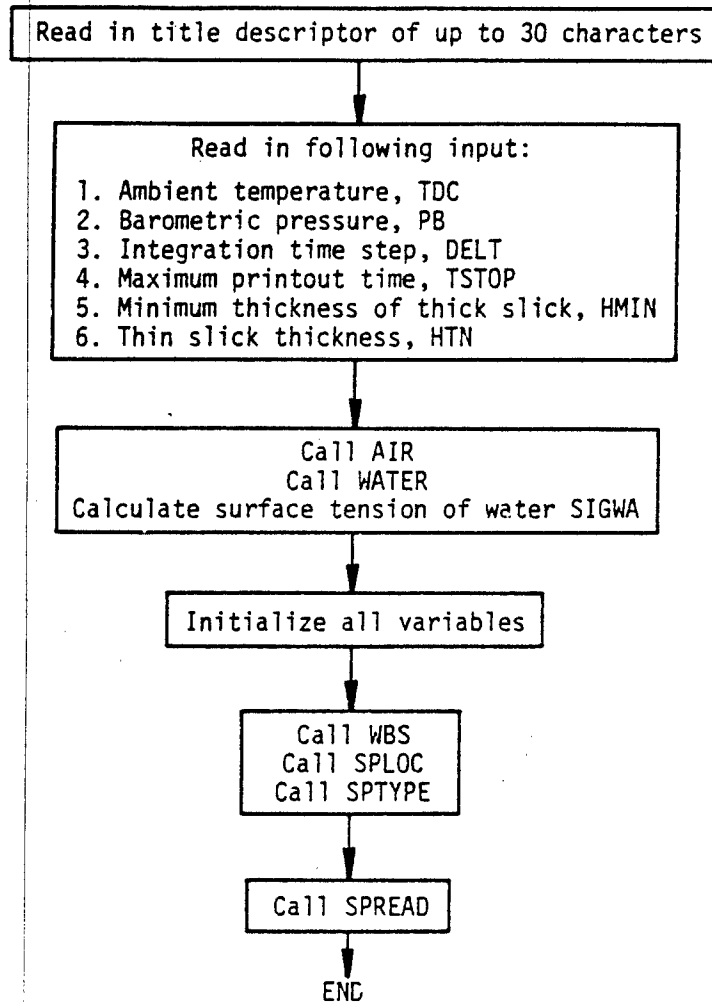
TABLE B.3 (CONTD)

XC,YC	Location of center of an instantaneous spill (open water), meters
XC	Movement of an instantaneous spill in a river, meters
—	Upstream and downstream edges of an instantan- eous spill in a river, meters
TEMP1,TEMP2	Upstream and downstream locations of a con- tinuous spill in a river, meters
XLE,YLE	Coordinates of leading edge of a triangular spill, meters
—	Time when slick impacts a coast
—	Time when thick slick thickness is less than HMIN

FIGURES B.1 TO B.16 ARE THE FLOW
CHARTS OF PROGRAM "DMODEL" and
ALL SUBROUTINES. THE SUBROUTINES
ARE GIVEN IN THE ORDER THEY ARE
FIRST ENCOUNTERED IN THE PROGRAM,
NOT IN ALPHABETICAL ORDER.

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Page B-9

FIGURE B.1 FLOW CHART FOR PROGRAM "DMODEL"



Subroutine "AIR"

This subroutine calculates the density and viscosity of air as a function of pressure and temperature.

Subroutine "WATER"

This subroutine calculates the density and viscosity of water as a function of temperature.

FIGURE B.2 FLOW CHART FOR SUBROUTINE "WBS"

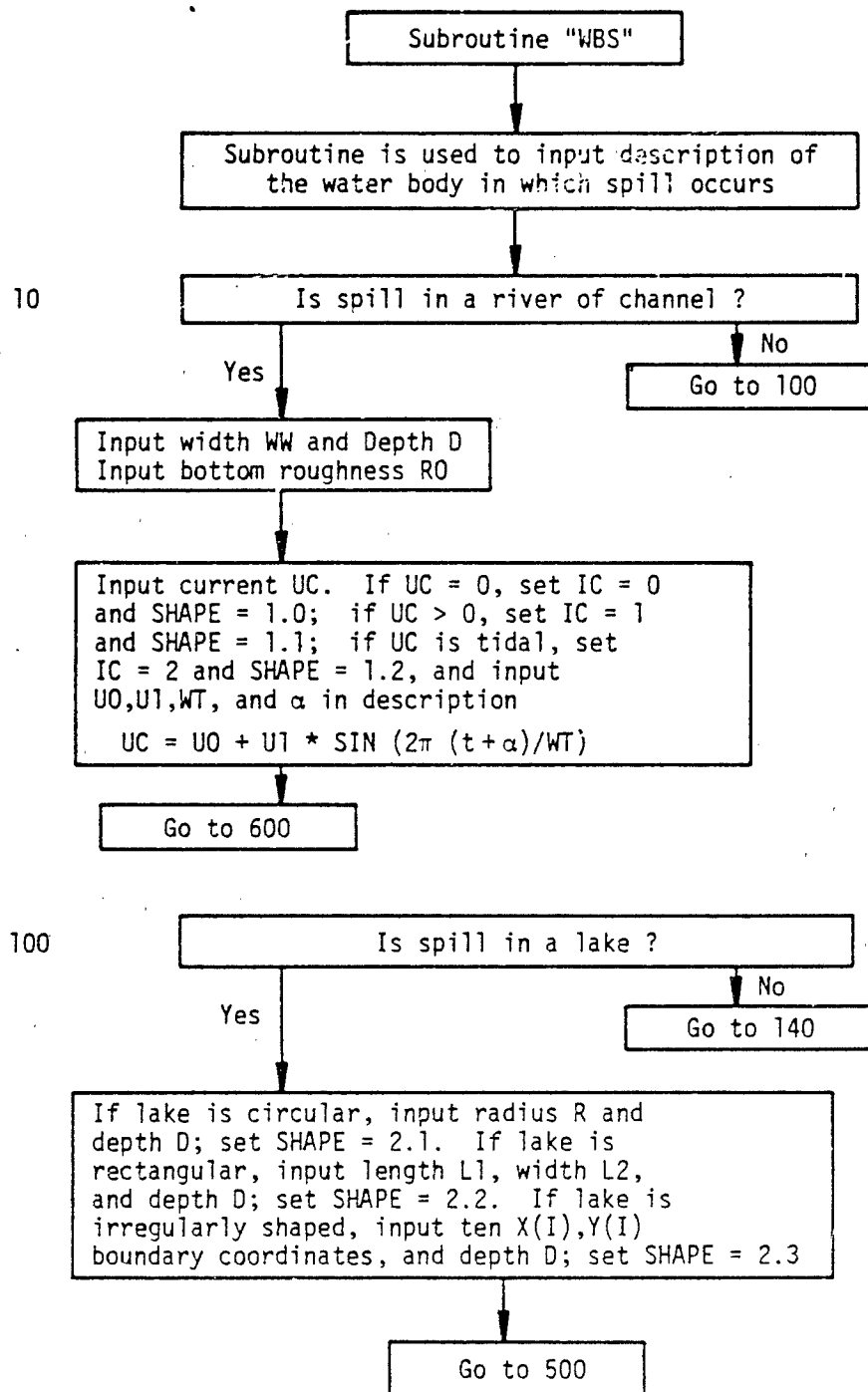


FIGURE B.2 (CONTD)

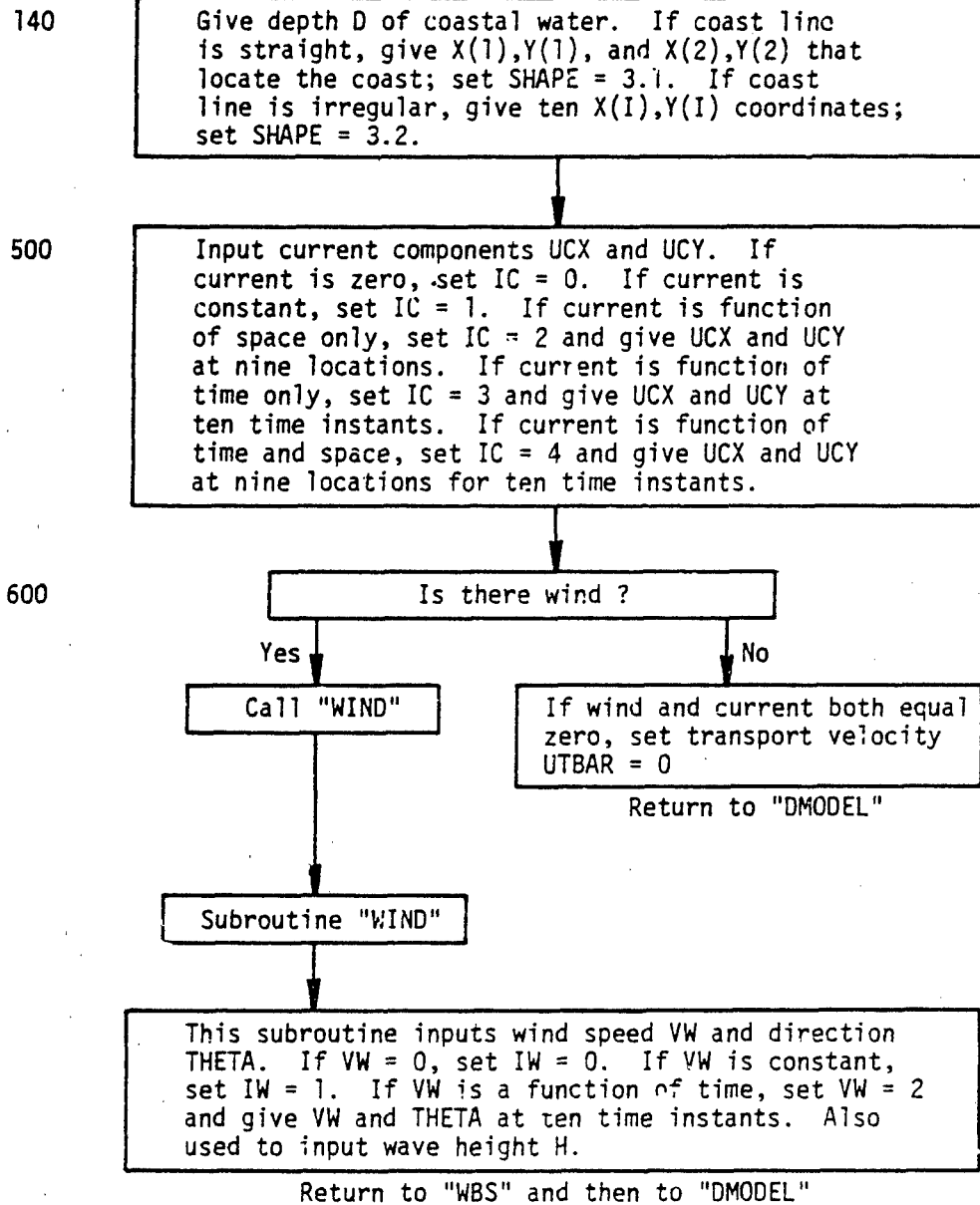


FIGURE B.3 FLOW CHARTS FOR SUBROUTINES "SPLOC" AND "SPTYPE"

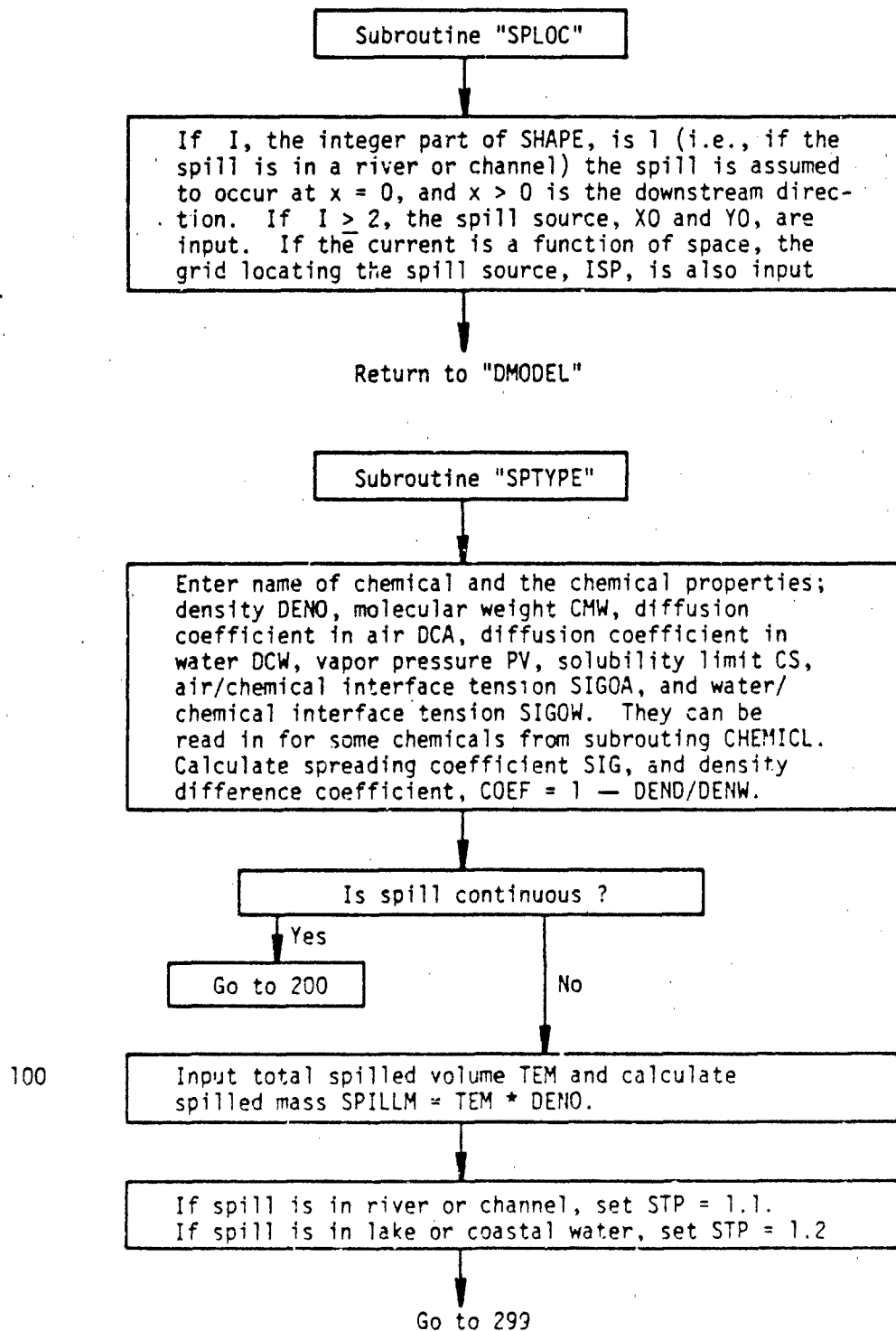


FIGURE B.3 (CONTD)

200

Input the rate of discharge TEM and total spill duration TSPILL. Calculate mass discharge rate SPILMR = TEM * DENO

If the current and wind are zero, and spill is in a river or channel, set STP = 2.1. If the current and wind are not zero and spill is in a river or channel, set STP = 2.2. If the current and wind are zero, and spill is in open water, set STP = 4.1. If the current and wind are not zero, and spill is open water, set STP = 4.2

299

Return to "DMODEL"

FIGURE B.4 FLOW CHARTS FOR SUBROUTINE "SPREAD"

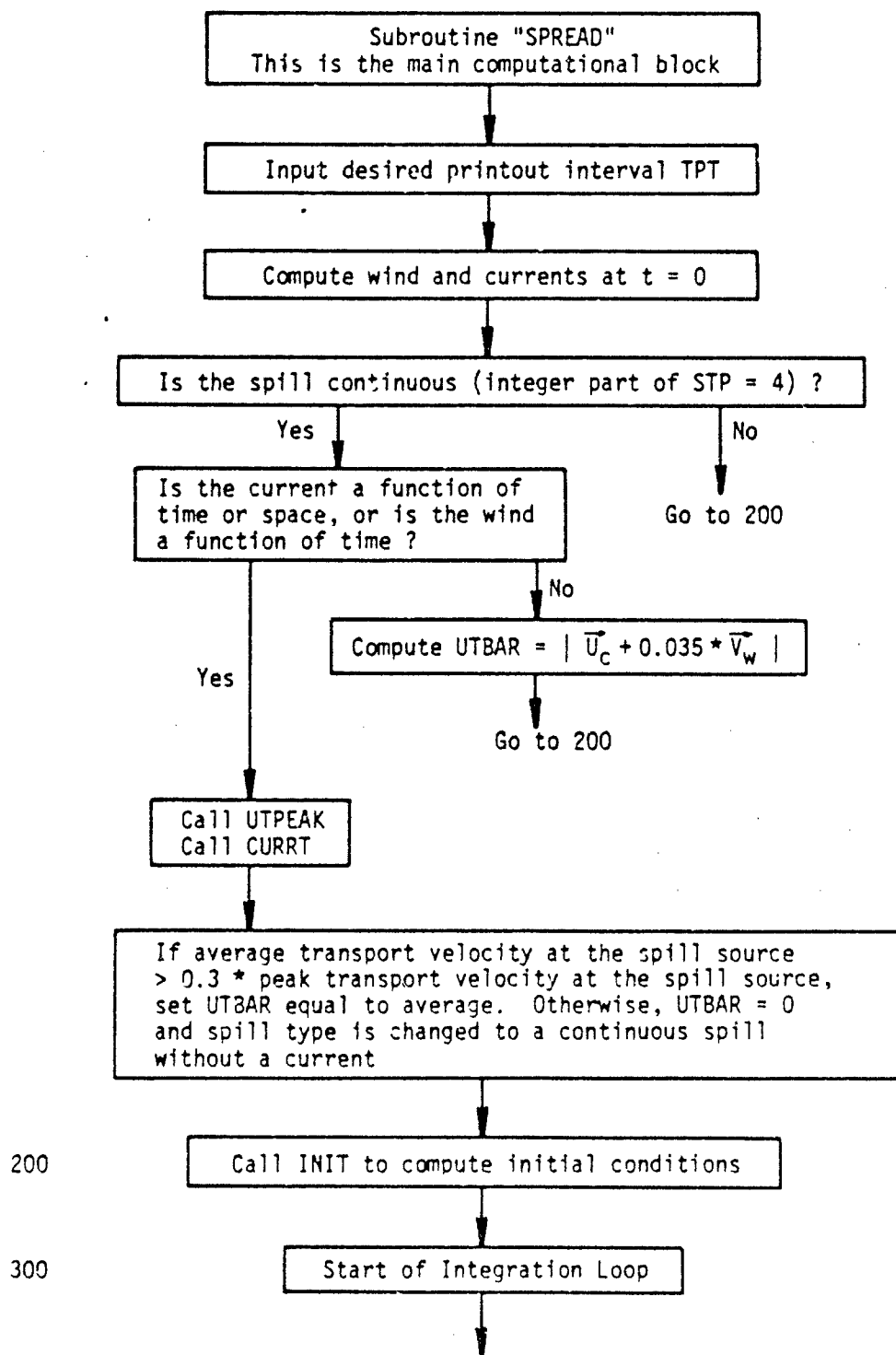


FIGURE B.4 (CONTD)

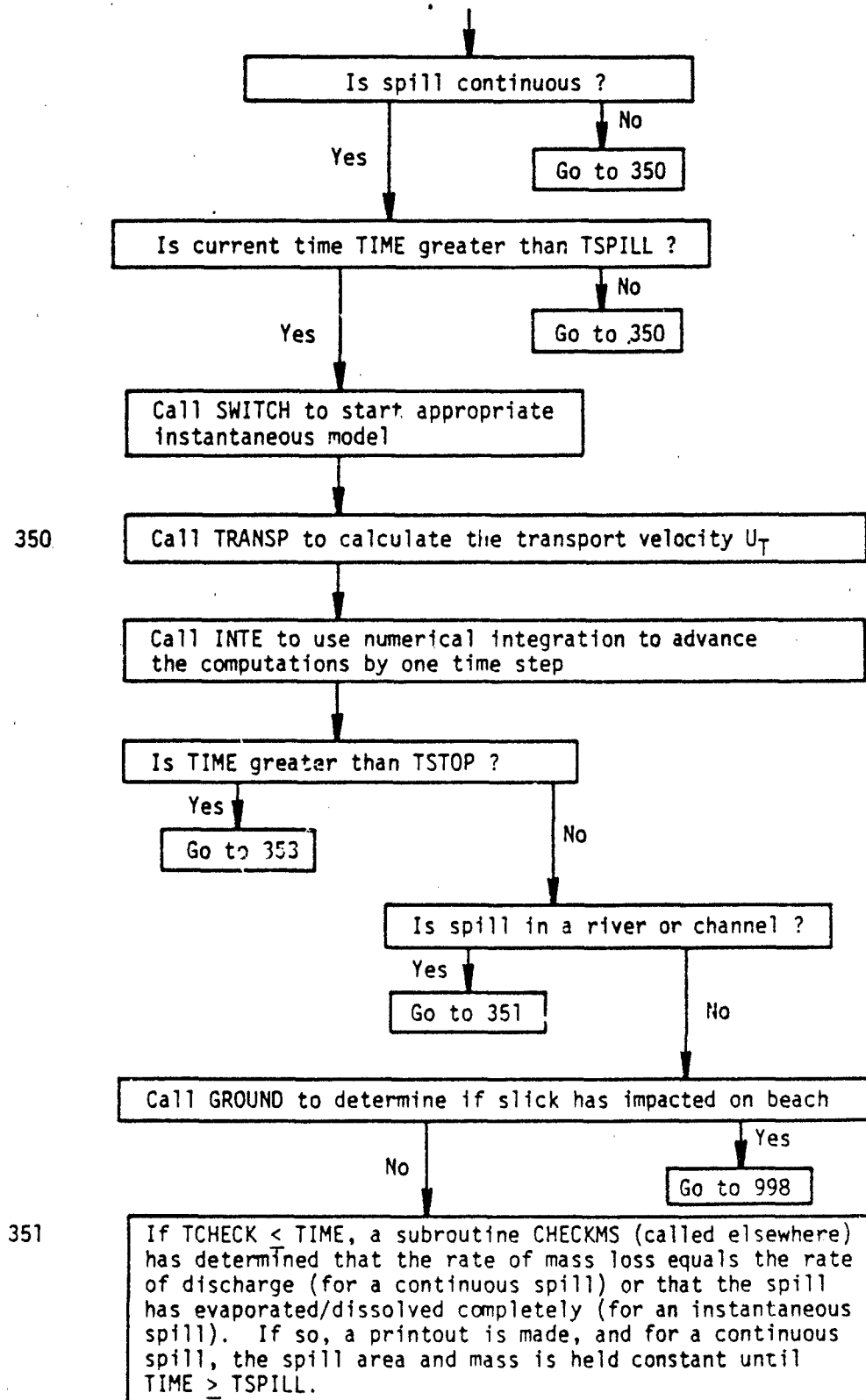


FIGURE B.4 (CONTD)

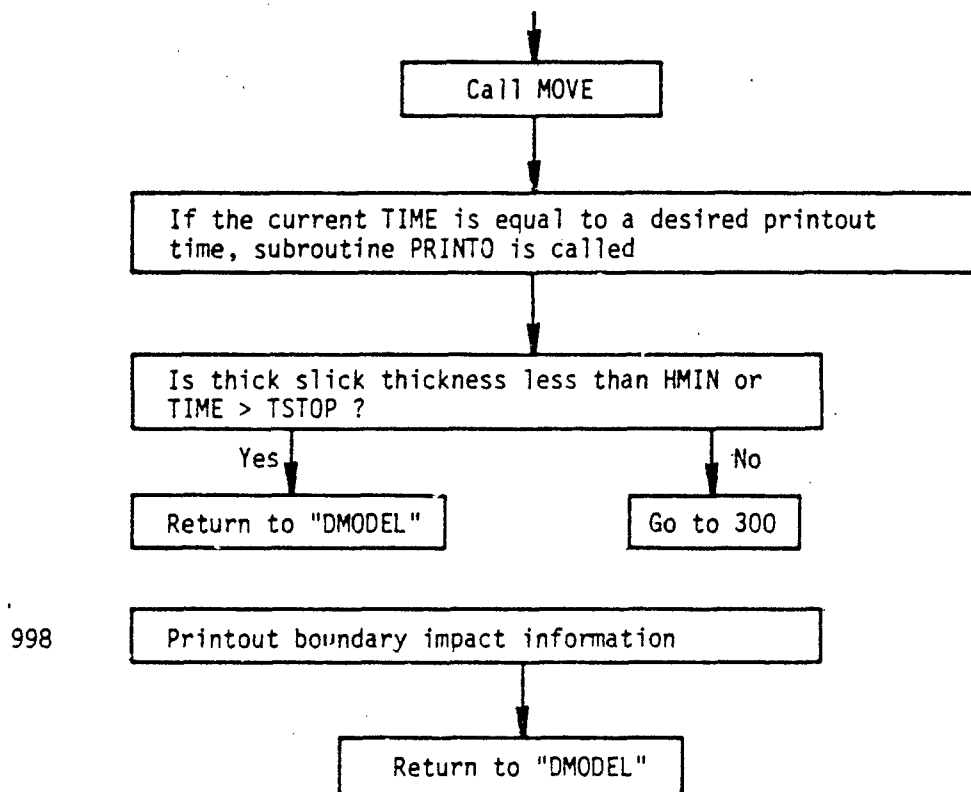


FIGURE B.5 FLOW CHARTS FOR SUBROUTINES
"UTPEAK" AND "CURRT"

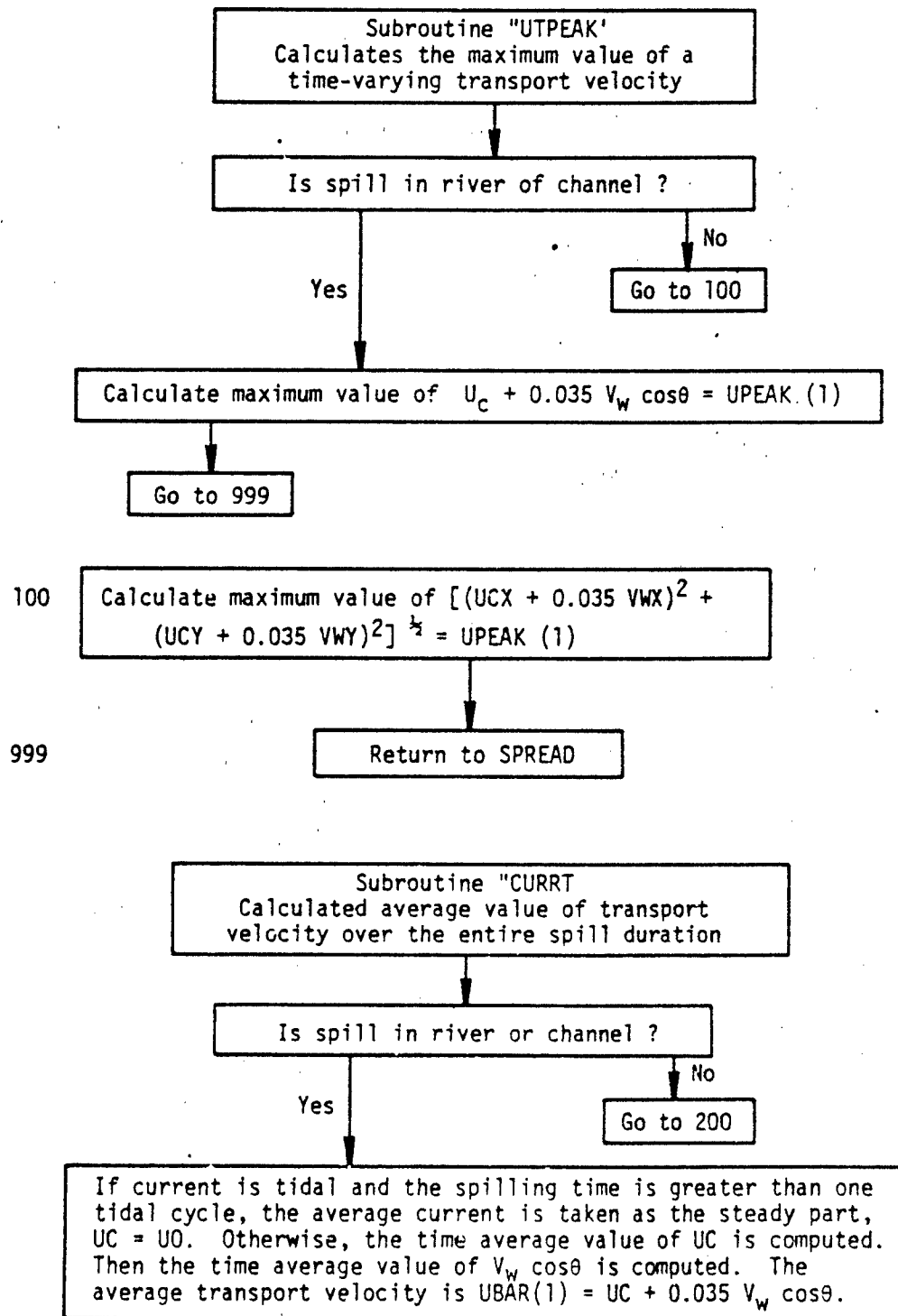


FIGURE B.5 (CONTD)

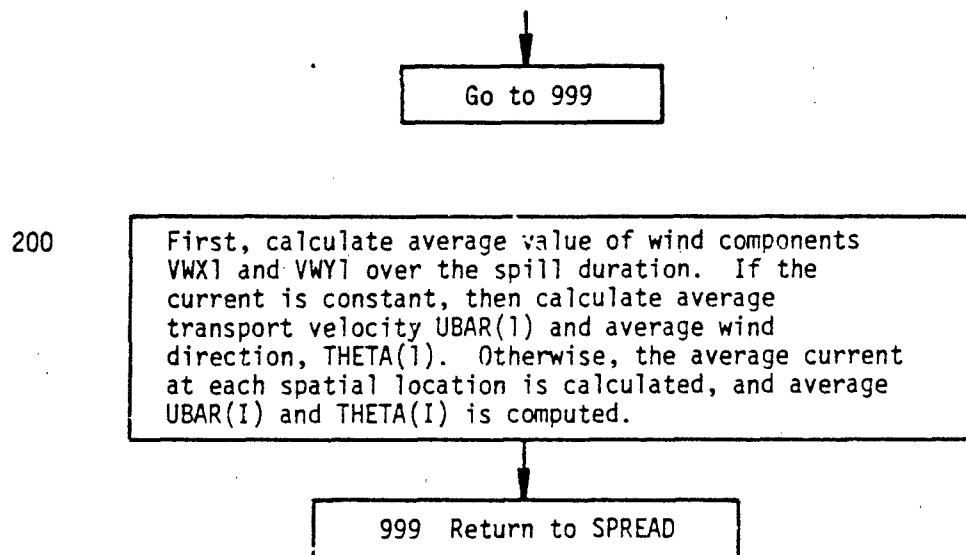
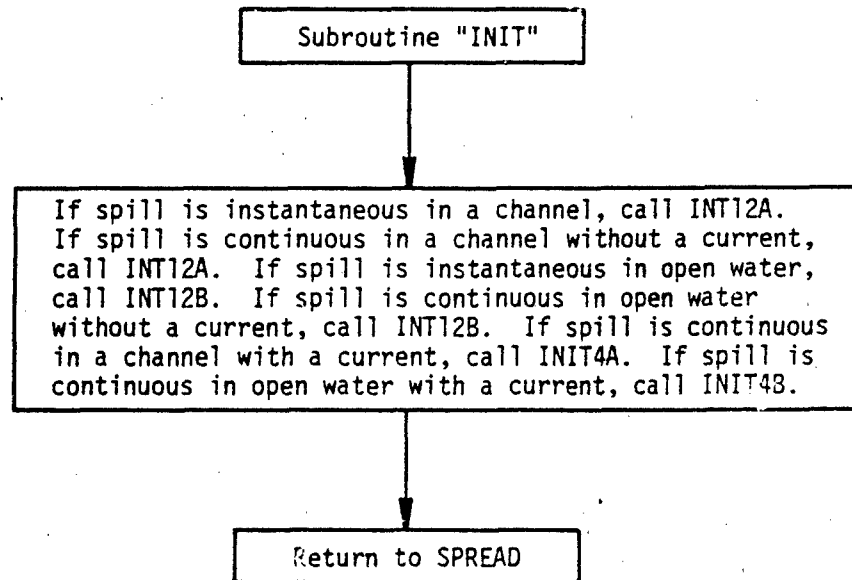


FIGURE B.6 FLOW CHART FOR SUBROUTINE "INIT"



Subroutine "INT12A"

This subroutine calculates initial conditions for spills in a channel. If the spill is continuous, and the time required for the spill to spread across the channel is greater than TSPILL, the spill is changed to instantaneous. In either case, if the time required for the spill to spread across the channel is greater than the gravity-inertial phase maximum time, the calculations are continued by numerical integration, just as in SPREAD, until the spill spreads across the channel.

FIGURE B.6 (CONTD)

Subroutine "INT12B"

This subroutine calculates initial conditions for spills in open water

Subroutine "INIT4A"

This subroutine calculates initial conditions for continuous spills in a channel with a current. If the time required for the spill to spread across the channel is greater than the gravity-inertial phase maximum time, the calculations are continued by numerical integration, just as in SPREAD, until the spill spreads across the channel

Subroutine "INIT4B"

This subroutine calculates initial conditions for continuous spills in open water without a current.

FIGURE B.7 FLOW CHART FOR SUBROUTINE "SWITCH"

Subroutine "SWITCH"

This subroutine switches a continuous spill model to an appropriate instantaneous spill model when $TIME > TSPILL$. If the spill is in open water, and the slick is wide compared to its length, the slick spreads as if it were in a channel until the slick shape is more regular. Afterwards, it spreads as an instantaneous slick in open water.

FIGURE B.8 FLOW CHART FOR SUBROUTINE "INTE"

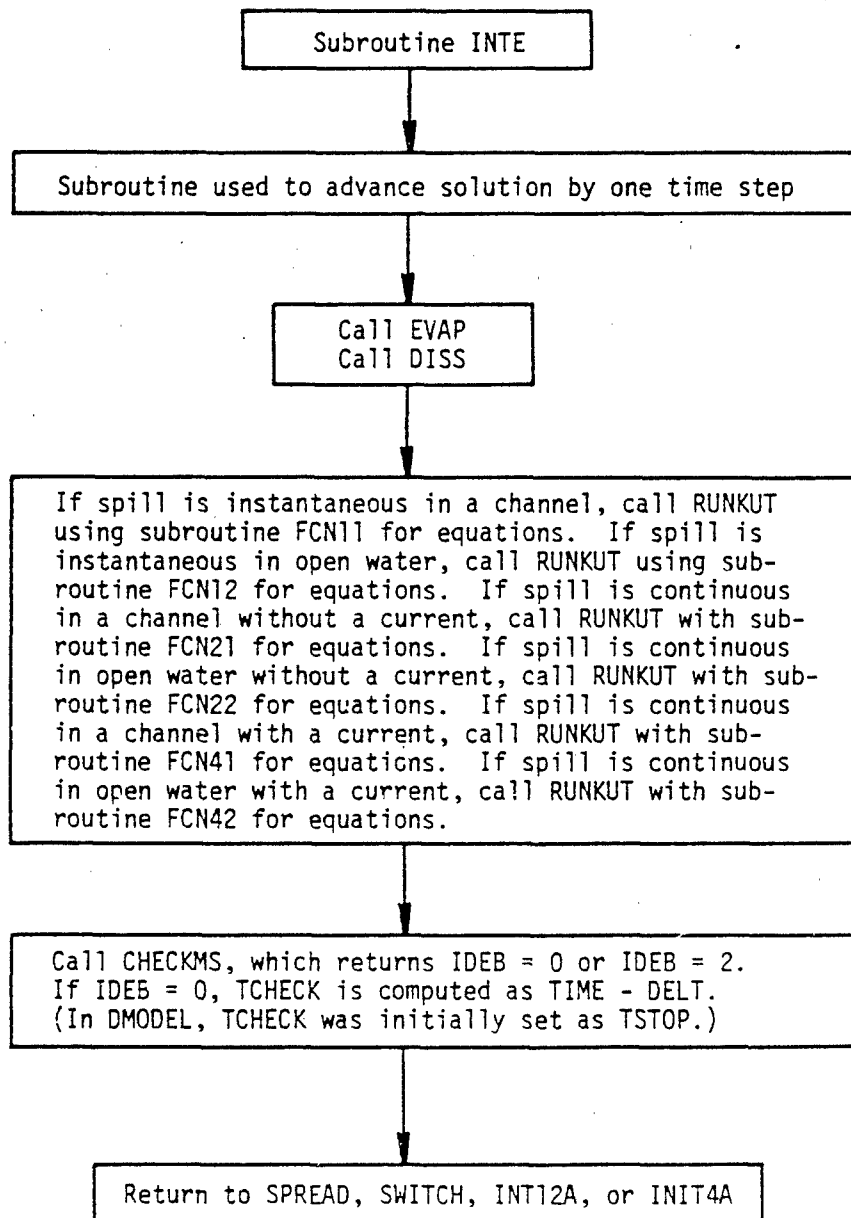


FIGURE B.9 FLOW CHART FOR INTEGRATION EQUATIONS

Subroutine FCN11

This subroutine contains the dA/dt and dh/dt equations for an instantaneous spill in a channel.

Subroutine FCN12

This subroutine contains the dA/dt and dh/dt equations for an instantaneous spill in open water.

Subroutine FCN21

This subroutine contains the dA/dt , $d\bar{A}/dt$, and dh/dt equations for a continuous spill in a channel without a current.

Subroutine FCN22

This subroutine contains the dA/dt , $d\bar{A}/dt$, and dh/dt equations for a continuous spill in open water without a current.

Subroutine FCN41

This subroutine contains the dA/dt , $d\bar{A}/dt$, and dh/dt equations for a continuous spill in a channel with a current.

Subroutine FCN42

This subroutine contains the dA/dt , $d\bar{A}/dt$, and dh/dt equations for a continuous spill in open water with a current.

FIGURE B.10 SUBROUTINES FOR MASS TRANSFER COEFFICIENTS

Subroutine EVAP

This subroutine computes the evaporation mass transfer coefficient EVAPM as a function of the relative wind speed UREL over the slick. (UREL is computed in TRANSP).

Subroutine DISS

This subroutine computes the dissolution mass transfer coefficient DISSOM as a function of wind, current, wave height, and bottom roughness.

FIGURE B.11 FLOW CHART FOR SUBROUTINE "TRANSP"

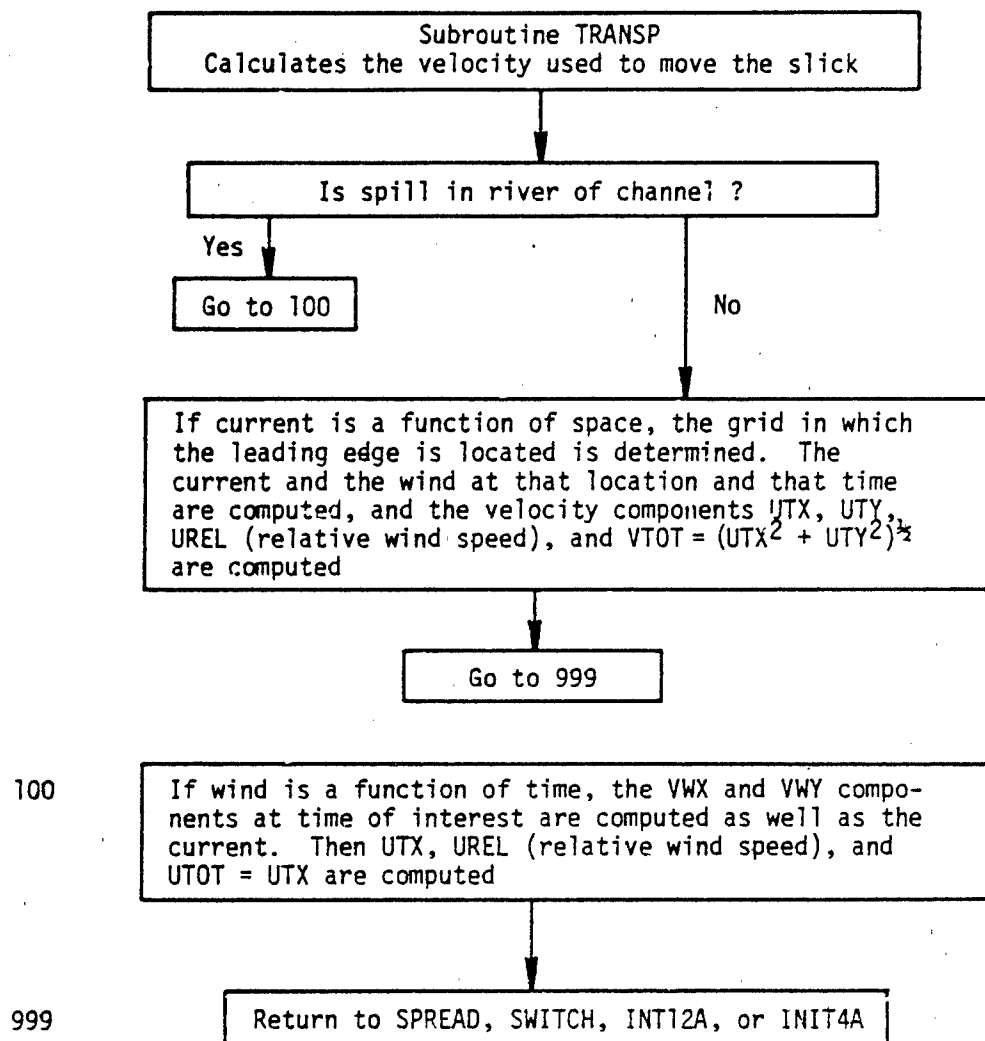


FIGURE B.12 FLOW CHART FOR SUBROUTINE "MOVE"

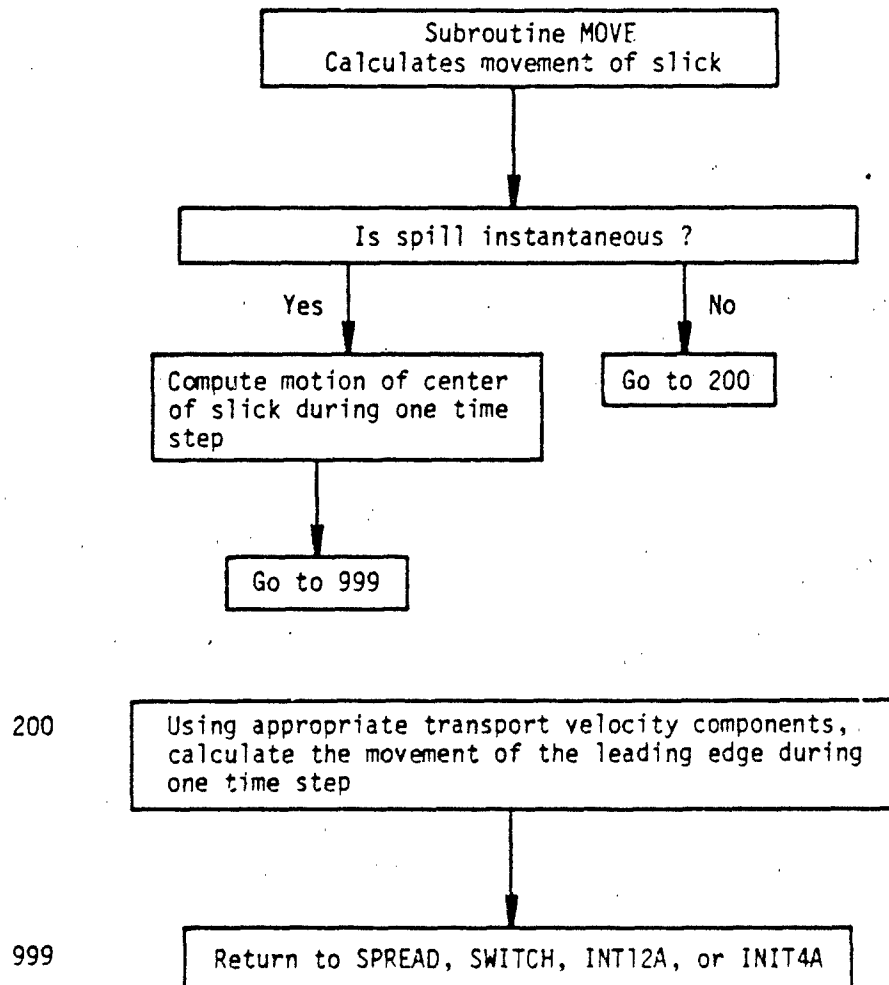


FIGURE B.13 FLOW CHART FOR "PRINTO"

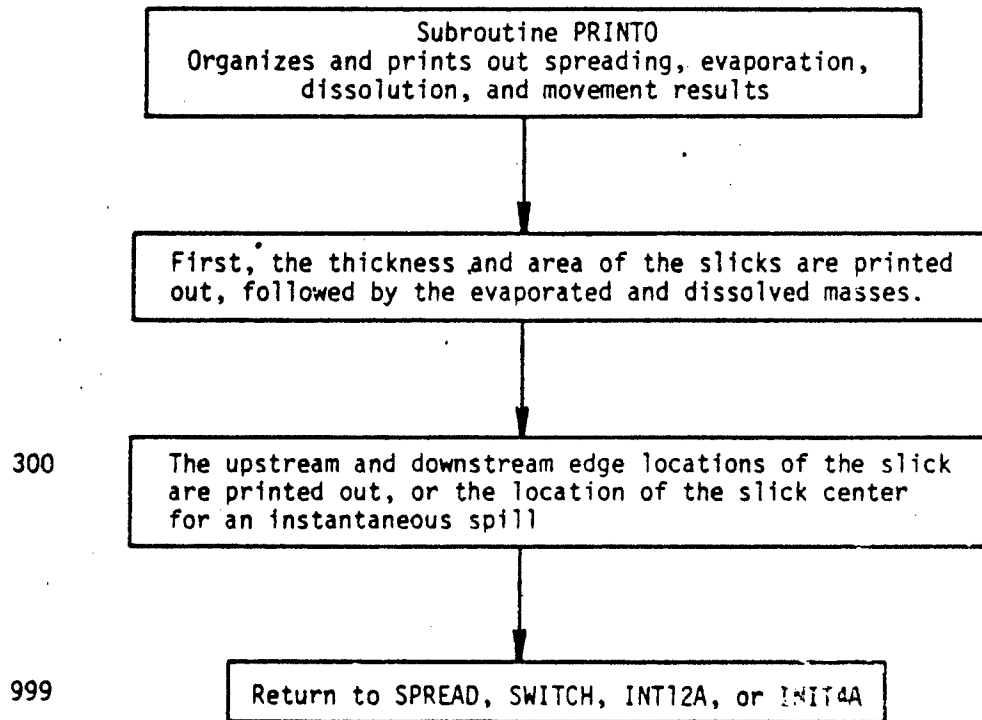


FIGURE B.14 FLOW CHART FOR SUBROUTINE "CHECKMS"

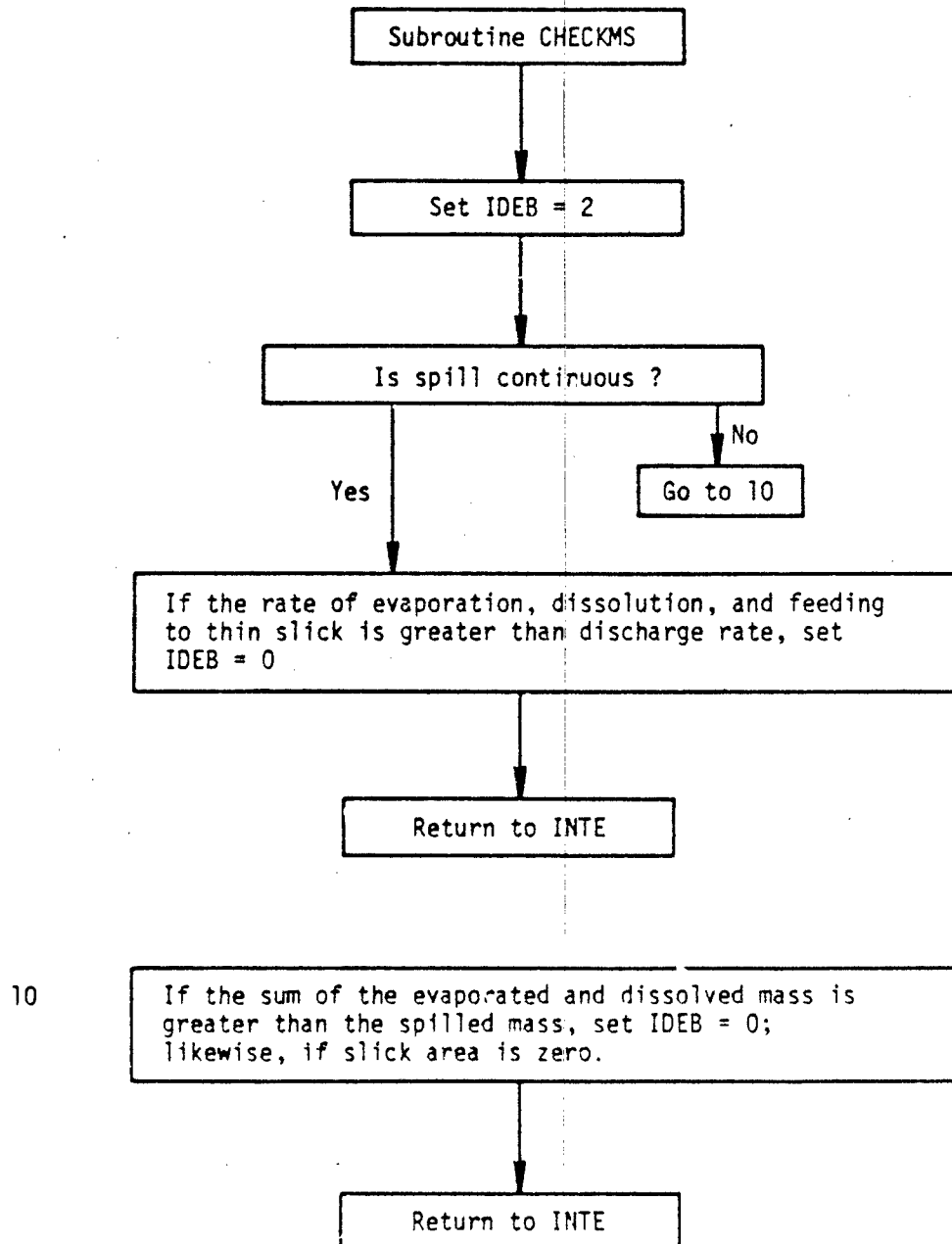
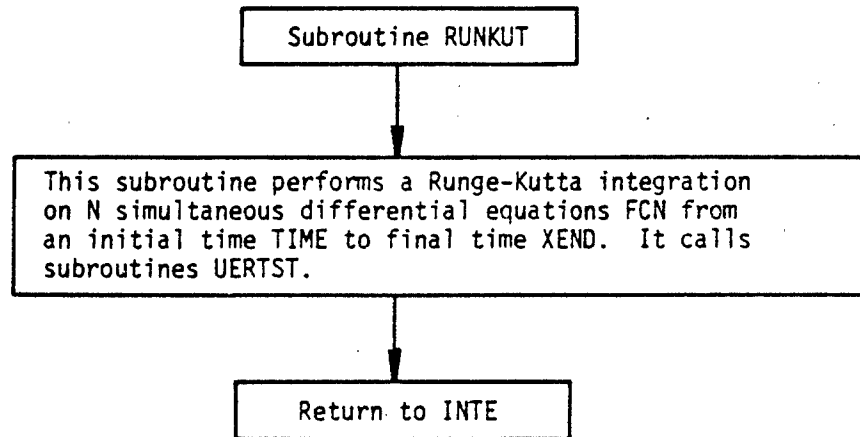


FIGURE B.15 FLOW CHART FOR "RUNKUT"



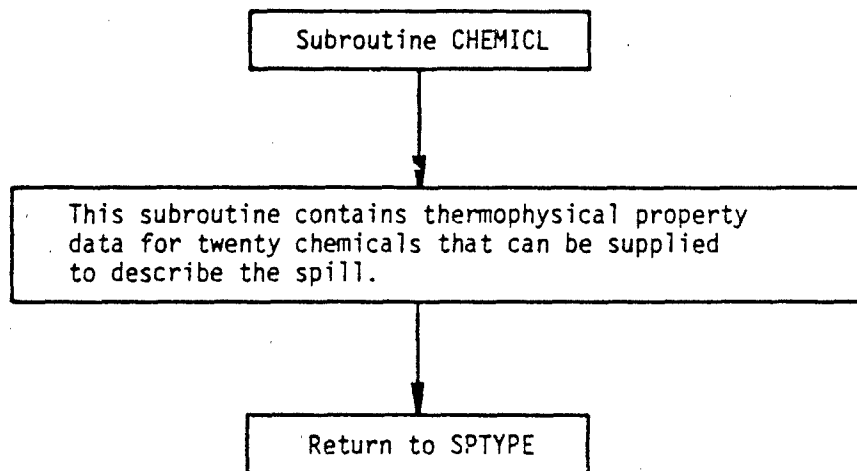
Subroutine UERTST

Determines if an error has occurred in RUNKUT; also calls UGETIO

Subroutine UGETIO

Manipulates input and output of RUNKUT; called by UERTST

FIGURE B.16 FLOW CHART FOR SUBROUTINE "CHEM1CL"



APPENDIX C

PROGRAM "DMODEL" LISTING

Subroutines of DMODEL are given in
alphabetical order

0001

PROGRAM DMODEL

```

C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                      DIFFUSION AND DISPERSION MODEL                      C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      THIS PROGRAM READS IN THE RUN TITLE AND THE INPUT
C      VALUES FOR:
C
C      TDC   = AMBIENT TEMPERATURE
C      PB    = BAROMETRIC PRESSURE
C      DELT  = INTEGRATION TIME STEP
C      TSTOP = MAXIMUM TIME FOR PRINTOUT (END OF RUN)
C      HMIN  = DES. RED MINIMUM THICKNESS OF THICK SLICK;
C              RUN ENDS WHEN THICKNESS BECOMES LESS THAN HMIN
C      HTN   = CONSTANT THICKNESS OF THIN SLICK, USUALLY EQUAL TO HMIN
C
C      THE PROGRAM ALSO CALCULATES THE SURFACE TENSION OF WATER=SIGWA,
C      AND CALLS SUBROUTINES "AIR" AND "WATER" TO CALCULATE AIR AND
C      WATER PROPERTIES. IT INITIALIZES ALL VARIABLES. IT CALLS
C      SUBROUTINES "WBS", "SPLOC", AND "SPTYPE", AND FINALLY CALLS
C      "SPREAD" TO MAKE THE SPREADING CALCULATIONS.
C
0002      COMMON/SIZE/R, D, WW, L1, L2, H, RO
0003      COMMON/CHEMI/DENO, DCA, DCW, CS, CMW
0004      COMMON/WATER/DENW, VISW, GR
0005      COMMON/ENVOR/PV, VISA, DENA, TDC
0006      COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0007      COMMON/CONSTAT/UC, VW, UBAR, UC, U1, WT, ALPH, THETA1
0008      COMMON/MLOSS/EVAPM, DISSOM
0009      COMMON/MOVE/UPSAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0010      COMMON/CURRENT/UBAR(10), DMOVE, UTOT, UTX, UTY, UREL
0011      COMMON/MASS/TOTALE, TOTALD, TOTALM, DMASS
0012      COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0013      COMMON/TRANSIT/UX(10, 10), UY(10, 10), VWX(10),
1          VWY(10), THETA(10), TI(10), ID, IT, IV,
2          XU(10), YU(10), TT(10)
0014      COMMON/ID/ID1, ID2, ID3
0015      COMMON/RUNGE/YY(5), C(24), W(5, 30)
0016      COMMON/SPREAD/TII, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0017      COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0018      COMMON/SENSE/EVA(40, 10), DIS(40, 10), THK(40, 10), TIN(40, 10),
1          PIP(40), TPT
0019      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
1          K12, K22
0020      DIMENSION NAME(30, 20)
0021      REAL K10, K20, K11, K21, K12, K22
C
C      C10-K22 ARE THE CONSTANTS IN THE SPREADING MODELS
C      *****
0022      C10=2. 37
0023      C20=3. 65
0024      C11=2. 37
0025      C21=3. 65
0026      C12=2. 37

```

```

0027      C22=3.65
0028      K10=1.53
0029      K20=1.21
0030      K11=1.24
0031      K21=1.09
0032      K12=2.37
0033      K22=3.65
0034      IFLAG = 1
          C      GR = GRAVITATIONAL ACCELERATION (M/SQ. SEC)
0035          GR = 9.80665
0036          INDEX = 0
0037          4      WRITE(6,5)
0038          5      FORMAT(1X,30HENTER THE TITLE FOR THIS RUN..)
0039          READ (5,7,ERR=4) (NAME(JJ, IFLAG),JJ=1,30)
0040          7      FORMAT(30A1)
0041          WRITE(1,8)(NAME(JJ, IFLAG),JJ=1,30)
0042          8      FORMAT(1H1,30A1,/)
0043          10     WRITE(6,11)
0044          11     FORMAT(1X,41HINPUT THE AMBIENT TEMPERATURE IN CELSIUS.)
0045          READ (5,*,ERR=10) TDC
0046          20     WRITE(6,21)
0047          21     FORMAT(1X,42HINPUT THE BAROMETRIC PRESSURE IN MILLIBARS,
          *      /,1X,47HOR ZERO, 0, FOR THE STANDARD SEA LEVEL PRESSURE/
          *1X,14HOF 1013.25 MB.)
0048          READ (5,*,ERR=20) PB
0049          IF(PB.LE.0.) PB=1013.25
0050          23     WRITE(6,24)
0051          24     FORMAT(1X,46HINPUT THE TIME INCREMENT IN SECONDS. TRY 1.0.)
0052          READ(5,*,ERR=23) DELT
0053          IF(DELT.LE.0.) DELT=1.0
0054          25     WRITE(6,26)
0055          26     FORMAT(1X,37HINPUT THE DESIRED RUN TIME IN MINUTES)
0056          READ(5,*,ERR=25)TSTOP
0057          TSTOP=TSTOP*60.
0058          27     WRITE(6,28)
0059          28     FORMAT(1X,
          1      59HINPUT MINIMUM ALLOWABLE THICKNESS OF THICK SLICK IN METERS.)
0060          READ(5,*,ERR=27)HMIN
0061          31     WRITE(6,32)
0062          32     FORM/T(1X,40HINPUT THICKNESS OF THIN SLICK IN METERS.)
0063          READ(5,*,ERR=31)HTN
          C
          C      CALL SUBROUTINE AIR TO CALCULATE AIR PROPERTIES
          C
0064          C      CALL AIR (PB, TDC, DENA, VISA)
          C
          C      CALL SUBROUTINE WATER TO CALCULATE WATER PROPERTIES
          C
0065          C      CALL WATER (TDC, DENW, VISW)
          C      *****
          C      SIGWA = SURFACE TENSION BETWEEN WATER AND AIR
          C      *****
0066          C      SIGWA = ( 75.64 - 0.144 * TDC ) * 1.E-3
          C
          C      SET UP ALL THE INITIAL AND DEFAULT VALUES

```

```

C
0067 UC = 0.0
0068 VW = 0.0
0069 UTBAR = 0.0
0070 THETA1 = 0.0
0071 XLE = 0.0
0072 YLE = 0.0
0073 XTE = 0.0
0074 YTE = 0.0
0075 XC = 0.0
0076 YC = 0.0
0077 XO = 0.0
0078 YO = 0.0
0079 TOTALM = 0.0
0080 TOTALE = 0.0
0081 EVAPM = 0.0
0082 DISSOM = 0.0
0083 TOTALD = 0.0
0084 SPILLM = 0.0
0085 SPILMR = 0.0
0086 IC = 0
0087 IW = 0
0088 ID = 1
0089 IT = 1
0090 IV = 1
0091 DO 30 I=1,10
0092 DO 29 J=1,10
0093 UX(I,J) = 0.0
0094 UY(I,J) = 0.0
0095 29 CONTINUE
0096 TI(I) = 0.0
0097 TT(I) = 0.0
0098 UPEAK(I) = 0.0
0099 UBAR(I) = 0.0
0100 VWX(I) = 0.0
0101 VWY(I) = 0.0
0102 THETA(I) = 0.0
0103 30 CONTINUE
C
0104 TIME = 0.0
0105 TCHECK = TSTOP
0106 TSPILL = TSTOP
C
C CALL SUBROUTINE WBS TO OBTAIN WATER BODY DESCRIPTION
C
0107 CALL WBS
C
C CALL SUBROUTINE SPLOC TO SPECIFY SPILL LOCATION
C
0108 CALL SPLOC
C
C CALL SUBROUTINE SPTYPE TO DETERMINE SPILL TYPE AND CHEMICAL
C PROPERTIES
C
0109 CALL SPTYPE (PB)

```

	C	
	C	CALL SUBROUTINE SPREAD TO SOLVE SPREADING MODEL
	C	
0110		CALL SPREAD
	C	
	C	
0111	999	CONTINUE
0112		STOP
0113		END

0009 DATA WM /76. 526, 78. 114, 54. 092, 116. 160, 90. 19, 88. 54, 84. 162,
1 82. 146, 102. 177, 64. 515, 62. 134, 100. 205, 86. 178, 98. 189,
2 128. 259, 114. 232, 72. 151, 92. 141, 120. 195, 106. 168/
C DOA IS DIFFUSIVITY IN AIR AT REFERENCE TEMPERATURE (20C) -
C IN SQ. CM. / SEC.
0010 DATA DOA/0. 097, 0. 087, 0. 0. 0. 0. 064, 0. 0. 0. 0. 0. 081, 0. 085, 0. 063,
1 0. 0913, 0. 0983, 0. 064, 0. 070, C. 072, 0. 058, 0. 058,
2 0. 075, 0. 083, 0. 065, 0. 072/
C DOW IS DIFFUSIVITY IN WATER AT REFERENCE TEMPERATURE (20C) -
C (SQ. CM. / SEC.) * 1E3
0011 DATA DOW/1. 019, 1. 02, 1. 062, 0. 712, 0. 0. 0. 0. 0. 84, 0. 870, 0. 744,
1 1. 128, 1. 533, 0. 700, 0. 764, 0. 799, 0. 597, 0. 638, 0. 84,
2 0. 85, 0. 695, 0. 756/
C VPA, VPB AND VPC ARE USED TO CALCULATE VAPOR PRESSURE PV HAS
C A UNIT OF (NEWTON / SQ. M.)
C
0012 DATA VPA/10. 84, 10. 03055, 10. 11873, 10. 15, 11. 06, 9. 2864,
1 9. 9662, 10. 01107, 9. 9744, 10. 82, 10. 75, 10. 02167,
2 10. 00091, 9. 9479, 10. 06383, 10. 04358, 9. 97786,
3 10. 07954, 10. 16572, 10. 13398/
0013 DATA VPB/1540. , 1211. 033, 1041. 117, 1343. , 1877. , 783. 45, 1201. 53,
1 1229. 973, 1139. 34, 1375. , 1461. , 1264. 90, 1171. 17,
2 1270. 763, 1431. 82, 1351. 99, 1064. 84, 1344. 8, 1593. 958,
3 1462. 266/
0014 DATA VPC/273. 2, 220. 79, 242. 274, 207. 0. 273, 0. 179, 7. 222, 65,
1 224. 10, 218. 7, 273. 2, 273. 0, 216. 54, 224. 41, 221. 42,
2 202. 01, 209. 15, 233. 01, 219. 48, 207. 08, 215. 11/
C SL IS THE SOLUBILITY IN G / 100 G OF H2O
0015 DATA SL / . 33, . 175, 0. , . 6, . 06, 0. , . 015, 0. , . 2, . 60, 1. 5, . 0052,
1 . 014, 0. , 0. , . 002, . 036, . 045, 0. , . 0196/
C TF1 IS THE REFERENCE TEMPERATURE FOR SOLUBILITY
0016 DATA TF1/25. , 20. , 0. , 20. , 0. , 0. , 28. 34, 0. , 20. , 20. , 20. , 18. ,
1 0. , 0. , 0. , 16. , 16. , 20. , 0. , 25. /
C
C CAO AND CA1 ARE USED TO CALCULATE TEMPERATURE DEPENDENT
C SOLUBILITY
C
0017 DATA CAO/0. 0, -. 8213, 15*0. 0, -1. 57767, 2*0. 0/
0018 DATA CA1/0. 0, . 00337, 15*0. 0, . 0114, 2*0. 0/
C
C STA IS THE SURFACE TENSION BETWEEN CHEMICAL AND AIR
C AT REFERENCE TEMPERATURE TF2 - IN DYNE / CM
C
0019 DATA STA/2. 89, 2. 888, 0. 0, 2. 37, 2. 61, 0. 0, 2. 46, 2. 678, 1. 71, 1. 95, 2. 35,
1 1. 93, 1. 84, 2. 385, 2. 29, 2. 17, 1. 60, 2. 852, 2. 883, 2. 860/
0020 DATA TF2/15. 0, 7*20. , 25. 05, 11*20. /
C SAO AND SA1 ARE USED TO CALCULATE SURFACE TENSION AT
C DIFFERENT TEMPERATURE
0021 DATA SAO/0. 0, 31. 54, 4*0. 0, 27. 62, 29. 23, 19. 89, 0. 0, 0. 0, 22. 1,
1 20. 44, 26. 11, 24. 72, 23. 52, 18. 25, 30. 90, 30. 91, 31. 23/
0022 DATA SA1/0. 0, . 133, 4*0. 0, . 1188, . 1223, . 1048, 2*0. 0, . 098,
1 . 1022, . 113, . 09347, . 09509, . 11021, . 1189, . 1040,
2 . 1104/
C
C STW IS THE SURFACE TENSION BETWEEN CHEMICAL AND WATER AT

```

C      REFERENCE TEMPERATURE TF3 - DYNE / CM
C
0023      DATA STW/5.71,3.5,0.0,4.0,3.0,0.0,5.0,0.0,1.71,4.00,2.50,5.10,
1          5.11,0.0,3.50,5.08,5.02,3.61,0.0,3.64/
0024      DATA TF3/22.75,20.,0.0,19.85,20.,0.,24.85,0.0,25.05,
1          -15.20.,19.85,20.,0.,20.,20.,19.85,25.,0.,29.85/
C      PAF IS THE PITZER ACENTRIC FACTOR
0025      DATA PAF/.13.,.212.,.255.,.479.,.3,0.,.213.,.21.,.34.,.19.,.19,
1          .351.,.296.,.233.,.444.,.394.,.251.,.257.,.39.,.331/
C      CTK IS THE CRITICAL TEMPERATURE - IN K
0026      DATA CTK/514.15,562.09,443.75,561.15,562.95,0.,553.45,
1          560.41,500.05,460.35,499.15,540.15,507.35,572.25,
2          594.56,568.76,469.65,591.72,664.45,616.97/
0027      DO 1112 I = 1, 2
0028          NAME(I) = NC(I, ICS)
0029      1112 CONTINUE
0030      PHI = (1.0-(293.15/CTK(ICS)))*(2.0/7.0)-(1.0-(TDC+273.15)/
1          CTK(ICS))*(2.0/7.0)
0031      IF (PHI.EQ.0.) GO TO 1115
0032      ZZZ = .29056 - .08775 * PAF(ICS)
C      DENO = CHEMICAL DENSITY IN KG/CU. M.
0033      DENO = (RHO(ICS) * (ZZZ ** PHI))
0034      GO TO 1116
0035      1115 DENO = RHO(ICS)
0036      1116 CONTINUE
C
C      PV = VAPOR PRESSURE - IN NEWTON / SQ. M.
0037      PV = (VPA(ICS) - VPB(ICS) / (TDC + VPC(ICS)))
0038      PV = (10. ** (PV)) / 10.0
C
C      CS = SOLUBILITY LIMIT - IN KG / CU. M.
0039      IF (CA0(ICS).EQ.0.0.AND.CA1(ICS).EQ.0.0) GO TO 1114
0040      SL(ICS) = 10. ** (CA0(ICS) + CA1(ICS) * TDC)
0041      1114 CS = SL(ICS) * DENW / 100.0
C
C      CMW = MOLECULAR WEIGHT
0042      CMW = WM(ICS)
C
C
C      DCA = DIFFUSIVITY IN AIR (SQ. M. / SEC)
0043      DCA = (DOA(ICS) * (1.01325E6) / 293.15 ** 1.5) *
1          ((TDC + 273.15) ** 1.5 / (PB * 1000.0))
0044      DCA = DCA * 1.E-4
C
C      NOTE : PB IS IN MILLIBAR
C          1.01325*1.E6 IS THE REFERENCE PRESSURE IN DYNE/CM. CM.
C
C      DCW = DIFFUSIVITY IN WATER (SQ. M. / SEC.)
0045      DCW = (DOW(ICS) * .001002 / 293.15) * ((TDC + 273.15) /
1          (VISW * DENW))
0046      DCW = DCW * 1.E-9
C
C
C      SIGOA = SURFACE TENSION BETWEEN CHEMICAL AND AIR
C          (IN NEWTON / M.)

```

```

0047      IF (SAO(ICS) .EQ. 0.0 .AND. SA1(ICS) .EQ. 0.0) GO TO 1117
0048      SIGOA = (SAO(ICS) - SA1(ICS) * TDC) * (1.E-3)
0049      GO TO 1118
0050      SIGOA = STA(ICS) * (1.0E-2)
0051      1117      CONTINUE
           C
           C
           C      SIGOW = SURFACE TENSION BETWEEN CHEMICAL AND WATER
           C      (IN NEWTON / M.)
0052      SIGOW = STW(ICS) * (1.0E-2)
0053      RETURN
0054      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      SUBROUTINE CURRENT C
C      THIS SUBROUTINE COMPUTES THE AVERAGE TRANSPORT C
C      VELOCITY OVER ENTIRE SPILL DURATION C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      THIS SUBROUTINE IS CALLED BY "SPREAD". IT CALCULATES THE
C      AVERAGE VALUE OF THE VELOCITY USED IN THE SPREADING MODELS
C      TO COMPARE WITH THE PEAK COMPUTED IN UTPEAK.
C
C      ** VARIABLE NAME **
C
C      UBAR(I) = AVERAGE VALUE OVER TIME OF UC + 0.035*VW (COMPONENTS)
C      IN EACH OF THE 9 SLICES OR BOXES. FOR A RIVER, A
C      DUMMY BOX(I=1) IS USED.
C
0001 SUBROUTINE CURRT
0002 COMMON/CURRENT/UBAR(10), DMOVE, UTOT, UTX, UTY, UREL
0003 COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0004 COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0005 COMMON/CONSTAT/UC, VW, UBAR, UO, U1, WT, ALPH, THETA1
0006 COMMON/TRANSIT/UX(10,10), UY(10,10), VWX(10),
1 VWY(10), THETA(10), TI(10), ID, IT, IV,
2 XU(10), YU(10), TT(10)
0007 COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0008 COMMON/UAVE/UCX1, UCY1, VWX1, VWY1
C
C
0009 IF (IC.EQ.0.AND.IW.EQ.0) GO TO 999
0010 ISHAP = SHAPE
0011 IF (ISHAP.GT.1) GO TO 200
C
C
C      -----
C      IN RIVERS OR CHANNELS
C      -----
C
0012 IF (IC.EQ.1) GO TO 60
0013 IF (TSPILL.GT.WT) GO TO 50
C
C      *****
C      AVERAGE VALUE OF TIDAL VELOCITY OVER ONE TIDAL PERIOD
C      *****
0014 UC = UO
0015 GO TO 60
0016 50 CONTINUE
C
C      *****
C      AVERAGE VALUE OF TIDAL VELOCITY OVER DISCHARGE TIME
C      *****
0017 UC = UO+U1*WT/6.28318*(-COS(6.28318/WT*(TSPILL+ALPH))
1 +COS(6.28318*ALPH/WT))
0018 60 IF (IW.LE.1) GO TO 70
0019 VWT = 0.
0020 THET1T = 0.
0021 DO 62 I = 1,10
0022 IF (TSPILL.LT.TT(I)) GO TO 65
0023 VWT = VWT +VWX(I)

```

```

0024      THET1T = THET1T + THETA(I)
0025      62      CONTINUE
0026      65      VW = VWX(I-1) + (TSPILL-TT(I-1))*(VWX(I)-VWX(I-1))/
1          (TT(I)-TT(I-1))
0027      1      THETA1 = THETA(I-1) + (TSPILL-TT(I-1))*(THETA(I)-THETA(I-1))
1          / (TT(I)-TT(I-1))
C          *****
C          TIME AVERAGE VALUE CALCULATED OF WIND AND WIND ANGLE UP TO
C          END OF DISCHARGE TIME
C          *****
0028      VW = (VNT+VW)/I
0029      THETA1 = (THET1T+THETA1)/I
C          -----
0030      70      UBAR(1) = UC + 0.035 * VW * THETA1
C          -----
0031      GO TO 999
C          -----
C          IN OPEN WATER
C          -----
0032      200      CONTINUE
0033      IF (IW.GT.1) GO TO 210
0034      VWX1 = VWX(1)
0035      VWY1 = VWY(1)
0036      GO TO 300
0037      210      VWX1 = 0.0
0038      VWY1 = 0.0
0039      DO 240 J = 1,10
0040      IF (TSPILL.LT.TT(J)) GO TO 250
0041      VWX1 = VWX1 + VWX(J)
0042      VWY1 = VWY1 + VWY(J)
0043      240      CONTINUE
0044      250      VWX1 = VWX1 + VWX(J-1)+(TSPILL-TT(J-1))*(VWX(J)-VWX(J-1))
1          / (TT(J)-TT(J-1))
0045      1      VWY1 = VWY1 + VWY(J-1)+(TSPILL-TT(J-1))*(VWY(J)-VWY(J-1))
1          / (TT(J)-TT(J-1))
C          *****
C          TIME AVERAGE VALUE OF WIND COMPONENTS UP TO END OF DISCHARGE
C          TIME
C          *****
0046      VWX1 = VWX1/J
0047      VWY1 = VWY1/J
0048      300      CONTINUE
0049      IF (IC.GT.1) GO TO 310
0050      UU1 = UX(1,1)
0051      UU2 = UY(1,1)
0052      UCX1 = UU1
0053      UCY1 = UU2
C          *****
C          COMPUTE UBAR WHEN CURRENT IS CONSTANT
C          *****
0054      UBAR(1) = SQRT((UU1+0.035*VWX1)**2+(UU2+0.035*VWY1)**2)

```

```

0055      THETA(1) = ATAN((UU2+0.035*VWY1)/(UU1+0.035*VWY1))
          C-----
0056      GO TO 999
0057      310 DO 390 I = 1,9
0058          IF (IC.GT.2) GO TO 320
0059          UU1 = UX(I,1)
0060          UU2 = UY(I,1)
0061      GO TO 360
0062      320 UU1 = 0.0
0063          UU2 = 0.0
0064          DO 340 J=1,IT
0065              IF (TSPILL.LT.TI(J)) GO TO 350
0066              UU1 = UU1 + UX(I,J)
0067              UU2 = UU2 + UY(I,J)
0068      340 CONTINUE
0069      350 UU1 = UU1 + UX(I,J-1)+(TSPILL-TI(J-1))*(UX(I,J)-UX(I,J-1))
          1      / (TI(J)-TI(J-1))
0070          UU2 = UU2 + UY(I,J-1)+(TSPILL-TI(J-1))*(UY(I,J)-UY(I,J-1))
          1      / (TI(J)-TI(J-1))
          C-----
          C *****
          C COMPUTE AVERAGE CURRENT IN EACH BOX OR SLICE
          C *****
0071      UU1 = UU1/J
0072      UU2 = UU2/J
0073      360 IF(I.NE.SP)GOTO 380
0074      UCX1 = J/1
0075      UCY1 = J/2
          C-----
          C *****
          C COMPUTE AVERAGE UBAR IN EACH BOX OR SLICE
          C *****
          C-----
0076      380 UBAR(I) = SQRT((UU1+0.035*VWX1)**2+(UU2+0.035*VWY1)**2)
0077      THETA(I) = ATAN((UU2+0.035*VWY1)/(UU1+0.035*VWX1))
          C-----
0078      390 CONTINUE
0079      999 RETURN
0080      END

```

```

C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          SUBROUTINE DISS
C          THIS SUBROUTINE IS USED TO COMPUTE DISSOLUTION LOSS
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          THIS SUBROUTINE IS CALLED BY "INTE". IT CALCULATES THE
C          DISSOLUTION MASS TRANSFER RATE COEFFICIENT. THE RELATIVE
C          WIND IS CALCULATED IN "TRANSP".
C          *****
C          DISSOM = DISSOLUTION MASS TRANSFER RATE COEFFICIENT (KG / SQ. M-
C
0001          SUBROUTINE DISS
0002          COMMON/SIZE/R, D, WW, L1, L2, H, RO
0003          COMMON/CHEMI/DENO, DCA, DCW, CS, CMW
0004          COMMON/WATER/DENW, VISW, QR
0005          COMMON/ENVOR/PV, VISA, DENA, TDC
0006          COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0007          COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0008          COMMON/MLOSS/EVAPM, DISSOM
0009          COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0010          COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0011          COMMON/TRANSIT/UX(10, 10), UY(10, 10), VWX(10),
1              VWY(10), THETA(10), TI(10), ID, IT, IV,
2              XU(10), YU(10), TT(10)
0012          COMMON/ID/ID1, ID2, ID3
0013          COMMON/EVADIS/DAN, UXA, SCHMIW, CSA, DWN, UXW, SCHMIW, CSW
0014          COMMON/CURRENT/UBAR(10), DMOVE, UTOT, UTX, UTY, UREL
C
0015          DATA D1, D2, D3, D4, D5, D6, D7, D8/.85, 1., 2.35, .8., .065, .55, .2, 11.2/
0016          I = IW+1
0017          J = SHAPE
C
C          ** SCHMIW = SCHMIDT NO. FOR WATER **
C
0018          SCHMIW = VISW/DCW
0019          CSW = CS/DENW
C
C
0020          GO TO (10, 100, 100) J
C
C          -----
C          DISSOLUTION IN RIVERS OR CHANNELS
C          -----
0021          10 CONTINUE
C
C          ** DWN = DALTON NO. FOR RIVER **
C
0022          DWN = 0.06266/(SCHMIW**(2./3.))
0023          K = IC+1
0024          GO TO (11, 12, 13) K
C          --- NO CURRENT ---
0025          11 DISSOM = 0.0
0026          GO TO 999
C          --- CONSTANT CURRENT ---

```

```

0027 12 GO TO 20
      C      --- TID AL CURRENT ---
0028 13 UC = U0+U1*SIN(2.0*3.14159/WT*(TIME+ALPH))
0029 20 UXW = UC/(5.66*ALOG10(2.0*D/RO)+4.92)
0030      GO TO 500

      C
      C
      C      -----
      C      DISSOLUTION IN OPEN WATER
      C      -----

0031 100 CONTINUE
0032      GO TO (110,120,120) I
      C      --- NO RELATIVE WIND ---
0033 110 DISSOM =0.0
0034      GO TO 999
      C      --- RELATIVE WIND---
0035 120 IF (UREL.GT.3.064) GO TO 155
      C      --- UREL . LE . 3.064 METER/SEC ---
0036      UXW = SQRT(DENA/DENW)*UREL*SQRT((1.25E-3)/(UREL**0.2))
0037      GO TO 160
      C      --- UREL . GT . 3.064 METER/SEC ---
0038 155 UXW = SQRT(DENA/DENW)*UREL*SQRT((D4+D5*UREL)/1000.0)
      C
0039 160 IF (UREL.GT.5.0) GO TO 165
      C      --- UREL . LE . 5.0 METER/SEC ---
0040      BW = 12.5*(SCHMIW**(.2/.3))+2.125*ALOG(SCHMIW)-5.3
0041      GO TO 170
      C      --- UREL . GT . 5.0 METER/SEC ---
0042 165 CONTINUE
0043      SCT = D1
0044      HPLUS =H*UXW/VISW
0045      BW = D6*((SCHMIW**(.2/.3))-D7)*SQRT(HPLUS)-
      1      2.5*SCT*ALOG(HPLUS)+D8*SCT

      C
      C
0046 170 ZW = D2*UXW/VISW
      C
      C      ** DWN = DALTON NO. FOR OPEN WATER **
      C
0047      DWN = 1.0/(2.5*SCT*ALOG(ZW)+BW+D3)
      C
      C
0048 500 DISSOM = DWN * DENW *UXW *CSW
      C
0049 999 RETURN
0050      END

```


0032	75	BA = D6*(SCHMIA**((2./3.)-D7)*SQRT(HX)-2.5*SCT*ALOG(HX)
	1	+D8*SCT
	C	
0033	80	CONTINUE
0034		ZA = D2 * UXA / VISA
0035		SCT = D1
	C	
	C	** DAN = DALTON NO. FOR AIR **
	C	
0036	85	DAN = 1.0/((2.5*SCT*ALOG(ZA)+BA+D3)
	C	
	C	
0037	100	EVAPM = DAN * DENA * UXA * CSA
	C	
	C	
0038	999	RETURN
0039		END

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          SUBROUTINE FCN11
C          SIMULTANEOUS EQUATIONS FOR MODEL 1. A
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          THIS SUBROUTINE IS CALLED BY "RUNKUT" THROUGH "INTE". IT CONTA
C          THE GRAVITY-VISCOUS SPREADING EQUATIONS FOR AN INSTANTANEOUS
C          SPILL IN A RIVER.
C
0001      SUBROUTINE FCN11 (N, TIME, YY, YPRIME)
0002      COMMON/SPREAD/TII, ATK, HTK, ATN, HTN, KMIN, INDEX, IFLAG
0003      COMMON/STYPE/SPILLM, SPILMR, TSFILL, WS, STP, SPM
0004      COMMON/CHEMI/DENO, DCA, DCW, CS, CMW
0005      COMMON/WATER/DENW, VISW, QR
0006      COMMON/ENVOR/PV, VISA, DENA, TDC
0007      COMMON/SIZE/R, D, WW, L1, L2, H, RO
0008      COMMON/MLOSS/EVAPM, DISSOM
0009      COMMON/MASS/TOTALE, TOTALD, TOTALM, DMASS
0010      COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0011      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
1          K12, K22
0012      COMMON/PRIM/PRIME(5), IDEB, KKK
0013      REAL YPRIME(5), YY(5)
0014      REAL K10, K20, K11, K21, K12, K22
0015      YPRIME(4) = EVAPM*YY(1)
0016      YPRIME(5) = DISSOM*YY(1)
0017      DLOSS = YPRIME(4)+YPRIME(5)
0018      YPRIME(2) = 2.76*(((SIG*WW*WW/DENW)**2/VISW)**(1./3.))
1          /((YY(2)**(1.0/3.0)))
C
0019      YPRIME(1) = 2.38*(C20**(.8./3.))*((QR*WW*WW*COEF)**2/VISW)
1          *(1./3.)*(YY(3)**(4./3.))/(YY(1)**(1./3.))
2          -DLOSS/(2.0*DENO*YY(3))
C
0020      YPRIME(3) = -(YY(3)*YPRIME(1)+DLOSS/DENO)/YY(1)
0021      DO 100 IID=1,5
C
C          ** PRIME ARE VARIABLES USED IN "CHEKMS" **
C
0022      PRIME(IID)=YPRIME(IID)
0023      100 CONTINUE
0024      RETURN
0025      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          SUBROUTINE FCN12
C          SIMULTANEOUS EQUATIONS FOR MODEL 1.8
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          THIS SUBROUTINE IS CALLED BY "RUNKUT" THROUGH "INTE". IT CONTA
C          THE GRAVITY-VISCOUS SPREADING EQUATIONS FOR AN INSTANTANEOUS SP
C          IN OPEN WATER.
C
0001      SUBROUTINE FCN12 (N,TIME,YY,YPRIME)
0002      COMMON/SPREAD/TII,ATK,HTK,ATN,HTN,HMIN,INDEX,IFLAG
0003      COMMON/STYPE/SPILLM,SPILMR,TSPILL,WS,STP,SPM
0004      COMMON/CHEMI/DENO,DCA,DCW,CS,CMW
0005      COMMON/WATER/DENW,VISW,GR
0006      COMMON/ENVOR/PV,VISA,DENA,TDC
0007      COMMON/SIZE/R,D,WW,L1,L2,H,RO
0008      COMMON/MLOSS/EVAPM,DISSOM
0009      COMMON/INTER/COEF,SIGWA,SIGOA,SIGOW,SIG
0010      COMMON/CK/C10,C20,C11,C21,C12,C22,K10,K20,K11,K21,
          1      K12,K22
0011      COMMON/PRIM/PRIME(5),IDEB,KKK
0012      REAL YPRIME(5),YY(5)
0013      REAL K10,K20,K11,K21,K12,K22
0014      PI=ACOS(-1.)
0015      YPRIME(4) = EVAPM*YY(1)
0016      YPRIME(5) = DISSOM*YY(1)
0017      DLOSS = YPRIME(4)+YPRIME(5)
0018      YPRIME(2) = 6.02*(((SIG/DENW)**2/VISW)**(1./3.))
          1      *(YY(2)**(1./3.))
C
0019      YPRIME(1) = 0.5*(((PI*(K20**2.))**2.)*(((GR*COEF)**2/VISW)
          1      *(1./3.))*((YY(3)**(4./3.))*((YY(1)**(1./3.))
          2      -2./3.*DLOSS/(DENO*YY(3)))
C
0020      YPRIME(3) = -(YY(3)*YPRIME(1)+DLOSS/DENO)/YY(1)
0021      DO 100 IID=1,5
C
C          ** PRIME ARE VARIABLES USED IN "CHEKMS" **
C
0022      PRIME(IID)=YPRIME(IID)
0023      100 CONTINUE
0024      RETURN
0025      END

```



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CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                               SUBROUTINE FCN41
C                               SIMULTANEOUS EQUATIONS FOR MODEL 4A
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      THIS SUBROUTINE IS CALLED BY "RUNKUT" THROUGH "INTE". IT CONT
C      THE GRAVITY-VISCOUS SPREADING EQUATIONS FOR A CONTINUOUS SPILL
C      A RIVER WITH CURRENT OR WIND.
C
0001      SUBROUTINE FCN41 (N, TIME, YY, YPRIME)
0002      COMMON/CONSTAT/UC, VW, UBAR, UO, U1, WT, ALPH, THETA1
0003      COMMON/SPREAD/T11, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0004      COMMON/STYPE/SPILLM, SPILMR, TSPJLL, WS, STP, SPM
0005      COMMON/CHEMI/DENO, DCA, DCW, CS, CMW
0006      COMMON/WATER/DENW, VISW, GR
0007      COMMON/ENVOR/PV, VISA, DENA, TDC
0008      COMMON/SIZE/R, D, WW, L1, L2, H, RO
0009      COMMON/MLOSS/EVAPM, DISSOM
0010      COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0011      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
1          K12, K22
0012      COMMON/PRIM/PRIME(5), IDEB, KKK
0013      REAL YPRIME(5), YY(5)
0014      REAL K10, K20, K11, K21, K12, K22
0015      YPRIME(4) = EVAPM*YY(1)
0016      YPRIME(5) = DISSOM*YY(1)
0017      DLOSS = YPRIME(4)+YPRIME(5)
0018      SPILLW = WW
15      C
0019      20 YPRIME(2) = 2.76*(((SIG*WW/DENW)**2/VISW)**(1./3.))
1          /((YY(2)**(1./3.))
0020      SPM=SPILMR-DLOSS-DENO*HTN*YPRIME(2)
0021      IF(SPM.LE.0.0) GOTO 998
C
0022      YPRIME(1) = 2.38*(C22**(.8./3.))*((GR*WW*COEF)**2/VISW)**(1./3.
1          *(YY(3)**(4./3.))/((YY(1)**(1./3.))
2          -DLOSS/(2.0*DENO*YY(3))
3          -0.5*(HTN/YY(3))*YPRIME(2)
4          + SPILMR/(2.0*DENO*YY(3))+ SPILLW * UBAR
C
0023      YPRIME(3) = -(YY(3)*YPRIME(1)+HTN*YPRIME(2)+
1          DLOSS/DENO-SPILMR/DENO)/YY(1)
0024      998 DO 100 IID=1,5
C
C      ** PRIME ARE VARIABLES USED IN "CHEKMS" **
C
0025      PRIME(IID)=YPRIME(IID)
0026      100 CONTINUE
0027      999 RETURN
0028      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                               SUBROUTINE FCN42
C                               SIMULTANEOUS EQUATIONS FOR MODEL 4B
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      THIS SUBROUTINE IS CALLED BY "RUNKUT" THROUGH "INTE".  IT CONT
C      THE EQUATIONS FOR GRAVITY-VISCOUS SPREADING OF A CONTINUOUS SP
C      IN OPEN WATER WITH A CURRENT OR WIND.
C
0001      SUBROUTINE FCN42 (N, TIME, YY, YPRIME)
0002      COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0003      COMMON/SPREAD/TII, ATX, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0004      COMMON/STYPE/SPILLR, SPILMR, TSPYLL, WS, STP, SPM
0005      COMMON/CHEMI/DENO, LCA, DCW, CS, CMW
0006      COMMON/WATER/DENW, VISW, OR
0007      COMMON/ENVOR/PV, VISA, DENA, TDC
0008      COMMON/SIZE/R, D, WW, L1, L2, H, RO
0009      COMMON/MLOSS/EVAPM, DISSOM
0010      COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0011      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
1          K12, K22
0012      COMMON/PRIM/PRIME(5), IDEB, KKK
0013      REAL YPRIME(5), YY(5)
0014      REAL K10, K20, K11, K21, K12, K22
0015      YPRIME(4) = EVAPM*YY(1)
0016      YPRIME(5) = DISSOM*YY(1)
0017      DLOSS = YPRIME(4)+YPRIME(5)
C
0018      YPRIME(2) = 2.06*(((SIG*(UTBAR**2)/DENW)**2/VISW)**(1./7.))
1          *(YY(2)**(3./7.))
C
0019      SPM = SPILMR - DLOSS-DENO*HTN*YPRIME(2)
C
0020      IF (SPM.LE.0.0) GO TO 998
C
0021      YPRIME(1) = ((11./8.)*(K22**((8./11.)))*(((OR*COEF*(UTBAR**2))**2
1          /VISW)**(1./11.)))*((SPM/(2.0*DENO))**(4./11.))
2          *(YY(1)**(3./11.))
C
0022      YPRIME(3) = -(YY(3)*YPRIME(1)+HTN*YPRIME(2)+
1          DLOSS/DENO-SPILMR/DENO)/YY(1)
C
0023      998 DO 100 IID=1,5
C
C          ** PRIME ARE VARIABLES USED IN "CHEKMS" **
C
0024      PRIME(IID)=YPRIME(IID)
0025      100 CONTINUE
0026      999 RETURN
0027      END

```



```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      SUBROUTINE GROUND IS USED TO                      C
C      DETERMINE WHETHER THE SLICK HAS HIT                C
C      THE BOUNDARY LINE(S)                                C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      THIS SUBROUTINE IS CALLED BY "SPREAD". IT DETERMINES IF THE
C      SLICK HAS HIT THE COASTLINE. IF IT HAS HIT, IT RETURNS
C      IH=99
C      OTHERWISE, IT RETURNS                               C
C      IH=0
C
0001      SUBROUTINE GROUND(IH)
0002      COMMON/SIZE/R, D, WW, L1, L2, H, RO
0003      COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0004      COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0005      COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0006      COMMON/RUNGE/YY(5), C(24), W(5, 30)
0007      COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0008      ISTP = STP
0009      IH = 0
0010      PI = 3.141592
0011      IF (STP.EQ.4.2) GO TO 7
C
C      ** IF STP IS NOT 4.2, ALL OPEN WATER SLICKS ARE CIRCULAR **
C      ** SO COMPUTE RADIUS OF SLICK = RAD **
C
0012      RAD = SQRT(YY(1)/PI)
0013      GO TO 9
C
C      ** IF STP IS 4.2, SLICK IS TRIANGULAR, SO COMPUTE WIDTH = RAD
C
0014      7      RAD = YY(1)/(UTBAR*TIME)
0015      XC = XLE
0016      YC = YLE
0017      9      IF (SHAPE.EQ.3.2.OR.SHAPE.EQ.2.3) GO TO 10
0018      GO TO 100
C
C      *****
C      FOR ARBITRARY LAKE OR COAST, COMPUTE DISTANCE FROM LEADING
C      EDGE (CONT.) OR CENTER (INST.) OF SLICK TO EACH BOUNDARY
C      POINT, AND DETERMINE IF RAD > THE DISTANCE. IF SO, SLICK
C      HAS HIT COAST
C      *****
0019      10     DO 20 I=1,10
0020      25     X1 = (XC-X(I))*(XC-X(I))+(YC-Y(I))*(YC-Y(I))
0021      20     IF ((R**2).GT.X1) GO TO 30
0022      GOTO 40
0023      30     IH = 99
0024      GO TO 999
0025      40     IH = 0
0026      GO TO 999
0027      50     IDH = 1
0028      GO TO 25
C
C      *****
C      FOR A STRAIGHT COAST, COMPUTE DISTANCE FROM LEADING EDGE (CONT.

```

```

C      OR CENTER (INST.) TO STRAIGHT LINE AND DETERMINE IF RAD > DISTANCE
C      IF SO, SLICK HAS HIT COAST.
C      *****
0029 100 IF (SHAPE.NE.3.1) GO TO 200
0030 120 SS = (Y(2)-Y(1))/(X(2)-X(1))
0031      X1 = (SS*(YC-Y(1))+X(1)*SS*SS-XC)/(SS*SS+1.0)
0032      Y1 = (SS*(XC-X(1))+YC*SS**2+Y(1))/(SS**2+1.0)
0033      SS = (XC-X1)*(XC-X1)+(YC-Y1)*(YC-Y1)
0034      IF ((RAD**2).LE.SS) GO TO 999
0035      IH = 99
0036      GO TO 999
0037 200 IF (SHAPE.NE.2.2) GO TO 300
C      *****
C      FOR A RECTANGULAR LAKE, CHECK DISTANCE FROM LEADING EDGE (CONT.)
C      OR CENTER (INST.) TO ALL 4 EDGES AND DETERMINE IF RAD > DISTANCE.
C      IF SO, SLICK HAS HIT COAST.
C      *****
0038      DO 220 I=1,4
0039      IF (I.EQ.4) GO TO 214
0040      IF (I.EQ.3) GO TO 213
0041      IF (I.EQ.2) GO TO 212
0042      X1=XC
0043      Y1=0.0
0044      GOTO 215
0045 212 X1=FLOAT(L1)
0046      Y1=YC
0047      GOTO 215
0048 213 X1=XC
0049      Y1=FLOAT(L2)
0050      GOTO 215
0051 214 X1=0.0
0052      Y1=YC
0053 215 SS = (XC-X1)*(XC-X1)+(YC-Y1)*(YC-Y1)
0054      IF ((RAD**2).LE.SS) GO TO 220
0055      IH = 99
0056      GO TO 999
0057 220 CONTINUE
0058      IH = 0
0059      GO TO 999
0060 300 CONTINUE
C      *****
C      IF (RAD + OFFSET OF LEADING EDGE (CONT.) OR CENTER (INST.) OF
C      SLICK FROM CENTER OF CIRCULAR LAKE) > RADIUS OF LAKE,
C      SLICK HAS HIT THE COAST.
C      *****
0061      X1 = RAD + SQRT((XC-X0)*(XC-X0)+(YC-Y0)*(YC-Y0))
0062      IF (X1.LE.R) GO TO 999
0063      IH = 99
0064 999 RETURN
0065      END

```



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0001      SUBROUTINE INT12A
C
C
C      *****
C      *      CALCULATE INITIAL CONDITIONS FOR MODELS 1A & 2A      *
C      *      INSTANTANEOUS OR CONTINUOUS IN RIVER OR CHANNEL      *
C      *      IF SPILL IS CONTINUOUS, UTBAR MUST BE ZERO          *
C      *****
C
C      THIS SUBROUTINE IS CALLED BY "INIT". IT CALCULATES THE INITIAL
C      CONDITIONS FOR INSTANTANEOUS OR CONTINUOUS SPILLS IN A CHANNEL.
C      FOR A CONTINUOUS SPILL, THE CURRENT AND WIND MUST BE ZERO;
C      OTHERWISE, "INIT4A" WILL BE CALLED.
C
0002      COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0003      COMMON/CHEMI/DENO, DCA, DCW, CS, CMW
0004      COMMON/WATER/DENW, VISW, GR
0005      COMMON/ENVOR/PV, VISA, DENA, TDC
0006      COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0007      COMMON/SPREAD/TII, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0008      COMMON/SIZE/R, D, WW, L1, L2, H, RO
0009      COMMON/RUNGE/YY(5), C(24), W(5, 30)
0010      COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0011      COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0012      COMMON/UAVE/UCX1, UCY1, VWX1, VWY1
0013      COMMON/PRIM/PRIME(5), IDEB, KKK
0014      COMMON/SENSE/EVA(40, 10), DIS(40, 10), THK(40, 10), TIN(40, 10),
1          PIP(40), TPT
0015      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
1          K12, K22
0016      COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0017      REAL K10, K20, K11, K21, K12, K22
C
C      ** STP = 1.1 (INST.) OR 2.1 (CONT.) FOR THIS SUBROUTINE (RIVERS)
C
0018      I = STP
0019      PI=ACOS(-1.)
0020      GO TO (201, 101) I
C
C      ---- MODEL 2A IS BEING USED ----
C      *** (CONTINUOUS SPILL IN THE CHANNEL) ***
C
0021      101 TIA = ((SPILMR/(DENW*WW))**2/(GR*COEF*VISW**(3./2.))**(2./3.))
          *((C21/C11)**8.)
C
C      ** TIA = END OF GRAVITY-INERTIA SPREADING FOR A CONT. SPILL **
C
0022      IF (TIA.GE.TSPILL) GO TO 110
0023      GO TO 210
0024      110 WRITE (1, 112)
0025      WRITE (6, 112)
0026      112 FORMAT (1H1//1X,
1          50H*****
1          1X, 48HTHE SPILL TIME IS SO SHORT THAT AN INSTANTANEOUS, /
2          1X, 31H SPILL WILL GIVE BETTER RESULTS)
C

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C      ** SPILL IS SWITCHED TO INSTANTANEOUS WITH      **
C      ** SPILLED MASS = DISCHARGE RATE * DISCHARGE TIME **
C
0027      STP = 1.1
0028      SPILLM = SPILMR * TSPILL
C
C      ----- MODEL 1A IS BEING USED -----
C      ** (INSTANTANEOUS SPILL IN THE CHANNEL) **
C
0029      201      CONTINUE
0030      VO = SPILLM/DENQ
0031      TIA=((VO/WW)**4./((VSW**3.)*(GR*COEF)**2.))*((1./7.)*
*      ((C20/C10)**(24./7.)))
C
C      ** TIA = END OF GRAVITY-INERTIA SPREADING FOR AN INST. SPILL **
C
0032      210      I = STP
0033      GO TO (240,220) I
C      ----- CALCULATE TIB AND RIB BY USING MODEL 2B -----
C      (2A IS THE CURRENT MODEL)
C
C      *****
C      FOR A CONTINUOUS SPILL, USE OPEN WATER MODEL TO COMPUTE TIME
C      FOR SPILL TO SPREAD ACROSS RIVER. FIRST, COMPUTE THE CONDITIONS
C      AT END OF GRAVITY-INERTIA PHASE FOR OPEN WATER.
C      *****
0034      220      TIB = SQRT(SPILMR/(GR*COEF*DENW*VSW))*((K21/K11)**6.)
C
C      ** TIB = END OF GRAVITY-INERTIAL PHASE FOR A CONT. SPILL **
C      **      IN OPEN WATER      **
C
0035      AIB = (((SPILMR/DENW)**5/(VSW**3*GR*COEF))**0.25)*
*      (PI*C21**2.*(C21/C20)**7.)
0036      RIB = SQRT(AIB/PI)
C
C      ** RIB = RADIUS OF GRAVITY-INERTIA PHASE SLICK FOR CONT. **
C      **      SPILL IN OPEN WATER      **
C
0037      GO TO 260
C
C      ----- CALCULATE TIB AND RIB BY USING MODEL 1B -----
C      (1A IS THE CURRENT MODEL)
C
C      *****
C      FOR AN INSTANTANEOUS SPILL, USE OPEN WATER MODEL TO COMPUTE TIME
C      FOR SPILL TO SPREAD ACROSS RIVER. FIRST, COMPUTE THE CONDITIONS
C      AT END OF GRAVITY-INERTIA PHASE FOR OPEN WATER.
C      *****
0038      240      TIB = (VO/(GR*COEF*VSW))*((1./3.))*((K20/K10)**4.)
0039      AIB = (VO**2./3.)*(GR*VO*COEF/(VSW**2))*((1./6.))*
*      (PI*K20**2.*(K20/K10)**2.)
0040      RIB = SQRT(AIB/3.141593)
C
C      ** TIB = END OF GRAVITY-INERTIA PHASE FOR INST. SPILL IN **
C      **      OPEN WATER      **
C      ** RIB = RADIUS OF GRAVITY-INERTIA PHASE SLICK FOR INST. **

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C      **      SPILL IN OPEN WATER      **
C
0041 260 CONTINUE
0042 IF (RIB.LT.(WW/2 0)) GO TO 400
C
C *****
C IF RIB < WW/2, THE SLICK WILL SPREAD SOME MORE AS AN OPEN
C WATER SLICK, BUT NUMERICAL INTEGRATION IS REQUIRED.
C *****
0043 IF (TIB.GE.TIA) GO TO 280
C
C *****
C IF TIB > TIA, OPEN-WATER SLICK HAS SPREAD ALL THE WAY ACROSS
C RIVER, BUT NEED TO REDUCE TIME SOME TO FIND ACTUAL TIME TO
C SPREAD ACROSS RIVER.
C *****
0044 TII = TIA
C
C ** TIB < TIA, SO INITIAL TIME TII = TIA **
C
0045 GO TO (261,262) I
C
C      USE MODEL 1A TO COMPUTE INITIAL AREA AND THICKNESS
C
0046 261 ATK=2.*C20*((C20/C10)**(9./7.))*((VO**4.*WW**2.)*(1./7.))*
$      ((GR*COEF*VO/VISW**2.)*(1./7.))
0047 HTK = VO/ATK
C
C *****
C ATK AND HTK ARE INSTANTANEOUS SPILL THICK SLICK AREA AND
C THICKNESS AT TIME SLICK HAS SPREAD ACROSS RIVER.
C *****
0048 IF(IC.GE.2) GOTO 265
C
C *****
C XC = NEW SPILL CENTER LOCATION XC AFTER BEING TRANSPORTED
C DOWNSTREAM (INSTANTANEOUS)
C *****
0049 XC=XO + (UCX1+0.025*VWX1)*TIA
0050 GOTO 270
0051 265 XC=XO+(UO*TIA-(WT/(2.*PI*TIA))*(COS(2.*PI*(TIA+ALPH)/WT)
1      -COS(2.*PI*ALPH/WT))+0.035*VWX1)*TIA
0052 GO TO 270
C
C      USE MODEL 2A TO COMPUTE INITIAL AREA & THICKNESS
C
0053 262 ATK = 2.*C21*((C21/C11)**7.)*(WW*(SPILMR/(WW*DENW)))*(5./3.)/
1      (VISW*((GR*COEF)**(1./3.)))
0054 HTK = (SPILMR*TII-DENO*8.0*ATK*HTN)/(DENO*ATK)
C
C *****

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C      ATK AND HTK ARE CONTINUOUS SPILL THICK SLICK AREA AND THICKNESS
C      AT TIME SLICK HAS SPREAD ACROSS RIVER.
C      *****
0055  270  ATN = 8.0*ATK
C
C      ** ATN = THIN SLICK AREA **
C
0056      GO TO 300
0057  280  CONTINUE
0058      TII = TIB * SQRT(WW/(2.0*RIB))
0059      ATK = AIB*TII/TIB
C
C      ** INITIAL TIME AND AREA WHEN RIB > WW/2 AND TIB > TIA. **
C
0060      GO TO (281,282) I
C
C      USE MODEL 1. A TO CALCULATE INITIAL THICKNESS(INSTANTANEOUS)
C
0061  281  HTK = VO/ATK
0062      GO TO 285
C
C      USE MODEL 2. A TO CALCULATE INITIAL THICKNESS AND
C      CORRECT FOR MASS IN THIN SLICK(CONTINUOUS)
C
0063  282  HTK = (SPILMR*TII-DENO*8.0*ATK*HTN)/(DENO*ATK)
0064  283  CONTINUE
0065      ATN = 8.0 * ATK
C
0066  290  IF (I.EQ.1) GO TO 300
0067      IF (TII.LT.TSPILL) GO TO 300
0068      WRITE (1,112)
C
C      *****
C      TIME REQUIRED TO SPREAD ACROSS RIVER > DISCHARGE TIME.
C      SWITCH TO AN INSTANTANEOUS MODEL AND START OVER
C      *****
0069      STP = 1.1
0070      SPILLM = SPILMR * TSPILL
0071      GO TO 201
C
0072  300  CONTINUE
0073      TIIT = TII/60.
0074      WRITE (1,301) ATK,TIIT
0075      WRITE (6,301) ATK,TIIT
0076  301  FORMAT (/1H1/1X,
1  60H*****
2  /1X,35HTHE THICK SLICK HAS SPREAD OVER THE,
2  15H CHANNEL WIDTH. /1X,21HIT COVERS AN AREA OF ,
2  F15.2,2X,13HSQUARE METERS, /1X,15HAFTER A TIME OF,
3  F15.7,2X,7HMINUTES)
0077      GO TO 699
C
0078  400  CONTINUE

```

```

C
C *****
C ROUTINE TO NUMERICALLY INTEGRATE OPEN WATER MODELS IN
C GRAVITY-VISCOUS PHASE UNTIL SLICK SPREADS ACROSS RIVER
C *****
C
0079      TII = TIB
0080      ATK = AIB
0081      GO TO (401,402) I

C          USE MODEL 1B TO CALCULATE INITIAL THICKNESS(INSTANTANEOUS)
C
0082      401      HTK = VO/ATK
0083              GO TO 405

C          USE MODEL 2B TO CALCULATE INITIAL THICKNESS
C          (CORRECT FOR MASS IN THIN SLICK) (CONTINUOUS)
C
0084      402      HTK = (SPILMR*TII-DENO*8.0*ATK*HTN)/(DENO*ATK)
0085      405      CONTINUE
C
0086      TIME=TII
0087      YY(1)=ATK
0088      YY(2)=8.0*ATK
0089      YY(3)=HTK
0090      YY(4) = 0.0
0091      YY(5) = 0.0

C
C      ** TEMPORARILY CHANGE TO OPEN WATER MODEL **
C
0092      IF (STP.EQ.1.1) STP=1.2
0093      IF (STP.EQ.2.1) STP=2.2
0094      CALL TRANSP

C
C      ** INTEGRATE OVER ONE TIME STEP **
C
0095      410      CALL INTE(XEND)
C
C      ** CHECK FOR EVAPORATION PROBLEMS **
C
0096      IF (IDEB.EQ.0) THEN
0097          KKK=3
0098          IF (STP.EQ.1.2) STP=1.1
0099          IF (STP.EQ.2.2) STP=2.1
0100          GO TO 699
0101      ELSE
0102      ENDIF

C
C      ** CHECK TO SEE IF SLICK HAS SPREAD ACROSS RIVER **
C
0103      IF (SQRT(YY(1)/3.141593).GE.(WW/2.0)) GO TO 420

C
C      ** SEE IF PRINTOUT TIME HAS OCCURRED **
C
0104      IJ = TIME

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0105      IK = TPT
0106      MD = MOD(IJ, IK)
0107      IF (MD.NE.0) GO TO 410
0108      CALL MOVE
0109      CALL PRINTO
0110      GO TO 410
0111      420  CONTINUE
0112      TB=TIME
          C
          C      ** CHANGE BACK TO INSTANTANEOUS MODEL IN RIVER **
          C
0113      STP = 1.1
0114      GO TO (442, 422) I
          C
0115      422  IF (TB.GE.TSPILL) GO TO 424
          C
          C      ** CHANGE BACK TO CONTINUOUS MODEL IN RIVER **
          C
0116      STP = 2.1
0117      SPILLM=SPILMR*TB
0118      GO TO 442
0119      424  CONTINUE
0120      WRITE (1, 112)
0121      WRITE (6, 112)
          C
          C      ** IF TIME > DISCHARGE TIME, SWITCH TO INSTANTANEOUS MODEL **
          C
0122      STP = 1.1
0123      SPILLM=SPILMR*TSPILL
0124      GO TO 201
0125      442  CONTINUE
          C
          C      ** SET INITIAL TIME = TII **
          C
0126      TII = TB
0127      ATK = YY(1)
0128      ATN = YY(2)
0129      HTK = YY(3)
0130      TOTALM = YY(1)*YY(3)*DENO
0131      DMASS = SPILLM-TOTALM
0132      TIIT = TII/60.
0133      WRITE (1, 444) ATK, TIIT, DMASS
0134      WRITE (6, 444) ATK, TIIT, DMASS
0135      444  FORMAT (1H1//1X,
1  60H*****
2  /1X, 32HTHE THICK SLICK HAS SPREAD OVER ,
3  32HCHANNEL WIDTH AND COVERS AN AREA/1X, 3HOF , E12. 5,
4  2X, 29HSQUARE METERS AFTER A TIME OF, E12. 5, 2X, 9H MINUTES. /,
3  1X, 39HTHE MASS LOST FROM THE SLICK UP TO THIS,
4  8H TIME IS, E12. 5, 2X, 9H KILOGRAMS)
0136      699  RETURN
0137      END

```

```

0001      SUBROUTINE INT12B
C
C
C      *****
C      *      INITIAL CONDITIONS FOR MODELS 1.B AND 2.B      *
C      *      SPILL IN OPEN WATER. IF SPILL IS              *
C      *      CONTINUOUS, CURRENT MUST BE ZERO.              *
C      *****
C
C      THIS SUBROUTINE IS CALLED BY "INIT". IT CALCULATES THE
C      INITIAL CONDITIONS FOR INSTANTANEOUS OR CONTINUOUS SPILLS
C      IN OPEN WATER. FOR A CONTINUOUS SPILL, THE CURRENT AND WIND
C      MUST BE ZERO, OR ELSE "INIT4B" WILL BE CALLED.
C
0002      COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0003      COMMON/CHEMI/DENO, DCA, DCW, CS, CMW
0004      COMMON/WATER/DENW, VISH, GR
0005      COMMON/SPREAD/TII, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0006      COMMON/ENVOR/PV, VISA, DENA, TDC
0007      COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0008      COMMON/SENSE/EVA(40,10), DIS(40,10), THK(40,10), TIN(40,10),
C      PIP(40), TPT
0009      COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0010      COMMON/UAVE/UCX1, UCY1, VWX1, VWY1
0011      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
C      K12, K22
0012      REAL K10, K20, K11, K21, K12, K22
0013      PI=ACOS(-1.)
C
C      ** STP = 1.2 (INST.) OR 2.2 (CONT.) -- OPEN WATER **
C
0014      I = STP
0015      GO TO (10,110) I
C
C      -----
C      FOR INSTANTANEOUS SPILL IN OPEN WATER
C      -----
0016      10  SPI = SPILLM
0017      VO = SPI/DENO
0018      15  TII = ((K20/K10)**4.)*(VO/(GR*COEF*VISH)) ** (1.0/3.0)
0019      20  ATK = PI*(K20**2.)*((K20/K10)**2.)*(VO**(2.0/3.0)) *
C      (GR*VO*COEF/(VISH*VISH))**(1.0/6.0)
0020      1  HTK = VO/ATK
C
C      *****
C      TII = END OF GRAVITY-INERTIA PHASE
C      ATK, HTK = THICK SLICK AREA AND THICKNESS AT END OF
C      GRAVITY-INERTIA PHASE
C      *****
0021      XC=XO+(UCX1+0.035*VWX1)*TII
0022      YC=YO+(UCY1+0.035*VWY1)*TII
C
C      ** XC, YC = NEW VALUES OF SLICK CENTER LOCATION **
C
0023      GO TO 149

```

```

C
C
C -----
C          FOR CONTINUOUS SPILL
C -----
0024 110 TII = ((K21/K11)**6.)*SQRT(SPILMR/(QR*COEF*DENW*VISW))
C
C ** TII = END OF GRAVITY-INERTIA PHASE **
C
0025 IF (TII.LT.TSPILL) GO TO 120
0026 WRITE (1,112)
0027 WRITE (6,112)
0028 112 FORMAT (1H1//1X,
1 50H*****,,/
2 1X,48HTHE SPILL TIME IS SO SHORT THAT AN INSTANTANEOUS,/
3 1X,30HSPILL WILL GIVE BETTER RESULTS)
C
C ** SINCE TII > DISCHARGE TIME, SWITCH TO INSTANTANEOUS MODEL **
C
0029 STP = 1.2
0030 SPILLM = SPILMR * TSPILL
0031 GO TO 10
0032 120 ATK = (PI*K21**2.*(K21/K11)**7.)*((SPILMR/DENW)**5
* /(VISW**3.*QR*COEF)) ** 0.25
0033 HTK = (SPILMR*TII-DENO*8.0*ATK*HTN)/(DENO*ATK)
0034 ATN = 8.0*ATK
C
C ** ATK, HTK = THICK SLICK AREA AND THICKNESS AT END OF **
C ** GRAVITY-INERTIA PHASE **
C ** ATN = THIN SLICK AREA AT END OF GRAVITY-INERTIA PHASE **
C
0035 149 CONTINUE
0036 RADIUS = SQRT(ATK/3.141593)
0037 TIIT = TII/60.
0038 WRITE (1,159) ATK,RADIUS,TIIT
0039 WRITE (6,159) ATK,RADIUS,TIIT
0040 159 FORMAT (//1X,38HTHICK SLICK HAS SPREAD OVER A CIRCULAR,
1 8H AREA OF,E12.5,14HSQUARE METERS,/
2 1X,17HWITH A RADIUS OF ,E12.5,6HMETERS,
3 16H AFTER THE FIRST,E12.5,7HMINUTES)
0041 RETURN
0042 END

```

```

0001      SUBROUTINE INIT4A
C          *****
C          *      CALCULATE INITIAL CONDITIONS FOR MODEL 4A
C          *      CONTINUOUS IN A CHANNEL WITH A TRANSPORT VELOCITY
C          *      OF UTBA
C          *****
C          THIS SUBROUTINE IS CALLED BY "INIT". IT COMPUTES INITIAL
C          CONDITIONS FOR A CONTINUOUS SPILL IN A RIVER WITH A CURRENT.
C
0002      COMMON/SIZE/R, D, WW, L1, L2, H, RO
0003      COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0004      COMMON/WATER/DENW, VISW, GR
0005      COMMON/CHEMI/DENO, DCA, DCW, CS, CMW
0006      COMMON/SPREAD/TII, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0007      COMMON/RUNGE/YY(5), C(24), W(5, 30)
0008      COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0009      COMMON/TRAVEL/WTX, Z
0010      COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0011      COMMON/SENSE/EVA(40, 10), DIS(40, 10), THK(40, 10), TIN(40, 10),
1          PIP(40), TPT
0012      COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0013      COMMON/PRIM/PRIME(5), IDEB, KKK
0014      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
1          K12, K22
0015      REAL K10, K20, K11, K21, K12, K22
0016      TIB = ((K22/K12)**(24./7.))*(SPILMR/(2.*DENW))**(4./7.)/
1          ((UTBAR**(4./7.))*(GR*COEF)**(2./7.))*(VISW**(3./7.)))
0017      ATKB = K22*((K22/K12)**(33./7.))*(SPILMR/(2.*DENW))**(9./7.)
1          /((UTBAR**(2./7.))*(GR*COEF)**(1./7.))*(VISW**(5./7.)))
C
C      ** TIB = END OF GRAVITY-INERTIA PHASE      **
C      ** ATKB = THICK SLICK AREA AT END OF GRAVITY- **
C      **          INERTIA PHASE                  **
C
0018      IF (TIB.LT.TSPILL) GO TO 50
0019      5  WRITE (1, 10)
0020      WRITE (6, 10)
0021      10  FORMAT (//1X, 44HSPILL TIME IS SO SHORT THAT AN INSTANTANEDUS,
1          /1X, 31HMODEL WILL GIVE BETTER RESULTS.)
C
C          *****
C          SINCE TIB > DISCHARGE TIME, SWITCH TO AN INSTANTANEDUS
C          SPILL (RETURN TO "INIT").
C          *****
C
0022      STP = 1.1
0023      SPILLM = SPILMR * TSPILL
0024      GO TO 299
C
C      ** WTK = WIDTH OF DOWNSTREAM END OF THICK SLICK **
C
0025      50  WTK = 2.0*ATKB/(UTBAR*TIB)
0026      IF (WTK.GT.WW) GO TO 55
0027      GO TO 100

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```

C
C *****
C SINCE WTK > RIVER WIDTH, TIME AND SLICK AREA NEED TO BE
C REDUCED ACCORDINGLY TO GET INITIAL CONDITIONS.
C *****
C
0028 55 TII = TIB*(WW/WTK)
0029 ATK = ATAB*(TII/TIB)**2
C
C ** TII AND ATK ARE INITIAL CONDITIONS FOR TIME AND THICK **
C ** SLICK AREA.
C
0030 IF (TII.GT.TSPILL) GO TO 90
0031 Z = UTBAR*TII
0032 TIIIT = TII/60.
0033 WRITE (1,60) ATK,TIIIT,Z
0034 WRITE (6,60) ATK,TIIIT,Z
0035 60 FORMAT(//1X,42HTHICK SLICK HAS SPREAD ACROSS THE CHANNEL ,
1 27HWIDTH AND COVERS AN AREA OF,E12.5/1X,
2 29HSQUARE METERS AFTER A TIME OF,E12.5,2X,8HMINUTES.,
3 /1X,25HTHE SLICK LEADING EDGE IS,E12.5,2X,
4 18HMETERS DOWNSTREAM.)
0036 HTK = (SPILMR*TII-DENO*8.0*ATK*HTN)/(DENO*ATK)
C
C ** HTK = INITIAL THICK SLICK THICKNESS CORRECTED FOR MASS **
C ** IN THIN SLICK
C
0037 ATN = 8.0 * ATK
C
C ** ATN = INITIAL THIN SLICK AREA
C
0038 GO TO 299
0039 90 CONTINUE
0040 TIB = TII
0041 GO TO 5
C
C *****
C SINCE SLICK WIDTH < RIVER WIDTH AT END OF GRAVITY-INERTIA
C PHASE, USE INTEGRATION OF OPEN-WATER GRAVITY-VISCOUS MODEL
C TO CONTINUE UNTIL WIDTH = RIVER WIDTH.
C *****
C
0042 100 TII = TIE
0043 ATK = ATK8
0044 HTK = (SPILMR*TII-DENO*8.0*ATK*HTN)/(DENO*8.0*ATK)
0045 TIME = TII
0046 YY(1) = ATK
0047 YY(2) = 8.0 * ATK
0048 YY(3) = HTK
C
C ** SWITCH TO OPEN-WATER MODEL **
C
0049 STP = 4.2
0050 CALL TRANSP
0051 105 CALL INTE(XEND)

```

```

C
C
C      ** CHECK FOR EVAPORATION TROUBLES **
0052      IF (IDEB.EQ.0) THEN
0053          KKK=3
0054          STP=4.1
0055          GOTO 299
0056      ELSE
0057      ENDIF

C
C
C      ** ONCE MORE, CHECK TO SEE IF TIME < DISCHARGE TIME **
0058      IF (TIME.GT. TSPILL) GOTO 5
0059      IF ((2.0*YY(1)/(UTBAR*TIME)).GT.WW) GO TO 110

C
C
C      ** GO TO 110 WHEN WIDTH > RIVER WIDTH **

0060      IJ = TIME
0061      IK = TPT
0062      MD = MOD(IJ,IK)
0063      IF (MD.NE.0) GO TO 105
0064      CALL MOVE
0065      CALL PRINTO
0066      GO TO 105
0067      STP = 4.1
110

C
C
C      *****
C      RETURN WITH INITIAL CONDITIONS TII = TIME, ATK = THICK SLICK
C      AREA, ATN=THIN SLICK AREA, AND ATK = THICK.
C      *****

0068      TII = TIME
0069      ATK = YY(1)
0070      ATN = YY(2)
0071      HTK = YY(3)
0072      TOTALM = YY(1)*YY(3)*DENO
0073      SPILLM=SPILMR * TIME
0074      DMASS = SPILLM - TOTALM
0075      TIIT = TII/60.
0076      Z = UTBAR * TII
0077      WRITE (1,120) ATK,TIIT,Z,DMASS
0078      WRITE (6,120) ATK,TIIT,Z,DMASS
0079      120      FORMAT(/1X,41HTHICK SLICK HAS SPREAD ACROSS THE CHANNEL,
1          28H WIDTH AND COVERS AN AREA OF,/1X,E12.5,
2          14HSQUARE METERS./1X,16HAFTER A TIME OF ,E12.5,8HMINUTES./,
3          25HTHE SLICK LEADING EDGE IS,E12.5,
4          18HMETERS DOWNSTREAM./1X,
5          47HTHE MASS LOST FROM THE SLICK UP TO THIS TIME IS,
6          E12.5,10HKILOGRAMS.)
0080      299      RETURN
0081      END

```

```

0001      SUBROUTINE INIT4B
          C *****
          C *          CALCULATE INITIAL CONDITIONS FOR MODEL 4B
          C *          CONTINUOUS SPILL IN OPEN WATER WITH A CURRENT
          C *          SPEED (TRANSPORT VELOCITY) OF UTBAR
          C *****
          C
          C THIS SUBROUTINE IS CALLED BY "INIT". IT COMPUTES THE INITIAL
          C CONDITIONS FOR A CONTINUOUS SPILL IN OPEN WATER WITH A CURRENT.
          C
0002      COMMON/SIZE/R, D, WW, L1, L2, H, R0
0003      COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0004      COMMON/WATER/DENW, VISW, OR
0005      COMMON/CHEMI/DENO, DCA, DCW, CS, CNW
0006      COMMON/SPREAD/TII, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0007      COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0008      COMMON/TRAVEL/WTX, Z
0009      COMMON/INTER/COEF, SIGWA, SIGOA, SIGOW, SIG
0010      COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0011      COMMON/TRANSIT/UX(10, 10), UY(10, 10), VWX(10),
          C 1          VWY(10), THETA(10), TI(10), ID, IT, IV,
          C 2          XU(10), YU(10), TT(10)
0012      COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0013      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
          C 1          K12, K22
0014      REAL K10, K20, K11, K21, K12, K22
0015      M=ISP
0016      10 TII = ((K22/K12)**(24./7.))*((SPILMR/(2.*DENW))**(4./7.))/
          C 1 ((UTBAR**(4./7.))*((OR*COEF)**(2./7.))*
          C 2 (VISW**(3./7.)))
          C
          C ** TII = END OF GRAVITY-INERTIA PHASE **
          C
0017      IF (TII.GE.TSPILL) GO TO 50
          C
          C IF TII > DISCHARGE TIME, SWITCH TO AN INSTANTANEOUS MODEL **
          C
0018      ATK = K22*((K22/K12)**(33./7.))*(SPILMR/(2.*DENW))**(9./7.)
          C 1 /((UTBAR**(2./7.))*((OR*COEF)**(1./7.))*(VISW**(5./7.)))
0019      HTK = (SPILMR*TII-DENO*8.0*ATK*HTN)/(DENO*ATK)
0020      ATN = 8.0 * ATK
0021      WTK = 2.0 * ATK/(UTBAR*TII)
          C
          C *****
          C ATK = INITIAL THICK SLICK AREA
          C HTK = INITIAL THICK SLICK THICKNESS
          C ATN = INITIAL THIN SLICK AREA
          C WTK = INITIAL THICK SLICK DOWNSTREAM WIDTH
          C *****
          C
          C *****
          C XLE AND YLE ARE DOWNSTREAM COORDINATES OF LEADING EDGE
          C WITH RESPECT TO CURRENT DIRECTION.
          C *****

```

```

C
0022      Z = UTBAR*TII
0023      XLE = XC + (UX(M,1)+0.035*VWX(1))*TII
0024      YLE = YC + (UY(M,1)+0.035*VWY(1))*TII
0025      TIIT = TII/60.
0026      WRITE (1,20) ATK,TIIT,WTk,Z
0027      WRITE (6,20) ATK,TIIT,WTk,Z
0028      20  FORMAT(//1X,41HTHICK SLICK HAS SPREAD OVER AN ELONGATED ,
1          19HTRIANGULAR AREA OF ,E12.5, /
2          1X,29HSQUARE METERS AFTER A TIME OF,E12.5,8HMINUTES. , /
3          1X,31HTHE THICK SLICK LEADING EDGE IS,E12.5,2X,
4          18HMETERS WIDE AND IS,E12.5,2X,7HMETERS /
5          1X,11HDOWNSTREAM. )
0029      WRITE (1,22) ATN
0030      22  FORMAT (//1X,31HTHE THIN SLICK AREA IS.EQUAL TO,E12.5,
1          1X,14HSQUARE METERS.
0031      TEMP1 = DENO*(ATK*HTK-ATN*HTN)
0032      TEMP2 = SPILMR*TII
0033      GO TO 99
0034      50  WRITE (1,52)
0035      WRITE (6,52)
0036      52  FORMAT(//1X,45HSPILL TIME IS SO SHORT THAT AN INSTANTANEOUS ,
1          1X,31HMODEL WILL GIVE BETTER RESULTS. )
C
C      ** MAKE SWITCH TO INSTANTANEOUS MODEL **
C
0037      STP = 1.2
0038      SPILLM = SPILMR * TSPILL
0039      99  RETURN
0040      END

```



```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      SUBROUTINE INTE (XEND)
C      SUBROUTINE TO SOLVE SIMULTANEDUS 1ST ORDER DIFFERENTIAL
C      EQUATIONS BY USING RUNGE-KUTTA METHOD
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      THIS SUBROUTINE IS CALLED BY "SPREAD" AND THE INITIAL CONDITIO
C      SUBROUTINES "INT12A" AND "INIT4A". IT SENDS THE APPROPRIATE
C      GRAVITY-VISCOUS MODEL EQUATIONS TO A RUNGE-KUTTA INTEGRATION
C      ROUTINE "RUNKUT" TO COMPUTE THE THICK SLICK AREA AND OTHER
C      VARIABLES AS A FUNCTION OF TIME. AFTER EACH PASS, 'TIME' IS
C      INCREMENTED BY 'DELT'. THE "FCN" SUBROUTINES IN THE "RUNKUT"
C      CALL ARE THE EQUATIONS OF THE GRAVITY-VISCOUS MODELS. THE
C      MATRIX 'YY' IN THE CALL IS:
C      ** YY(1) = THICK SLICK AREA, SQ. M
C      ** YY(2) = THIN SLICK AREA, SQ. M
C      ** YY(3) = THICK SLICK THICKNESS, M
C
C      THE MATRIX 'YPRIME' IN THE "FCN" SUBROUTINES IS:
C      ** YPRIME(1) = D(YY(1))/DT
C      ** YPRIME(2) = D(YY(2))/DT
C      ** YPRIME(3) = D(YY(3))/DT
C      ** YPRIME(4) = RATE OF EVAPORATION LOSS, KG/SEC
C      ** YPRIME(5) = RATE OF DISSOLUTION LOSS, KG/SEC
C
0001      SUBROUTINE INTE(XEND)
0002      COMMON/RUNGE/YY(5), C(24), W(5,30)
0003      COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0004      COMMON/MASS/TOTALE, TOTALD, TOTALM, DMASS
0005      COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0006      COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0007      COMMON/MLOSS/EVAPM, DISSOM
0008      COMMON/CHEMI/DENO, DCA, DCW, CS, CMW
0009      COMMON/PRIM/PRIME(5), IDEB, KKK
0010      COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
1          K12, K22
0011      COMMON/SPREAD/T11, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0012      REAL K10, K20, K11, K21, K12, K22
0013      EXTERNAL FCN11, FCN12, FCN21, FCN22, FCN41, FCN42
C
C
C      ----- CALL SUBROUTINE TO CALCULATE EVAPORATION LOSS -----
0014      CALL EVAP
C      ----- CALL SUBROUTINE TO CALCULATE DISSOLUTION LOSS -----
0015      CALL DISS
0016      10  CONTINUE
C
0017      N=5
0018      NW = 5
0019      IND = 1
0020      TOL = 1.E-7
C
0021      XEND = TIME + DELT
C      ----- MODEL 1. A -----
0022      IF (STP.NE.1.1) GO TO 20

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C          ----- MODEL 1. A -----
0023      CALL RUNKUT(N, FCN11, TIME, YY, XEND, TOL, IND, C, NW, W, IER)
0024      GO TO 99
0025      20  IF (STP. NE. 1. 2) GO TO 30
C          ----- MODEL 1. B -----
0026      CALL RUNKUT(N, FCN12, TIME, YY, XEND, TOL, IND, C, NW, W, IER)
0027      GO TO 99
0028      30  IF (STP. NE. 2. 1) GO TO 40
C          ----- MODEL 2. A -----
0029      CALL RUNKUT(N, FCN21, TIME, YY, XEND, TOL, IND, C, NW, W, IER)
0030      GO TO 99
0031      40  IF (STP. NE. 2. 2) GO TO 70
C          ----- MODEL 2. B -----
0032      CALL RUNKUT(N, FCN22, TIME, YY, XEND, TOL, IND, C, NW, W, IER)
0033      GO TO 99
0034      70  IF (STP. NE. 4. 1) GO TO 80
C          ----- MODEL 4. A -----
0035      CALL RUNKUT(N, FCN41, TIME, YY, XEND, TOL, IND, C, NW, W, IER)
0036      GO TO 99
0037      80  CONTINUE
C          ----- MODEL 4. B -----
0038      CALL RUNKUT(N, FCN42, TIME, YY, XEND, TOL, IND, C, NW, W, IER)
0039      99  CONTINUE
0040      TOTALE = YY(4)
0041      TOTALD = YY(5)
0042      TOTALM = DENO*YY(1)*YY(3)
0043      ISTOP = STP
0044      110  CONTINUE
0045      CALL CHEKMS
0046      IF (IDEB. GT. 1) GOTO 999
C
C      *****
C      IF IDEB = 0, 'TCHECK' IS MADE LESS THAN 'TIME' OTHERWISE,
C      'TCHECK' REMAINS EQUAL TO 'TSTOP' AS SPECIFIED IN "DMODEL".
C      *****
0047      111  TCHECK = TIME - DELT
0048      999  CONTINUE
0049      RETURN
0050      END

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0022      C      200      CONTINUE
0023      C      IF (J.GT.1) GO TO 400
0024      C      IF (IC.GT.1 AND IW.GT.1) GO TO 250
      C      ***      MOVEMENT MODEL M.3. A      ***
      C      1. IN RIVER OR CHANNEL
      C      2. UC AND VW DO NOT VARY WITH TIME
0025      C      DMOVE = 3.10
0026      C      XLE = UTOT*TIME
0027      C      XTE = 0.0
0028      C      GO TO 999
0029      C      250      CONTINUE
      C
0030      C      280      IF (UBAR(1).LT.(0.3*UPEAK(1))) GO TO 300
      C
      C      ***      MOVEMENT MODEL M.3 (B.1)      ***
      C      1. IN RIVER OR CHANNEL
      C      2. UBAR .GE. (0.3*UPEAK)
      C
      C      *****
      C      WHEN UBAR > 0.3 * UPEAK, TIME VARIATION IS NEGLECTED AND
      C      AVERAGE TRANSPORT VELOCITY IS USED TO COMPUTE MOVEMENT
      C      DUE TO CURRENT. CORRECTION FOR APPARENT MOVEMENT DUE TO
      C      SPREADING IS MADE IN "PRINTO".
      C      *****
      C
0031      C      DMOVE = 3.21
0032      C      XLE = (UBAR(1) + 0.035*VW*COS(THETA1))*TIME
0033      C      XTE = 0.0
0034      C      GO TO 999
      C
      C      ***      MOVEMENT MODEL M.3 (B.2)      ***
      C      1. IN RIVER OR CHANNEL
      C      2. UBAR .LT. (0.3*UPEAK)
      C
      C      *****
      C      WHEN UBAR < 0.3 * UPEAK, TIME VARYING 'UTOT' IS USED TO
      C      COMPUTE INCREMENTAL MOTION OF LEADING EDGE DUE TO CURRENT.
      C      CORRECTION FOR APPARENT MOVEMENT DUE TO SPREADING IS MADE
      C      IN "PRINTO".
      C      *****
      C
0035      C      300      CONTINUE
0036      C      DMOVE = 3.22
0037      C      XLE = XLE + UTOT*DELT
0038      C      GO TO 999
      C
      C      ***      OPEN WATER, CONTINUOUS SPILL      ***
      C
0039      C      400      IF (IC.LE.2 AND IW.LE.1) GO TO 455
0040      C      GO TO 500
      C
      C      ***      MOVEMENT MODEL M.4. A      ***
      C      1. IN OPEN WATER
      C      2. UC AND VW DO NOT VARY WITH TIME
0041      C      455      DMOVE = 4.10

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0042 470 XLE = XLE + UTX*DELT
0043 YLE = YLE + UTY*DELT
0044 GO TO 999
0045 500 CONTINUE
0046 IF (IW.GT.1) GO TO 505
0047 W1 = VWX(1)
0048 W2 = VWY(1)
0049 GO TO 530

C
C ** SINCE WIND = F(TIME), INTERPOLATE TO FIND WIND SPEED AT **
C ** CORRECT TIME. **
C

0050 505 CONTINUE
0051 DO 510 I = 1,10
0052 IF (TBEF.LE.TT(I)) GO TO 520
0053 510 CONTINUE
0054 520 W1 = VWX(I-1)+(VWX(I)-VWX(I-1))*(TBEF-TT(I-1))/
1 (TT(I)-TT(I-1))
0055 W2 = VWY(I-1)+(VWY(I)-VWY(I-1))*(TBEF-TT(I-1))/
1 (TT(I)-TT(I-1))

C
C ** W1 AND W2 ARE INTERPOLATED WIND SPEEDS IN X AND Y DIRECTION
C
0056 530 CONTINUE
0057 IF (IC.EQ.1.OR.IC.EQ.3) ISP = 1

C
C ** IF CURRENT IS NOT F(SPACE), BOX OR SLICE LOCATION = 1 **
C

0058 IF (STP.LE.2.2) GO TO 600

C
C *** MOVEMENT MODEL M.4 (B.1) ***
C 1. IN OPEN WATER
C 2. UT(I) .GE. UPEAK(I)
C I IS THE REGION NO.WHERE THE LEADING
C EDGE WAS.....

0059 DMOVE = 4.21
0060 XLE = XLE + UTX*DELT
0061 YLE = YLE + UTY*DELT
0062 GO TO 999

C
C *** MOVEMENT MODEL M.4 (B.2) ***
C 1. IN OPEN WATER
C 2. UT(I) .LT. UPEAK(I)
C 3. THE SLICK IS CIRCULAR
C 4. SPREADING MODEL 2.B WAS USED AND UBAR = 0.

0063 600 CONTINUE
0064 DMOVE = 4.22
0065 XLE = XLE+UTX*DELT
0066 YLE = YLE+UTY*DELT
0067 UO = UTX/SGRT(UTX**2.+UTY**2.)
0068 U1 = UTY/SGRT(UTX**2.+UTY**2.)
0069 999 RETURN
0070 END

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0031      RAD2 = SQRT((YY(1)+YY(2))/3.14159)
0032      WRITE (1,5) TEMP, DIFFT,YY(1),YY(3),RAD1
0033      WRITE (6,5) TEMP, DIFFT,YY(1),YY(3),RAD1
0034      5  FORMAT(////2X,7HTIME = ,F10.2,8H MINUTES,2X,F7.3,8H SECONDS/9X,
           1 18HTHICK SLICK AREA =,E12.5,6H SQ. M.,2X,
           2 23HTHICK SLICK THICKNESS =,E12.5,7H METERS/9X,
           3 20HTHICK SLICK RADIUS =,E12.5,7H METERS)
0035      IF(I.EQ.1) GOTO 9
0036      WRITE (1,6) YY(2),RAD2
0037      WRITE (6,6) YY(2),RAD2
0038      6  FORMAT(9X,
           1 18HTHIN SLICK AREA =,E12.5,5HSQ. M.,/9X,
           2 20HTHIN SLICK RADIUS =,E12.5,6HMETERS)
0039      9  WRITE (1,7) TOTALM,TOTALE,EVAPM,TOTALD,DISSOM
0040      WRITE (6,7) TOTALM,TOTALE,EVAPM,TOTALD,DISSOM
0041      7  FORMAT(/9X,27HTOTAL MASS OF THICK SLICK =,E12.5,4H KG./9X,
           2 27HTOTAL EVAPORATED MASS =,E12.5,4H KG.,/9X,
           3 27HRAE OF EVAPORATION =,E12.5,15H KG/(SEC-SQ. M.),/9X,
           4 27HTOTAL DISSOLVED MASS =,E12.5,4H KG.,/9X,
           5 27HRAE OF DISSOLUTION =,E12.5,15H KG/(SEC-SQ. M.))
0042      IF(I.EQ.1) GOTO 10
0043      WRITE(1,8)TMASS
0044      WRITE(6,8)TMASS
0045      8  FORMAT(9X,27HTOTAL MASS OF THIN SLICK =,E12.5,4H KG.)
0046      10 WRITE(1,20)TOTS
0047      20 FORMAT(/9X,27HTOTAL MASS =,E12.5,4H KG.)
0048      WRITE(6,20)TOTS
0049      GO TO 300

C
C
C      SPREADING MODEL 4.8
C      (CONTINUOUS SPILL IN OPEN WATER WITH CURRENT)
C      ** ELONGATED SLICK **
C
C
0050      50 CONTINUE
0051      XW = 2.0*YY(1)/(UTBAR*TIME)
0052      XW1 = YY(2)*2.0/(UTBAR*TIME)
0053      WRITE (1,55) TEMP,DIFFT,YY(1),YY(3),XW
0054      WRITE (6,55) TEMP,DIFFT,YY(1),YY(3),XW
0055      WRITE (1,57) YY(2),XW1
0056      WRITE (6,57) YY(2),XW1
0057      55  FORMAT(////2X,7HTIME = ,F10.2,8H MINUTES,2X,F7.3,8H SECONDS/9X,
           1 18HTHICK SLICK AREA =,E12.5,6H SQ. M.,2X,
           2 23HTHICK SLICK THICKNESS =,E12.5,7H METERS/9X,
           3 30HTHICK SLICK DOWNSTREAM WIDTH =,E12.5,1X,6HMETERS)
0058      57  FORMAT(9X,
           1 18HTHIN SLICK AREA =,E12.5,6H SQ. M./9X,
           2 30HTHIN SLICK DOWNSTREAM WIDTH =,E12.5,1X,6HMETERS)
0059      WRITE (1,7) TOTALM,TOTALE,EVAPM,TOTALD,DISSOM
0060      WRITE (6,7) TOTALM,TOTALE,EVAPM,TOTALD,DISSOM
0061      WRITE(1,8)TMASS
0062      WRITE(6,8)TMASS
0063      WRITE(1,20)TOTS
0064      WRITE(6,20)TOTS

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```

0065      GO TO 300
          C
          C
          C      SPREADING MODELS 1. A, 2. A
          C      (1A = INSTANTANECUS SPILL IN RIVER;
          C      2A = CONTINUOUS SPILL IN RIVER WITH NO CURRENT)
          C
0066      100  CONTINUE
0067      WRITE (1,105) TEMP, DIFFT,YY(1),YY(3)
0068      WRITE (6,105) TEMP, DIFFT,YY(1),YY(3)
0069      105  FORMAT (///2X,7H TIME = ,F10.2,8H MINUTES,2X,F7.3,8H SECONDS/9X,
          C      1 18H THICK SLICK AREA =,E12.5,6H SQ. M.,2X,
          C      2 23H THICK SLICK THICKNESS =,E12.5,7H METERS)
0070      IF (I.EQ.1) GO TO 107
0071      WRITE (1,106) YY(2)
0072      WRITE (6,106) YY(2)
0073      106  FORMAT (9X,
          C      1 18H THIN SLICK AREA =,E12.5,5H SQ. M.)
0074      107  WRITE (1,7) TOTALM,TOTALE,EVAPM,TOTALD,DISSOM
0075      WRITE (6,7) TOTALM,TOTALE,EVAPM,TOTALD,DISSOM
0076      IF (I.EQ.1) GO TO 30
0077      WRITE (1,8) TMASS
0078      WRITE (6,8) TMASS
0079      30    WRITE (1,20) TOTS
0080      WRITE (6,20) TOTS
          C
0081      300  CONTINUE
0082      IJ = TIME
0083      IK = TPT
0084      IF (IJ.EQ.IK) GO TO 298
0085      MD = MOD(IJ,IK)
0086      IF (MD.NE.0) GO TO 299
0087      298  CONTINUE
0088      INDEX = INDEX + 1
0089      PIP(INDEX) = TIME
0090      EVA(INDEX,IFLAG) = TOTALE
0091      DIS(INDEX,IFLAG) = TOTALD
0092      THK(INDEX,IFLAG) = TOTALM
0093      TIN(INDEX,IFLAG) = TMASS
0094      299  CONTINUE
          C
          C      TRACKING MOVEMENT
          C
          C
          C      *****
          C      'DMOVE' INDICES ARE DEFINED IN "MOVE".
          C      *****
          C
0095      IF (DMOVE.EQ.1.0.OR.DMOVE.EQ.1.1) GO TO 301
0096      IF (DMOVE.EQ.2.0) GO TO 311
0097      GO TO 321
          C
          C      ** HERE TO 314 PERTAIN TO INSTANTANEOUS SPILLS **
          C
0098      301  WRITE (1,303) XC,YC

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0099      WRITE (6,303) XC,YC
0100      303      FORMAT (//9X,
1          41HTHE CENTER OF THE SLICK IS LOCATED AT X =,
2          E12. 5, 15H METERS AND Y =, E12. 5, 7H METERS)
0101      GO TO 500
          C
0102      311      WRITE (1,313) XC
0103      WRITE (6,313) XC
0104      313      FORMAT (//9X, 25HTHE WHOLE SLICK HAS MOVED, E12. 5,
1          6HMETERS)
0105      LTH=YY(1)/WW
0106      WRITE(1,314) LTH/2+XC, XC-LTH/2
0107      WRITE(6,314) LTH/2+XC, XC-LTH/2
0108      314      FORMAT(9X, 40HTHE DOWNSTREAM EDGE OF THE SLICK IS AT =, E12. 5,
*          7H METERS, 1X, 30H AND THE UPSTREAM EDGE IS AT =, E12. 5, 7H METERS)
0109      GO TO 500
0110      321      CONTINUE
0111      IF (DMOVE. LE. 3. 215) GO TO 323
0112      IF (DMOVE. LT. 3. 900) GO TO 325
0113      IF (DMOVE. LT. 4. 215) GO TO 333
0114      GO TO 335
          C
          C      ** REST OF STATEMENTS RELATE TO CONTINUOUS SPILLS **
          C
0115      323      TEMP1 = XLE
0116      TEMP2 = 0. 0
          C
          C      ** NOW CORRECT IF THERE IS NO CURRENT, SO SLICK IS SPREAD **
          C      ** OUT SYMMETRICALLY ABOUT SOURCE.      **
          C
0117      IF(TEMP1.EQ.0. 0) THEN
0118          TEMP1 = YY(1)/(2. 0*WW)
0119          TEMP2 = -YY(1)/(2. 0*WW)
0120      ELSE
0121          TEMP1=YY(1)/WW
0122      ENDIF
0123      GO TO 327
0124      325      TEMP1 = XLE+YY(1)/(2. 0*WW)
0125      TEMP2 = XLE-YY(1)/(2. 0*WW)
          C
          C      ** IN A TIDAL RIVER, THE TRAILING EDGE CANNOT MOVE **
          C      ** DOWNSTREAM, JUST UPSTREAM.      **
          C
0126      IF (TEMP2. GT. 0. 0) TEMP2=0. 0
0127      327      WRITE (1,329) TEMP1,TEMP2
0128      WRITE (6,329) TEMP1,TEMP2
0129      329      FORMAT (//9X,
1          47HTHE LEADING EDGE OF THE SLICK IS LOCATED AT X =,
2          E12. 5, 6HMETERS/
3          9X,
4          48HTHE TRAILING EDGE OF THE SLICK IS LOCATED AT X =,
5          E12. 5, 6HMETERS)
0130      GO TO 500
0131      333      CONTINUE
0132      WRITE (1,334) XLE,YLE

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```

0133      WRITE (6,334) XLE,YLE
0134      334      FORMAT (//9X,
1          47HTHE LEADING EDGE OF THE SLICK IS LOCATED AT X =,
2          E12.5,2X,10MMETERS AND/53X,3HY =,E12.5,2X,6MMETERS/5X,
3          61HTHE TRAILING EDGE OF THE SLICK IS LOCATED AT THE SPILL ORI
4          )
0135      GO TO 500
0136      335      TEMP1 = XLE+UO*SQRT(YY(1)/3.14159)+XC
0137      TEMP2 = YLE+U1*SQRT(YY(1)/3.14159)+YC
0138      TEMP3=(SQRT(XLE**2.+YLE**2.)-2.*SQRT(YY(1)/3.14159))*UO
0139      TEMP4=(SQRT(XLE**2.+YLE**2.)-2.*SQRT(YY(1)/3.14159))*U1
0140      IF((TEMP3-XC)*UO GE. 0.) TEMP3=XC
0141      IF((TEMP4-YC)*U1 GE. 0.) TEMP4=YC
0142      337      WRITE (1,339) TEMP1,TEMP2,TEMP3,TEMP4
0143      WRITE (6,339) TEMP1,TEMP2,TEMP3,TEMP4
0144      339      FORMAT (//9X,
1          47HTHE LEADING EDGE OF THE SLICK IS LOCATED AT X =,
2          E12.5,2X,10MMETERS AND/53X,3HY =,E12.5,2X,6MMETERS/5X,
3          48HTHE TRAILING EDGE OF THE SLICK IS LOCATED AT X =,
4          E12.5,2X,10MMETERS AND 54X,3HY =,E12.5,2X,6MMETERS)
0145      500      CONTINUE
0146      799      RETURN
0147      END

```

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C
SUBROUTINE RUNKUT
```

[illegible]

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C      THIS SUBROUTINE IS A STANDARD RUNGE-KUTTA INTEGRATION ROUTINE
C      CALLED BY "INTE".  IT CALLS "UERTST" AND "UOETIO".
C      ** N = NO. OF SIMULTANEOUS FIRST-ORDER DIFFERENTIAL EQUATIONS
C      ** FCN = SUBROUTINE WHERE DIFFERENTIAL EQUATIONS ARE GIVEN
C      ** X = STARTING TIME
C      ** Y = MATRIX OF DIFFERENTIAL EQUATIONS
C      ** XEND = STARTING TIME + DELT
C      ** TOL, IND, C, NW, W, IER = NUMERICAL AND ERROR DATA FOR
C      ** CHECKING CONVERGENCE

```

```

0001      SUBROUTINE RUNKUT(N,FCN,X,Y,YEND,TOL,IND,C,NW,W,IER)
0002      INTEGER      N,IND,NW,IER
0003      INTEGER      K
0004      DIMENSION Y(N),C(24),W(NW,9),RK(39)
0005      DATA          ZERO/0.0/,ONE/1.0/,TWO/2.0/,THREE/3.0/,
0006      DATA          FOUR/4.0/,FIVE/5.0/,SEVEN/7.0/,
0007      DATA          TEN/10.0/,HALF/0.5/,P9/0.9/,
0008      DATA          C4D15/.2666667E0/,
0009      DATA          C2D3/.6666667E0/,
0010      DATA          C5D4/.8333333E0/,
0011      DATA          C1D6/.1666667E0/,
0012      DATA          C1D15/.6666667E-1/,
0013      DATA          C2D96/120.4273/,
0014      DATA          REP8/2.77556E-17/,
0015      DATA          RTOL/1.056791E-22/,
0016      DATA          RK( 1)/.1666667E+00/,
0017      DATA          RK( 2)/.5333333E-01/,
0018      DATA          RK( 3)/.2133333E+00/,
0019      DATA          RK( 4)/.8333333E+00/,
0020      DATA          RK( 5)/.2666667E+01/,
0021      DATA          RK( 6)/.2500000E+01/,
0022      DATA          RK( 7)/.2578123E+01/,
0023      DATA          RK( 8)/.9166667E+01/,
0024      DATA          RK( 9)/.6640625E+01/,
0025      DATA          RK(10)/.8854167E+00/,
0026      DATA          RK(11)/.2400000E+01/,
0027      DATA          RK(12)/.8000000E+01/,
0028      DATA          RK(13)/.6560458E+01/,
0029      DATA          RK(14)/.3055556E+00/,
0030      DATA          RK(15)/.3450980E+00/,
0031      DATA          RK(16)/.3508667E+00/,
0032      DATA          RK(17)/.1653333E+01/,
0033      DATA          RK(18)/.9435882E+00/,
0034      DATA          RK(19)/.3240000E+00/,
0035      DATA          RK(20)/.2337882E+00/,
0036      DATA          RK(21)/.2033465E+01/,
0037      DATA          RK(22)/.6976744E+01/,
0038      DATA          RK(23)/.3648180E+01/

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0039      DATA      RK(24)/. 1373816E+00/
0040      DATA      RK(25)/. 2863023E+00/
0041      DATA      RK(26)/. 1441786E+00/
0042      DATA      RK(27)/. 7500000E-01/
0043      DATA      RK(28)/. 3899287E+00/
0044      DATA      RK(29)/. 3194444E+00/
0045      DATA      RK(30)/. 1350384E+00/
0046      DATA      RK(31)/. 1078330E-01/
0047      DATA      RK(32)/. 6980519E-01/
0048      DATA      RK(33)/. 6250000E-02/
0049      DATA      RK(34)/. 6963012E-02/
0050      DATA      RK(35)/. 6944444E-02/
0051      DATA      RK(36)/. 6138107E-02/
0052      DATA      RK(37)/. 6818182E-01/
0053      DATA      RK(38)/. 1078330E-01/
0054      DATA      RK(39)/. 6980519E-01/
0055      IER = 0
0056      IF (IND.LT.1.OR.IND.GT.6) GO TO 290
0057      GO TO (5,5,40,145,265,265), IND
0058      5 IF (N.GT.NW.OR.TOL.LE.ZERO) GO TO 295
0059      IF (IND.EQ.2) GO TO 15
0060      DO 10 K=1,9
0061      C(K) = ZERO
0062      10 CONTINUE
0063      GO TO 30
0064      15 CONTINUE
0065      DO 20 K=1,9
0066      C(K) = ABS(C(K))
0067      20 CONTINUE
0068      IF (C(1).NE.FOUR.AND.C(1).NE.FIVE) GO TO 30
0069      DO 25 K=1,N
0070      C(K+30) = ABS(C(K+30))
0071      25 CONTINUE
0072      30 CONTINUE
0073      C(10) = REPS
0074      C(11) = RTOL
0075      C(20) = X
0076      DO 35 K=21,24
0077      C(K) = ZERO
0078      35 CONTINUE
0079      GO TO 45
0080      40 IF (C(21).NE.ZERO.AND.(X.NE.C(20).OR.XEND.EQ.C(20))) GO TO 285
0081      C(21) = ZERO
0082      45 CONTINUE
0083      50 CONTINUE
0084      IF (C(7).EQ.ZERO.OR.C(24).LT.C(7)) GO TO 55
0085      IND = -1
0086      GO TO 9005
0087      55 CONTINUE
0088      IF (IND.EQ.6) GO TO 60
0089      CALL FCN (N,X,Y,W(1,1))
0090      C(24) = C(24)+ONE
0091      60 CONTINUE
0092      C(13) = C(3)
0093      IF (C(3).NE.ZERO) GO TO 120

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0094      TEMP = ZERO
0095      IF (C(1).NE.ONE) GO TO 70
0096      DO 65 K=1,N
0097          TEMP = AMAX1(TEMP,ABS(Y(K)))
0098      65 CONTINUE
0099      C(12) = TEMP
0100      GO TO 115
0101      70 IF (C(1).NE.TWO) GO TO 75
0102      C(12) = ONE
0103      GO TO 115
0104      75 IF (C(1).NE.THREE) GO TO 85
0105      DO 80 K=1,N
0106          TEMP = AMAX1(TEMP,ABS(Y(K))/C(2))
0107      80 CONTINUE
0108      C(12) = AMIN1(TEMP,ONE)
0109      GO TO 115
0110      85 IF (C(1).NE.FOUR) GO TO 95
0111      DO 90 K=1,N
0112          TEMP = AMAX1(TEMP,ABS(Y(K))/C(K+30))
0113      90 CONTINUE
0114      C(12) = AMIN1(TEMP,ONE)
0115      GO TO 115
0116      95 IF (C(1).NE.FIVE) GO TO 105
0117      DO 100 K=1,N
0118          TEMP = AMAX1(TEMP,ABS(Y(K))/C(K+30))
0119      100 CONTINUE
0120      C(12) = TEMP
0121      GO TO 115
0122      105 CONTINUE
0123      DO 110 K=1,N
0124          TEMP = AMAX1(TEMP,ABS(Y(K)))
0125      110 CONTINUE
0126      C(12) = AMIN1(TEMP,ONE)
0127      115 CONTINUE
0128      C(13) = TEN*AMAX1(C(11),C(10)*AMAX1(C(12)/TOL,ABS(X)))
0129      120 CONTINUE
0130      C(15) = C(5)
0131      IF (C(5).EQ.ZERO) C(15) = ONE
0132      IF (C(6).NE.ZERO.AND.C(5).NE.ZERO) C(16) = AMIN1(C(6),TWO/C(5))
0133      IF (C(6).NE.ZERO.AND.C(5).EQ.ZERO) C(16) = C(6)
0134      IF (C(6).EQ.ZERO.AND.C(5).NE.ZERO) C(16) = TWO/C(5)
0135      IF (C(6).EQ.ZERO.AND.C(5).EQ.ZERO) C(16) = TWO
0136      IF (C(13).LE.C(16)) GO TO 125
0137      IND = -2
0138      GO TO 9005
0139      125 CONTINUE
0140      IF (IND.GT.2) GO TO 130
0141      C(14) = C(4)
0142      IF (C(4).EQ.ZERO) C(14) = C(16)*TOL**C1D6
0143      GO TO 140
0144      130 IF (C(23).GT.ONE) GO TO 135
0145      TEMP = TWO*C(14)
0146      IF (TOL.LT.C2D96*C(19)) TEMP = P9*(TOL/C(5))*C1D6*C(14)
0147      C(14) = AMAX1(TEMP,HALF*C(14))
0148      GO TO 140

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0149      135 CONTINUE
0150      C(14) = HALF*C(14)
0151      140 CONTINUE
0152      C(14) = AMIN1(C(14),C(16))
0153      C(14) = AMAX1(C(14),C(13))
0154      IF (C(8).EQ.ZERO) GO TO 145
0155      IND = 4
0156      GO TO 9005
0157      145 CONTINUE
0158      IF (C(14).GE.ABS(XEND-X)) GO TO 150
0159      C(14) = AMIN1(C(14),HALF*ABS(XEND-X))
0160      C(17) = X+SIGN(C(14),XEND-X)
0161      GO TO 155
0162      150 CONTINUE
0163      C(14) = ABS(XEND-X)
0164      C(17) = XEND
0165      155 CONTINUE
0166      C(18) = C(17)-X
0167      DO 160 K=1,N
0168          W(K,9) = Y(K)+C(18)*W(K,1)*RK(1)
0169      160 CONTINUE
0170      CALL FCN (N,X+C(18)*C1D6,W(1,9),W(1,2))
0171      DO 165 K=1,N
0172          W(K,9) = Y(K)+C(18)*(W(K,1)*RK(2)+W(K,2)*RK(3))
0173      165 CONTINUE
0174      CALL FCN (N,X+C(18)*C4D15,W(1,9),W(1,3))
0175      DO 170 K=1,N
0176          W(K,9) = Y(K)+C(18)*(W(K,1)*RK(4)-W(K,2)*RK(5)+W(K,3)*RK(6))
0177      170 CONTINUE
0178      CALL FCN (N,X+C(18)*C2D3,W(1,9),W(1,4))
0179      DO 175 K=1,N
0180          W(K,9) = Y(K)+C(18)*(-W(K,1)*RK(7)+W(K,2)*RK(8)-W(K,3)*RK(9)
1          +W(K,4)*RK(10))
0181      175 CONTINUE
0182      CALL FCN (N,X+C(18)*C5D6,W(1,9),W(1,5))
0183      DO 180 K=1,N
0184          W(K,9) = Y(K)+C(18)*(W(K,1)*RK(11)-W(K,2)*RK(12)+W(K,3)*RK(13)
1          -W(K,4)*RK(14)+W(K,5)*RK(15))
0185      180 CONTINUE
0186      CALL FCN (N,X+C(18),W(1,9),W(1,6))
0187      DO 185 K=1,N
0188          W(K,9) = Y(K)+C(18)*(-W(K,1)*RK(16)+W(K,2)*RK(17)-W(K,3)
1          *RK(18)-W(K,4)*RK(19)+W(K,5)*RK(20))
0189      185 CONTINUE
0190      CALL FCN (N,X+C(18)*C1D15,W(1,9),W(1,7))
0191      DO 190 K=1,N
0192          W(K,9) = Y(K)+C(18)*(W(K,1)*RK(21)-W(K,2)*RK(22)+W(K,3)*RK(23)
1          -W(K,4)*RK(24)+W(K,5)*RK(25)+W(K,7)*RK(26))
0193      190 CONTINUE
0194      CALL FCN (N,X+C(18),W(1,9),W(1,8))
0195      DO 195 K=1,N
0196          W(K,9) = Y(K)+C(18)*(W(K,1)*RK(27)+W(K,3)*RK(28)+W(K,4)*RK(29)
1          +W(K,5)*RK(30)+W(K,7)*RK(31)+W(K,8)*RK(32))
0197      195 CONTINUE
0198      C(24) = C(24)+SEVEN

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0199      DO 200 K=1,N
0200      W(K,2) = W(K,1)*RK(33)+W(K,3)*RK(34)-W(K,4)*RK(35)+W(K,5)
1      *RK(36)+W(K,6)*RK(37)-W(K,7)*RK(38)-W(K,8)*RK(39)
0201 200 CONTINUE
0202      TEMP = ZERO
0203      IF (C(1).NE.ONE) GO TO 210
0204      DO 205 K=1,N
0205      TEMP = AMAX1(TEMP,ABS(W(K,2)))
0206 205 CONTINUE
0207      GO TO 260
0208 210 IF (C(1).NE.TWO) GO TO 220
0209      DO 215 K=1,N
0210      IF (Y(K).EQ.ZERO) GO TO 280
0211      TEMP = AMAX1(TEMP,ABS(W(K,2)/Y(K)))
0212 215 CONTINUE
0213      GO TO 260
0214 220 IF (C(1).NE.THREE) GO TO 230
0215      DO 225 K=1,N
0216      TEMP = AMAX1(TEMP,ABS(W(K,2))/AMAX1(C(2),ABS(Y(K))))
0217 225 CONTINUE
0218      GO TO 260
0219 230 IF (C(1).NE.FOUR) GO TO 240
0220      DO 235 K=1,N
0221      TEMP = AMAX1(TEMP,ABS(W(K,2))/AMAX1(C(K+30),ABS(Y(K))))
0222 235 CONTINUE
0223      GO TO 260
0224 240 IF (C(1).NE.FIVE) GO TO 250
0225      DO 245 K=1,N
0226      TEMP = AMAX1(TEMP,ABS(W(K,2)/C(K+30)))
0227 245 CONTINUE
0228      GO TO 260
0229 250 CONTINUE
0230      DO 255 K=1,N
0231      TEMP = AMAX1(TEMP,ABS(W(K,2))/AMAX1(ONE,ABS(Y(K))))
0232 255 CONTINUE
0233 260 CONTINUE
0234      C(19) = TEMP*C(14)+C(15)
0235      IND = 5
0236      IF (C(19).GT.TOL) IND = 6
0237      IF (C(9).NE.ZERO) GO TO 9005
0238 265 CONTINUE
0239      IF (IND.EQ.6) GO TO 275
0240      X = C(17)
0241      DO 270 K=1,N
0242      Y(K) = W(K,9)
0243 270 CONTINUE
0244      C(22) = C(22)+ONE
0245      C(23) = ZERO
0246      IF (X.NE.XEND) GO TO 50
0247      IND = 3
0248      C(20) = XEND
0249      C(21) = ONE
0250      GO TO 9005
0251 275 CONTINUE
0252      C(23) = C(23)+ONE

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```
0253      IF (C(14).GT.C(13)) GO TO 50
0254      IND = -3
0255      GO TO 9005
0256      280 CONTINUE
0257      IER = 132
0258      GO TO 9000
0259      285 CONTINUE
0260      IER = 131
0261      GO TO 9000
0262      290 CONTINUE
0263      IER = 130
0264      GO TO 9000
0265      295 CONTINUE
0266      IER = 129
0267      9000 CONTINUE
0268      9005 CONTINUE
0269      RETURN
0270      END
```



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CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C      SUBROUTINE SPLOC
C      SPILL LOCATION DEFINITION
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      THIS SUBROUTINE IS CALLED BY "DMODEL". IT INPUTS THE SPILL
C      SOURCE LOCATION. IF THE SPILL IS IN A RIVER (SHAPE < 2), THE
C      SPILL OCCURS AT X = 0, Y=0 AND X > 0 IS DOWNSTREAM. IF THE SPI
C      IS IN A LAKE OR COAST, THE X,Y LOCATION OF SOURCE IS INPUT.
C      IF THE CURRENT = F(SPACE), THE BOX OR SLICE IN WHICH THE SOURC
C      LIES IS ALSO REQUESTED.
C      ** XO,YO = INITIAL SPILL LOCATION. M
C      ** ISP = BOX OR SLICE NO. WHEN CURRENT = F(SPACE) IN OPEN WA
C
0001      SUBROUTINE SPLOC
0002      COMMON/CONTOUR/SHAPE,X(10),Y(10),XC,YC,IC,IW,ISP,XO,YO
0003      COMMON/TRANSIT/UX(10,10),UY(10,10),VMX(10),
1          VWY(10),THETA(10),TI(10),ID,IT,IV,
2          XU(10),YU(10),TT(10)
0004      I = SHAPE
0005      IF (I.EQ.1) GO TO 99
0006      7      WRITE (6,10)
0007      10     FORMAT (1X,41H GIVE SPILL COORDINATES X AND Y, IN METERS)
0008      READ (5,*,ERR=7) XC,YC
0009      WRITE (1,12) XC,YC
0010      XO = XC
0011      YO = YC
0012      12     FORMAT (//5X,30H5. THE SPILL ORIGIN IS AT X = ,E12.5,
1          1X,10HMETERS AND, /31X,4HY = ,E12.5,1X,7HMETERS. )
0013      IF (IC.EQ.2.OR.IC.EQ.4) GO TO 27
0014      ISP = 1
0015      GO TO 99
0016      27     WRITE (6,30)
0017      30     FORMAT(1X,62HWHAT BOX (LAKE) OR SLICE (COAST) DOES THE SPILL C
          *QIN LIE IN?)
0018      READ (5,*,ERR=27) ISP
0019      99     RETURN
0020      END

```



```

C      NEXT 11 STATEMENTS CALCULATE DUMMY VARIABLES NEEDED TO
C      CALCULATE THE VELOCITY USED IN THE SPREADING MODELS --
C      UBAR, AT STATEMENT 100 -- WHEN NEITHER THE CURRENT NOR
C      THE WIND DEPEND ON TIME.
C      *****
0031      IF(J.GE.2) M=ISP
C
C      *****
C      ISP = BOX OR SLICE OF SPILL LOCATION WHEN CURRENT = F(SPACE)
C      *****
0032      IF(J.EQ.1) M=1
0033      UCX1=UX(M,1)
0034      UCY1=UY(M,1)
0035      VWX1 = VWX(1)
0036      VWY1 = VWY(1)
0037      IF(J.EQ.1) THEN
0038          VWX1=VW * COS(THETA1)
0039          UCX1=UC
0040      ELSE
0041      ENDIF
0042      IF (I .EQ. 4) GO TO 103
0043      GO TO 200
0044      103      IF (J.NE.1) GO TO 2
0045              IF(IC.GT.1.OR.IW.GT.1) GO TO 3
0046              GO TO 100
0047      2        IF(IC.GT.2.OR.IW.GT.1) GO TO 3
0048              GO TO 100
0049              CONTINUE
C
C      *****
C      NEXT 7 STATEMENTS CALCULATE THE VELOCITY USED IN THE SPREADING
C      MODELS -- UBAR -- WHEN THE CURRENT OR WIND IS A FUNCTION OF TII
C      *****
C
C      CALL SUBROUTINE UTPEAK TO COMPUTE MAXIMUM
C      TRANSPORT VELOCITY WHEN THE CURRENT OR
C      WIND IS A FUNCTION OF TIME
0050      CALL UTPEAK
C
C      CALL SUBROUTINE CURRENT TO CALCULATE
C      AVERAGE TRANSPORT VELOCITY OVER ENTIRE
C      SPILL DURATION
0051      CALL CURRT
0052      4        CONTINUE
C
0053      IF(J.GE.2) M=ISP
0054      IF(J.EQ.1) M=1
0055      IF(UBAR(M).LT.(0.3*UPEAK(M))) GO TO 50
0056      UBAR = UBAR(M)
0057      GO TO 200
C
C      -----
C      UBAR .LT. (0.3*UPEAK)
C      SET UT = 0 AND CHANGE SPREAD MODEL TO MODEL

```

```

C      WITHOUT CURRENT.....
C      -----
0058 50 DO 55 KK=1, ID
0059      UBAR(KK) = 0.0
0060 55 CONTINUE
0061      UTPAR = 0.0
0062      IF( STP.EQ.4.1 ) STP=2.1
0063      IF( STP.EQ.4.2 ) STP=2.2
0064      PRINT *, 'CHANGE TO MODEL ', STP
0065      GO TO 200
0066 100 UTPAR = SGRT((UCX1+0.035*VWX1)**2+
1          (UCY1+0.035*VWY1)**2)
0067 200 CONTINUE
C
C
C      ---- CALL SUBROUTINE INIT TO CALCULATE
C      INITIAL CONDITIONS ----
C
0068      WRITE (1,299)
0069 299 FORMAT(1H1/10X,
1 60H*****
2 /10X, 1H*, 16X, 22HSPREADING MODEL OUTPUT, 16X, 1H*/10X,
3 60H*****
0070 CALL INIT
0071 IF(KKK.EQ.3) GOTO 351
C
C *****
C 'KKK' IS A CODE THAT DETERMINES IF AN INSTANTANEOUS SPILL HAS
C EVAPORATED OR, FOR A CONTINUOUS SPILL, IF THE EVAPORATION RATE
C DISCHARGE RATE, DURING THE INITIAL CONDITION TIME PERIOD. IT
C IS COMPUTED IN "INT12A" AND "INIT4A".
C *****
C
0072 TIME=TII
0073 YY(1)=ATK
0074 YY(2)=ATN
0075 YY(3)=HTK
0076 YY(4) = 0.0
0077 YY(5) = 0.0
C
0078 300 ISTEP=STP
0079 IF(ISTP.EQ.1) GO TO 350
C      ---- WHEN ISTEP=1 SPILL IS INSTANTANEOUS ----
0080 SPM = SPILMR
0081 310 IF (TIME.LT.TSPILL) GO TO 350
C
C *****
C FROM HERE TO 350 IS EXECUTED ONLY IF SPILL IS CONTINUOUS
C AND DISCHARGE HAS JUST STOPPED.
C *****
C
C      ---- SPILL WAS CONTINUOUS. HOWEVER IT HAS STOPPED. ----
C      ---- CALL 'SWITCH' AND CHANGE TO APPROPRIATE
C      INSTANTANEOUS SPILL MODEL ----
C

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0082      CALL SWITCH
0083      350      CONTINUE
           C
           C
0084      CALL SUBROUTINE TRANSP TO CALCULATE SURFACE TRANSPORT VELOC.
           C
           C      CALL TRANSP
           C
           C      ---- CALL 'INTE' TO SOLVE SIMULTANEOUS
           C      DIFFERENTIAL EQUATIONS ----
0085      CALL INTE(XEND)
0086      IF (TIME.GE.TSTOP) GO TO 353
0087      IF (SHAPE.LT.1.9) GO TO 351
           C
           C      *****
           C      SKIP THE SLICK HITTING THE COAST LINE ROUTINE "GROUND"
           C      WHEN SPILL IS IN RIVER.
           C      *****
0088      CALL GROUND(IH)
           C
           C      *****
           C      IF IH > 0. THE SLICK HAS HIT THE COAST LINE.
           C      *****
0089      IF (IH.GT.0) GO TO 998
           C
           C      *****
           C      FROM HERE TO 353 IS A ROUTINE THAT PRINTS OUT THAT AN
           C      INSTANTANEOUS SLICK HAS EVAPORATED (355) OR THE EVAPORATION
           C      RATE HAS INCREASED TO EQUAL THE DISCHARGE RATE FOR A CONTINUOUS
           C      SPILL. THE CRITERION IS
           C      TCHECK > TIME
           C      AND IS DETERMINED IN SUBROUTINE "CHEKMS".
           C      *****
0090      351      IF (TCHECK.GT.TIME) GO TO 353
0091      TEMP = T.ME/60.
0092      IF (ISTP.EQ.1) GO TO 352
0093      TMPT=TSPILL/60.
0094      WRITE (1,354) TEMP, TMPT
0095      WRITE (6,354) TEMP, TMPT
0096      SPILLM = SPILMR * TIME
0097      TIME = TSPILL
0098      TCHECK = TSTOP
0099      GO TO 310
0100      352      CONTINUE
0101      DELTIM = (SPILLM - TOTALE - TOTALD) / (EVAPM*YY(1)
1          + DISSOM * YY(1))
0102      TOTALE=TOTALE + DELTIM * EVAPM * YY(1)
0103      TOTALD=TOTALD + DELTIM * DISSOM * YY(1)
0104      TMASS = 0.
0105      TOTALM = 0.
0106      YY(1) = 0.
0107      YY(2) = 0.
0108      YY(3) = 0.
0109      RAD1 = 0.

```

```

0110      RAD2 = 0.
0111      TIME= TIME + DELTIM
0112      TEMP = TIME / 60.
0113      WRITE (1,355) TEMP
0114      WRITE (6,355) TEMP
0115      GO TO 999
0116      353  CONTINUE
          C
          C
          C *****
          C BACK IN MAIN LOOP NOW -- EXCEPT FOR FORMATS 354 AND 355
          C *****
          C
          C ---- CALL 'MOVE' TO TRACK SPREADING ----
          C
0117      CALL MOVE
0118      354  FORMAT (////1X,
1  60H*****
2  /1X, 1H*, 2X,
3  48HTHE RATE OF MASS LOSS HAS INCREASED UNTIL IT IS , 8X, 1H*/1X,
4  1H*, 2X, 34HAPPROXIMATELY EQUAL TO THE RATE OF, 22X, 1H*, /1X, 1H*, 2)
5  25HSPILLING AT TIME EQUAL TO, E12. 5, 2X, 7HMINUTES, 10X, 1H*/1X, 1H*,
6  2X, 53HTHE SLICK SIZE REMAINS CONSTANT FROM NOW UNTIL SPILLING,
7  1X, 1H*/1X, 1H*, 2X, 14HSTOPS AT TIME=, E12. 5,
8  25H MINUTES AND THE PRINTOUT, 5X, 1H*/1X, 1H*, 2X,
9  49HRESUMES WHEN THE SLICK SIZE BEGINS TO VARY AGAIN, , 7X, 1H*/1X,
1  60H*****
0119      355  FORMAT(////1X,
1  60H*****
2  /1X, 1H*,
3  58HALL THE SPILLED MASS HAS BEEN EVAPORATED AND(OR) DISSOLVED,
4  1H*/1X, 1H*,
5  30HAT TIME APPROXIMATELY EQUAL TO, E12. 5, 2X, 7HMINUTES,
6  7X, 1H*/1X,
7  60H*****
0120      IF (TIME.LT.TPT) GO TO 400
          C
          C *****
          C NEXT 6 STATEMENTS DETERMINE IF PRINTOUT IS REQUIRED AND BREAK
          C TIME INTO MINUTES AND SECONDS FOR PRINTOUT
          C *****
          C
0121      IJ = TIME
0122      IK = TPT
0123      DIC = ABS(TIME - FLOAT(IJ))
0124      IF (DIC .GT. DELT) GO TO 400
0125      MD =MOD(IJ, IK)
0126      IF (MD .NE. 0) GO TO 400
          C      ---- TIME TO PRINT OUT SOME RESULTS ----
0127      CALL PRINTO
          C
          C *****
          C DETERMINE IF THICKNESS OF THICK SLICK IS LESS THAN HMIN.
          C IF SO, STOP.
          C *****
          C

```

```

0128      400      IF (ISTP.EG. 4. AND. TIME.LT. TSPILL) GOTO 510
0129      IF (YY(3).LT. HMIN) THEN
0130          WRITE(1,500)HMIN, TIME
0131          WRITE(6,500)HMIN, TIME
0132      500      FORMAT(///5X,
1          29HTHE THICK SLICK IS LESS THAN ,E12. 5, 11H M AT TIME=,E13. 6,
2          8H SECONDS)
0133          GO TO 999
0134      ELSE
0135      ENDIF

C
C
C      *****
C      STOP IF TIME >= RUN TIME
C      *****
C
0136      510      IF (TIME.GT. TSTOP) GO TO 999
0137      GO TO 300
0138      998      CONTINUE

C
C      *****
C      STOP IF SLICK HITS COASTLINE
C      *****
C
0139      TEMP = TIME/60.0
0140      WRITE (1,997) TEMP
0141      WRITE (6,997) TEMP
0142      997      FORMAT(///1X,
1          60H*****
2          /1X, 1H*, 2X,
3          52HTHE SLICK HAS HIT THE BOUNDARY AT TIME APPROXIMATELY,
4          4X, 1H*/1X, 1H*. 2X, 8HEQUAL TO, 2X, E12. 5, 7HMINUTES, 27X, 1H*/1X,
5          60H*****
0143      999      CONTINUE
0144      RETURN
0145      END

```



```

C      SIGOW = CHEMICAL-WATER INTERFACIAL TENSION, N/M
C
C      CALCULATED CHEMICAL PARAMETERS ARE:
C
C      SIG = SPREADING COEFFICIENT
C            = SIGWA - SIGOA - SIGOW, N/M
C      COEF = 1 - DENO/DENW
C      NOTE : COEF IS CALLED DELTA IN THE REPORT.
C      *****
0018      WRITE (1,15)
0019      15      FORMAT (/5X,12HPROPERTIES :)
0020      1109    WRITE(6,1110) (J, NC(1,J), NC(2,J), J+1, NC(1,J+1), NC(2,J+1)
1              J=1,20,2)
0021      1110    FORMAT(1X,50HWE HAVE STANDARD PROPERTIES FOR THE FOLLOWING CH
1              SHICALS,/,10(1X,12,2H, ,2A10,2X,12,2H, ,2A10,/)
0022      WRITE(6,8)
0023      8      FORMAT(5X,25HENTER THE NO. YOU WANT OR,/,5X,14HNEGATIVE VALUE
1              38H - IF YOU WANT TO INPUT THE PROPERTIES,/,5X,
2              14H      99      ,25H - IF THE CHEMICAL IS NOT,
3              12H ON THE LIST)
0024      READ (5,*,ERR=1109) ICS
0025      IF (ICS .LT. 0) GO TO 17
0026      IF (ICS .GT. 90) GO TO 12
0027      CALL CHEMCL(ICS, NAME, PB, PHI, DENO, CS, CMW, DCA,
1              DCW, SIGOA, SIGOW)
0028      GO TO 1036
0029      12      WRITE (6,13)
0030      13      FORMAT(/1X,33HWHAT IS THE NAME OF THE CHEMICAL?)
0031      READ (5,14,ERR=12) NAME
0032      14      FORMAT (2A10)
0033      17      WRITE (6,18)
0034      18      FORMAT (1X,29HENTER ITS DENSITY IN KG/CU M.)
0035      READ (5,*,ERR=17) DENO
0036      700     WRITE (6,701)
0037      701     FORMAT (1X,41HINPUT ITS MOLECULAR WEIGHT IN KG/KG-MOLE.)
0038      READ (5,*,ERR=700) CMW
0039      22      WRITE (6,23)
0040      23      FORMAT(/1X,56HENTER DIFFUSION COEFFICIENT OF VAPOR IN AIR IN
1              CM/SEC.)
0041      READ (5,*,ERR=22) DCA
C
0042      30      WRITE (6,31)
0043      31      FORMAT(/1X,
1              59HENTER DIFFUSION COEFFICIENT OF LIQUID IN WATER IN SG M/SEC.)
0044      READ (5,*,ERR=30) DCW
C
0045      34      WRITE (6,35)
0046      35      FORMAT(/1X,45HIS PV (VAPOR) 1. A NUMBER OR 2. A FORMULA?)
0047      READ (5,*,ERR=34) I
0048      GO TO (36,38) I
0049      36      WRITE (6,37)
0050      37      FORMAT(/1X,17HENTER CONSTANT PV)
0051      READ (5,*,ERR=36) PV
0052      GO TO 39
0053      38      WRITE(6,138)

```

```

0054      138      FORMAT(/1X,31HPV IS A FUNCTION OF TEMPERATURE/
1              5X,25HPV=10.0**((A1-B1/(C1+TDC)))/
2              6X,32HENTER COEFFICIENTS A1, B1 AND C1)
0055      READ (5,*,ERR=38) A1,B1,C1
0056      PV = 10.0**((A1-B1/(C1+TDC))
0057      39      CONTINUE
0058      WRITE (6,40)
0059      40      FORMAT(/1X,47HINPUT THE SOLUBILITY LIMIT OF CHEMICAL IN WATER
1              11H (KG/CU.M.))
0060      READ (5,*,ERR=39) CS
0061      C.
0061      60      WRITE (6,61)
0062      61      FORMAT(/1X,44HINPUT (1) CHEMICAL/AIR INTERFACE TENSION AND,
1              /6X,36H(2) WATER/CHEMICAL INTERFACE TENSION,
2              /1X,16HUNIT : NEWTON/M )
0063      READ (5,*,ERR=60) SIGOA,SIGOW
0064      1036      CONTINUE
0065      WRITE (1,9) PB
0066      WRITE (6,9) PB
0067      9      FORMAT(/5X,23HBAROMETRIC PRESSURE : ,F12.3,2X,8HMILLIBAR,/)
0068      WRITE (1,11) TDC
0069      WRITE (6,11) TDC
0070      11      FORMAT(/5X,14HTEMPERATURE : ,F12.3,2X,9HDEGREES C,/)
0071      WRITE (1,16) NAME
0072      WRITE (6,16) NAME
0073      16      FORMAT (/5X,18HCHEMICAL NAME IS: ,2A10)
0074      WRITE (1,41) DENO
0075      WRITE (6,41) DENO
0076      WRITE (1,1013) CMW
0077      WRITE (6,1013) CMW
0078      1013      FORMAT (/5X,18HMOLECULAR WEIGHT =,F10.3,2X,10HKG/KG-MOLE)
0079      WRITE (1,42) DCA
0080      WRITE (6,42) DCA
0081      WRITE (1,44) DCW
0082      WRITE (6,44) DCW
0083      WRITE (1,46) PV
0084      WRITE (6,46) PV
0085      WRITE (1,48) CS
0086      WRITE (6,48) CS
0087      41      FORMAT (/5X,25HCHEMICAL DENSITY : ,F12.2,2X,8HKG/CU.M.
0088      42      FORMAT (/5X,25HDIFFUSION COEFF (AIR) : ,E12.5,2X,9HSG M./SEC
0089      44      FORMAT (/5X,25HDIFFUSION COEFF (WATER) : ,E12.5,2X,9HSG M./SEC
0090      46      FORMAT (/5X,25HCHEMICAL VAPOR PRESSURE =,F12.2,2X,
1              12HNEWTON/SG M )
0091      48      FORMAT (/5X,25HSOLUBILITY IN WATER : ,F12.2,2X,8HKG/CU.M.)
0092      WRITE (1,1035) SIGOA,SIGOW
0093      WRITE (6,1035) SIGOA,SIGOW
0094      1035      FORMAT (/5X,33HTHE INTERFACE TENSION WRT AIR IS ,E10.5,
1              2X,9HNEWTON/M.,/5X,
2              33HTHE INTERFACE TENSION WRT WATER IS ,E10.5,2X,
3              9HNEWTON/M )
0095      SIG = SIGWA-SIGOW-SIGOA
0096      WRITE (1,49) SIG
0097      WRITE (6,49) SIG
0098      49      FORMAT(/5X,29HTHE SPREADING COEFFICIENT IS ,E10.5,2X,9HNEWTON

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```

0099      1      )      COEF=1. 0-DENO/DENW
C
C
C      *****
C      THE SPILL PARAMETERS ARE:
C      *****
C
C      SPILLM = TOTAL MASS OF INSTANTANEOUS SPILL, KG
C      SPILLMR = DISCHARGE RATE OF CONTINUOUS SPILL, KG/SEC
C      TSPILL = TOTAL DISCHARGE TIME, SEC
C      *****
0100      50      WRITE (6,51)
0101      51      FORMAT(/1X,47HIS SPILL 1. INSTANTANEOUS OR 2. CONTINUOUS
0102      READ (5,*,ERR=50) ITYPE
0103      GO TO (100,200) ITYPE
C
C      -----
C      INSTANTANEOUS SPILL
C      -----
0104      100     CONTINUE
0105      WRITE (1,101)
0106      101     FORMAT (/5X,30H1. THE SPILL IS INSTANTANEOUS. )
0107      102     WRITE (6,103)
0108      103     FORMAT(/1X,44HINPUT THE TOTAL SPILLED VOLUME (CUBIC METER))
0109      READ (5,*,ERR=102) TEM
0110      SPILLM = DENO * TEM
0111      WRITE (1,104) SPILLM
0112      104     FORMAT (/5X,24H2. TOTAL MASS OF SPILL =,E12.5,2X,3HK0. )
C
0113      105     CONTINUE
0114      I = SHAPE
0115      IF (I.EQ.1) GO TO 120
C      ----- SPILL IS IN OPEN WATER -----
0116      STP = 1.2
0117      GO TO 299
0118      120     CONTINUE
C      ----- SPILL IS IN RIVER OR CHANNEL -----
0119      STP = 1.1
0120      GO TO 299
C
0121      200     CONTINUE
C
C      -----
C      CONTINUOUS SPILL
C      -----
0122      WRITE (1,201)
0123      201     FORMAT (/5X,27H1. THE SPILL IS CONTINUOUS. )
0124      204     WRITE (6,205)
0125      205     FORMAT(/1X,39HINPUT THE RATE OF DISCHARGE (CU. M. /SEC))
0126      READ (5,*,ERR=204) TEM
0127      SPILMR = DENO * TEM
0128      WRITE (1,206) SPILMR
0129      206     FORMAT (/5X,29H2. THE MASS DISCHARGE RATE =,F8.3,2X,
1      7HK0/SEC. )

```

0130	207	WRITE (6,208)
0131	208	FORMAT(/1X,44HINPUT THE TOTAL DURATION OF SPILL IN MINUTES)
0132		READ (5,*,ERR=207) TSPILL
0133		WRITE (1,210) TSPILL
0134	210	FORMAT (/5X,29H3. TOTAL DURATION OF SPILL = ,E12.5,4HMIN.)
0135		TSPILL=TSPILL*60.
	C	
0136	220	CONTINUE
0137		I=SHAPE
0138	222	IF (I.EQ.1) GO TO 250
	C	---- SPILL MUST BE IN OPEN WATER ----
0139	224	IF (IC.NE.0 OR IW.NE.0) GO TO 240
	C	---- NO CURRENT ----
0140		STP = 2.2
0141		GO TO 299
0142	240	CONTINUE
	C	---- THERE IS CURRENT ----
0143		STP = 4.2
0144		GO TO 299
	C	
0145	250	CONTINUE
	C	---- SPILL IS IN RIVER OR CHANNEL ----
0146	252	IF (IC.NE.0 OR IW.NE.0) GO TO 260
	C	---- NO CURRENT ----
0147		STP = 2.1
0148		GO TO 299
0149	260	CONTINUE
	C	---- THERE IS CURRENT ----
0150		STP = 4.1
	C	
0151	299	RETURN
0152		END

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          SUBROUTINE SWITCH                                C
C          THIS SUBROUTINE IS USED TO SWITCH THE CONTINUOUS  C
C          MODEL TO THE PROPER INSTANTANEOUS MODEL AFTER     C
C          THE SPILL STOPS. ....                             C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          THIS SUBROUTINE IS CALLED BY "SPREAD". IT CHANGES A CONTINUOUS
C          SPILL TO AN INSTANTANEOUS SPILL AFTER THE DISCHARGE STOPS, AND
C          COMPUTES THE CENTER OF THE NEW INSTANTANEOUS SPILL SLICK.
C
0001          SUBROUTINE SWITCH
0002          COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0003          COMMON/SIZE/R, D, WW, L1, L2, H, RO
0004          COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0005          COMMON/RANGE/YY(5), C(24), W(5, 30)
0006          COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0007          COMMON/CURRENT/UBAR(10), DMOVE, UTOT, UTX, UTY, UREL
0008          COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0009          COMMON/MLOSS/EVAPH, DISSOM
0010          COMMON/SENSE/EVA(40, 10), DIS(40, 10), THK(40, 10), TIN(40, 10),
1          PIP(40), TPT
0011          COMMON/SPREAD/TII, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0012          COMMON/CK/C10, C20, C11, C21, C12, C22, K10, K20, K11, K21,
1          K12, K22
0013          REAL K10, K20, K11, K21, K12, K22
C
0014          ISTOP = STP
C
C          *****
C          ISTOP = 2: CONTINUOUS SPILL WITH NO CURRENT;
C          ISTOP = 4: CONTINUOUS SPILL WITH CURRENT
C          *****
C
0015          IF (ISTOP.EQ.4) GO TO 100
0016          SPILLM = SPILMR * TSPILL
0017          IF (STP.EQ.2.1) STP=1.1
0018          IF (STP.EQ.2.2) STP=1.2
0019          GO TO 999
C
0020          100 CONTINUE
0021          IF (STP.EQ.4.2) GO TO 150
0022          SPILLM = SPILMR * TSPILL
0023          XC=YY(1)/(2.*WW)
C
C          *****
C          CENTER OF INSTANTANEOUS SLICK = CENTER OF CONTINUOUS SPILL
C          SLICK IF SLICK IS IN RIVER.
C          *****
C
0024          STP = 1.1
0025          GO TO 999
0026          150 CONTINUE
0027          IF (SPM.GT.0.0) GO TO 200
0028          STP = 1.2

```

```

0029          GO TO 999
          C
0030      200  CONTINUE
0031          TEMP1 = UTBAR * TSPILL
0032          TEMP2 = 3.0 * SQRT(YY(1))
0033          XC=(2./3.)*(XLE-X0)
0034          YC=(2./3.)*(YLE-Y0)
          C
          C *****
          C CENTER OF INSTANTANEOUS SLICK = CENTROID OF TRIANGULAR
          C CONTINUOUS SPILL SLICK IN OPEN WATER.
          C *****
0035          IF (TEMP1.LE.TEMP2) GO TO 250
0036          SPILLM = SPILMR * TSPILL
0037          STP = 1.2
0038          GO TO 999
          C
0039      250  CONTINUE
          C
          C *****
          C NEED TO LET SPILL SPREAD LIKE AN INSTANTANEOUS SPILL IN A
          C RIVER UNTIL IT SPREADS ENOUGH SO THAT 3*SQRT(THICK SLICK AREA)
          C IS GREATER THAN LENGTH OF SLICK.
          C *****
          C
0040          SPILLM = SPILMR * TSPILL
0041          STP = 1.1
0042      275  CALL TRANSP
0043          CALL INTE(XEND)
0044          CALL MOVE
0045          IJ = TIME
0046          IK = TPT
0047          MD=MOD(IJ, IK)
0048          DIC=ABS(TIME-FLOAT(IJ))
0049          IF(DIC.GT.DELT) GOTO 300
0050          IF (MD.NE.0) GO TO 300
0051          CALL PRINTO
0052      300  TEMP1 = UTBAR * TSPILL
0053          TEMP2 = 3.0 * SQRT(YY(1))
0054          IF(TIME.GT.TSTOP) GOTO 999
0055          IF (TEMP1.LE.TEMP2) GO TO 275
0056          STP = 1.2
0057          IF (TIME.GT.TSTOP) GO TO 999
0058          IF (YY(3).LT.HMIN) GO TO 999
          C
0059      999  CONTINUE
0060          RETURN
0061          END

```



```

0023      ID=3
0024      IF(J.GE.3) ID=9
0025      DO 35 LL=1, ID
0026      IF(ISTP.EQ.2.OR.ISTP.EQ.4) THEN
0027          XL = XLE
0028          YL = YLE
0029      ELSE
0030          XL = XC
0031          YL = YC
0032      ENDIF
0033      IF(XL.GE.XU(LL).AND.XL.LE.XU(LL+1)) LL1=LL
0034      IF(J.GE.3) GOTO 35
0035      IF(YL.GE.YU(LL).AND.YL.LE.YU(LL+1)) LL2=LL
0036      35      CONTINUE
0037      IF(J.GE.3) LL=LL1
0038      IF(J.GE.3) GOTO 38
0039      IF(LL2.EQ.1) LL=LL1
0040      IF(LL2.EQ.2) LL=LL1+3
0041      IF(LL2.EQ.3) LL=LL1+6
0042      38      CONTINUE
0043      39      IF (LT.EQ.1) GO TO 50
0044      40      DO 45 LT=1,10
0045          IF (TIME.GT.TI(LT)) GO TO 45
0046          GO TO 49
0047      45      CONTINUE
0048      49      CONTINUE
0049      C
0050      C      *****
0051      C      IF CURRENT IS ALSO A FUNCTION OF TIME, INTERPOLATE IN THE BOX
0052      C      OR SLICE TO FIND VALUE AT DESIRED TIME.
0053      C      *****
0054      C
0055      1      UU1 = UX(LL,LT-1)+(UX(LL,LT)-UX(LL,LT-1))*
0056      1      (TIME-TI(LT-1))/(TI(LT)-TI(LT-1))
0057      1      UU2 = UY(LL,LT-1)+(UY(LL,LT)-UY(LL,LT-1))*
0058      1      (TIME-TI(LT-1))/(TI(LT)-TI(LT-1))
0059      GO TO 55
0060      50      CONTINUE
0061      C
0062      C      ** UU1,UU2 = CURRENTS IN BOX OR SLICE AT DESIRED TIME **
0063      C
0064      55      UU1 = UX(LL,LT)
0065      56      UU2 = UY(LL,LT)
0066      60      IF (IW.GT.1) GO TO 70
0067      60      W1 = VWX(1)
0068      60      W2 = VWY(1)
0069      60      GO TO 90
0070      70      DO 75 I=1,10
0071      70      IF (TIME.GT.TT(I)) GO TO 75
0072      70      GO TO 79
0073      75      CONTINUE
0074      C
0075      C      ** IF WIND = F(TIME), INTERPOLATE TO FIND WIND AT DESIRED TIME
0076      C
0077      79      W1 = VWX(I-1)+(VWX(I)-VWX(I-1))*(TIME-TT(I-1))/

```



```

0064      1 (TT(I)-TT(I-1))
      W2 = VWY(I-1)+(VWY(I)-VWY(I-1))*(TIME-TT(I-1))/
0065      1 (TT(I)-TT(I-1))
      CONTINUE
      C
      C
0066      UTX = UU1 + 0.035*W1
0067      UTY = UU2 + 0.035*W2
0068      UREL = SQRT((UTX-W1)**2. + (UTY-W2)**2.)
0069      UTOT = SQRT (UTX**2+UTY**2)
      C
0070      GO TO 999
      C
      C
      C
0071      100
0072      CONTINUE
0073      IF (IC.LE.1) GO TO 120
0074      UC = UO + U1*SIN(6.28318/WT*(TIME+ALPH))
0075      120
0076      IF (IW.LE.1) THEN
0077          VWXX=VW*COS(THETA1)
0078          GOTO 140
0079      ELSE
0080      ENDIF
0081      DO 130 I=1,10
0082      IF (TIME.LT.TT(I)) GO TO 135
0083      CONTINUE
0084      130
0085      C
0086      C
0087      C
0088      C
0089      ** IF WIND = F(TIME), INTERPOLATE TO FIND WIND AT DESIRED TIP
0090      C
0091      C
0092      135
0093      VWXX = VWX(I-1)+(VWX(I)-VWX(I-1))*(TIME-TT(I-1))/
0094      1 (TT(I)-TT(I-1))
0095      VWYY = VWY(I-1)+(VWY(I)-VWY(I-1))*(TIME-TT(I-1))/
0096      1 (TT(I)-TT(I-1))
      C
      C
0097      140
0098      UTX = UC + 0.035*VWXX
0099      UREL = SQRT((UTX-VWXX)**2. +(VWYY)**2.)
0100      UTOT = UTX
      C
0101      999
0102      RETURN
0103      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          SUBROUTINE UERTST
C          PRINTS A MESSAGE TO INDICATE AN ERROR CONDITION IN
C          THE RUNGE-KUTTA ROUTINE "RUNKUT".
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          THIS SUBROUTINE IS PART OF THE RUNGE-KUTTA INTEGRATION
C          ROUTINE "RUNKUT".
C
0001      SUBROUTINE UERTST(IER,NAME)
C
C          SPECIFICATIONS FOR ARGUMENTS
C
0002      INTEGER IER
0003      DOUBLE PRECISION NAME
0004      DOUBLE PRECISION NAMSET,NAMEQ
0005      DATA NAMSET/6HUSERSET/
0006      DATA NAMEQ/6H      /
0007      DATA LEVEL/4/,IEGDF/0/,IEG/1H=/
0008      IF(IER.GT.999) GOTO 25
0009      IF(IER.LT.-32) GOTO 55
0010      IF(IER.LE.128) GOTO 5
0011      IF(LEVEL.LT.1) GOTO 30
0012      CALL UGETIO(1,NIN,IOUNIT)
0013      IF(IEGDF.EQ.1) WRITE(IOUNIT,35) IER,NAMEQ,IEG,NAME
0014      IF(IEGDF.EQ.0) WRITE(IOUNIT,35) IER,NAME
0015      GOTO 30
0016      5      IF(IER.LE.64) GOTO 10
0017      IF(LEVEL.LT.2) GOTO 30
C
C          PRINT WARNING MESSAGE WITH FIX
C
0018      CALL UGETIO(1,NIN,IOUNIT)
0019      IF(IEGDF.EQ.1) WRITE(IOUNIT,40) IER,NAMEQ,IEG,NAME
0020      IF(IEGDF.EQ.0) WRITE(IOUNIT,40) IER,NAME
0021      GOTO 30
0022      10      IF(IER.LE.32) GOTO 15
C
C          PRINT WARNING MESSAGE
C
0023      IF(LEVEL.LT.3) GOTO 30
0024      CALL UGETIO(1,NIN,IOUNIT)
0025      IF(IEGDF.EQ.1) WRITE(IOUNIT,45) IER,NAMEQ,IEG,NAME
0026      IF(IEGDF.EQ.0) WRITE(IOUNIT,45) IER,NAME
0027      GOTO 30
0028      15      CONTINUE
C
CC          CHECK FOR UERSET CALL
C
0029      IF(NAME.NE.NAMSET) GOTO 25
0030      LEVOLD=LEVEL
0031      LEVEL=IER
0032      IER=LEVOLD
0033      IF(LEVEL.LT.0) LEVEL=4
0034      IF(LEVEL.GT.4) LEVEL=4

```

```

0035      GOTO 30
0036      25      CONTINUE
0037      IF(LEVEL.LT.4) GOTO 30
          C
          C      PRINT MESSAGE FOR UNDEFINED
          C
0038      CALL UGETIO(1,NIN,IOUNIT)
0039      IF(IEGDF.EQ.1) WRITE(IOUNIT,50) IER,NAMEQ,IEQ,NAME
0040      IF(IEGDF.EQ.0) WRITE(IOUNIT,50) IER,NAME
0041      30      IEGDF=0
0042      RETURN
0043      35      FORMAT(19H *** TERMINAL ERROR,10X,7H( IER = ,I3,
          *      15H) FROM ROUTINE ,1A6,A1,1A6)
0044      40      FORMAT(36H *** WARNING WITH FIX ERROR (IER = ,I3,
          1      15H) FROM ROUTINE ,1A6,A1,1A6)
0045      45      FORMAT(18H *** WARNING ERROR,11X,7H( IER = ,I3,
          *      15H) FROM ROUTINE ,1A6,A1,1A6)
0046      50      FORMAT(20H *** UNDEFINED ERROR,9X,7H( IER = ,I5,
          *      15H) FROM ROUTINE ,1A6,A1,1A6)
0047      55      IEGDF=1
0048      60      NAMEQ=NAME
0049      65      RETURN
0050      END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          SUBROUTINE UGETIO                                C
C          RETRIEVES CURRENT VALUS AND SETS NEW VALUES FOR INPUT    C
C          AND OUTPUT UNIT IDENTIFIERS.                            C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C          THIS SUBROUTINE IS PART OF THE RUNGE-KUTTA NUMERICAL INTEGRATION
C          ROUTINE "RUNKUT".
C
0001          SUBROUTINE UGETIO(IOPT,NIN,NOUT)
0002          INTEGER IOPT,NIN,NOUT
0003          INTEGER NIND,NOUTD
0004          DATA NIND/1/,NOUTD/2/
0005          IF(IOPT.EQ.3) GOTO 10
0006          IF(IOPT.EQ.2) GOTO 5
0007          IF(IOPT.EQ.1) GOTO 9005
0008          NIN=NIND
0009          NOUT=NOUTD
0010          GOTO 9005
0011          5      NIND=NIN
0012          GOTO 9005
0013          10     NOUTD=NOUT
0014          9005   RETURN
0015          END

```

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                               SUBROUTINE UTPEAK
C    THIS SUBROUTINE IS DESIGNED TO DETERMINE THE MAXIMUM
C    TRANSPORT VELOCITY (WHEN IT IS A FUNCTION OF TIME)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C    THIS SUBROUTINE IS CALLED BY "SPREAD". IT CALCULATES THE
C    VELOCITY USED IN THE SPREADING MODELS,  $UC + 0.035 * VW$  (COMPONENT
C    AND FINDS THE MAXIMUM OF IT FOR LATER USE.
C    ** VARIABLE NAME: **
C    UTPEAK(I) = MAXIMUM VALUE OVER TIME OF  $UC + 0.035 * VW$  (COMPONENT
C    IN EACH OF THE 9 SLICES OR BOXES.
C    FOR A RIVER, I = 1.
C
0001 SUBROUTINE UTPEAK
0002 COMMON/STYPE/SPILLM, SPILMR, TSPILL, WS, STP, SPM
0003 COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0004 COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0005 COMMON/TRANSIT/UX(10, 10), UY(10, 10), VWX(10),
1          VWY(10), THETA(10), TI(10), ID, IT, IV,
2          XU(10), YU(10), TT(10)
0006 COMMON/MOVE/UPEAK(10), XLE, XTE, YLE, YTE, DELT, TIME, TSTOP, TCHECK
0007 COMMON/SPREAD/TII, ATK, HTK, ATN, HTN, HMIN, INDEX, IFLAG
0008 I = STP
0009 J=SHAPE
0010 IF (J.NE.1) GO TO 100
C
C
C    -----
C    IN RIVER OR CHANNEL
C    -----
0011 UPEAK(1)=0.0
0012 IF (IC.EQ.2.AND.IW.LE.1) GO TO 20
0013 GO TO 30
C
C    *****
C    CALCULATE UPEAK(1) = PEAK VALUE OF  $UC + 0.035 * VW$ 
C    FOR A TIDAL RIVER
C    *****
0014 20 UPEAK(1)=(UO+U1)+0.035*VW*COS(THETA1)
0015 GO TO 999
C
0016 30 CONTINUE
0017 DO 50 I=1,10
0018 IF (IC.EQ.1) GO TO 45
C
C    *****
C    CALCULATE AVERAGE VALUE OF VALUE OF TIDAL CURRENT FROM
C    T = 0 TO T = TT(1) AND ADD WIND COMPONENT TO COMPUTE
C    DUMMY VARIABLE UTOTAL. THEN SET UPEAK(1) EQUAL TO MAXIMUM
C    UTOTAL.
C    *****
0019 UC=UO+U1*WT/(2.0*3.14159)*(-COS(6.28318/WT*(TT(I)+ALPH))+

```

```

0020      1      COS(6.28318*ALPH/WT))
0021      45      UTOTAL=UC+0.035*VWX(I)*THETA(I)
0022      50      IF(UTOTAL.GT.UPEAK(1)) UPEAK(1)=UTOTAL
0023      CONTINUE
0023      GO TO 999

C
C
C      -----
C      IN OPEN WATER
C      -----
C

0024      100     CONTINUE
0025      DO 105 I=1,9
0026      UPEAK(I) = 0.0
0027      105     CONTINUE
0028      DO 200 I=1,9
0029      DO 180 J=1,10
0030      IF (IW.EQ.2) GO TO 120
0031      W1 = VWX(I)
0032      W2 = VWY(I)
0033      GO TO 140
0034      120     DO 125 K=1,10
0035      IF (TI(J).EQ.TT(K)) GO TO 135
0036      IF (TI(J).LE.TT(K)) GO TO 130
0037      125     CONTINUE
C
C      *****
C      INTERPOLATE TO FIND WIND SPEED AT TIME TI(I) CORRESPONDING T
C      CURRENT INPUT (TT(I) MAY NOT BE SAME AS TI(I) )
C      *****
C

0038      130     W1 = VWX(K-1)+(VWX(K)-VWX(K-1))*(TI(J)-TT(K-1))/
0039      1      (TT(K)-TT(K-1))
0039      W2 = VWY(K-1)+(VWY(K)-VWY(K-1))*(TI(J)-TT(K-1))/
0040      1      (TT(K)-TT(K-1))
0040      GO TO 140
0041      135     W1 = VWX(K)
0042      W2 = VWY(K)
0043      140     UU1 = UX(I,J)+0.035*W1
0044      UU2 = UY(I,J)+0.035*W2
0045      UTOT = SGRT(UU1**2+UU2**2)
C
C      *****
C      CALCULATE MAXIMUM VALUE OF UPEAK FOR EACH OF THE NINE BOXES
C      OR SLICES FOR THE WHOLE TIME DURATION
C      *****
C

0046      IF (UTOT.GT.UPEAK(I)) UPEAK(I)=UTOT
0047      180     CONTINUE
0048      200     CONTINUE
0049      999     RETURN
0050      END

```



```

C
C
C      FOR A RIVER OR CHANNEL:
C      WW = WIDTH, M
C      D = DEPTH, M
C      RO = BOTTOM ROUGHNESS, M
C      UC = CURRENT, M/SEC
C      *IF THE CURRENT IS TIDAL,
C      UC = UO + U1 * SIN(2. * PI * (T + ALPHA)/WT)
C      WHERE T = TIME, SEC
C      WT = PERIOD, SEC
C
0015 20      CONTINUE
0016      WRITE (1,22)
0017 22      FORMAT (//5X,29H1. THE SPILL IS IN A CHANNEL.)
0018 24      WRITE (6,25)
0019 25      FORMAT(/1X,51HGIVE THE WIDTH AND DEPTH OF THE CHANNEL (IN METE
      S))
0020      READ (5,*,ERR=24) WW,D
0021      WRITE (1,26) WW,D
0022 26      FORMAT (//5X,30H2. THE GEOMETRY OF THE CHANNEL/,8X,
      1      12HW = WIDTH = ,E12.5,6HMETERS/,8X,
      2      12HD = DEPTH = ,E12.5,6HMETERS)
0023 27      WRITE (6,127)
0024 127     FORMAT (/1X,50HINPUT THE BOTTOM ROUGHNESS(METERS) OF THE CHANN
      S,/,
      1      1X,51HINPUT ZERO, 0 IF YOU WANT TO USE THE DEFAULT VALUE.)
0025      READ (5,*,ERR=27) RO
0026      IF (RO.EQ.0.) RO=0.0584*D
0027 28      WRITE (6,29)
0028 29      FORMAT (/1X,36HIS THERE CURRENT IN THE CHANNEL? Y/N)
0029      READ (5,12,ERR=28) ICH
0030      IF (ICH.EQ.'Y') GO TO 40
C
C      --- NO CURRENT -----
C
0031      IC = 0
0032      SHAPE = 1.0
0033      UC=0.
C
0034      H=0.
0035 30      WRITE (1,32)
0036 32      FORMAT (//5X,30H3. THE CHANNEL HAS NO CURRENT.)
0037      GO TO 600
0038 40      CONTINUE
0039 41      WRITE (6,42)
0040 42      FORMAT (/1X,24HIS IT TIDAL CURRENT? Y/N)
0041      READ (5,12,ERR=41) ICH
0042      IF (ICH.EQ.'Y') GO TO 50
C
C      --- NON-TIDAL CURRENT ----
C
0043      SHAPE = 1.1
0044      IC = 1
0045 44      WRITE (6,45)

```

```

0046 45 FORMAT (/1X,31HCURRENT SPEED MUST BE CONSTANT. /
1 1X,29HINPUT CURRENT SPEED METER/SEC)
0047 READ (5,*,ERR=44) UC
0048 WRITE (1,48) UC
0049 48 FORMAT (/5X,27H3. IT IS NOT A TIDAL RIVER. /8X,
1 42HTHE CURRENT SPEED IS CONSTANT AND EQUAL TO.F10.3.
2 2X,10HMETER/SEC.)
0050 GO TO 600
C
C ---- TIDAL RIVER ----
C
0051 50 CONTINUE
0052 52 WRITE (6,54)
0053 54 FORMAT (/1X,39HTHE TIDAL VELOCITY CAN BE WRITTEN AS : /
1 8X,44HUC = UO + U1 * SIN (2*3.1416/WT*(TIME+ALPH))/
2 1X,50HINPUT UO (M/SEC), U1 (M/SEC), WT (MIN), ALPH (MIN)
0054 READ (5,*,ERR=52) UO,U1,WT,ALPH
0055 55 WRITE (1,56) UO,U1,WT,ALPH
0056 56 FORMAT (/5X,23H3. IT IS A TIDAL RIVER. /
1 8X,23HTHE CURRENT VELOCITY IS/
2 16X,44HUC = UO + U1 * SIN (2*3.1416/WT*(TIME+ALPH))/
3 8X,11HWHERE UO = ,F12.2,2X,9HMETER/SEC/
4 14X,5HU1 = ,F12.2,2X,9HMETER/SEC/
5 14X,5HWT = ,F12.2,2X,3HMIN/
6 14X,5HALPH=,F12.2,2X,3HMIN)
0057 WT=WT * 60.
0058 ALPH=ALPH * 60.
0059 IC = 2
0060 SHAPE = 1.2
0061 GO TO 600
C
C -----
C SPILL IS IN OPEN WATER
C -----
C
0062 100 CONTINUE
0063 101 IC=0
0064 102 WRITE (6,104)
0065 104 FORMAT (/1X,17HIS IT A LAKE? Y/N)
0066 READ (5,12,ERR=102) ICH
0067 IF (ICH.EQ.'N') GO TO 200
C
C --- SPILL IN LAKE ---
C
C FOR A LAKE:
C D = DEPTH, M
C R = RADIUS OF CIRCULAR LAKE, M
C L1,L2 = LENGTH AND WIDTH OF RECTANGULAR LAKE, M
C X(I),Y(I) = COORDINATES OF BOUNDARY OF IRREGULAR LAKE, M
C
0068 110 WRITE (6,112)
0069 112 FORMAT (/1X,26HIS IT A CIRCULAR LAKE? Y/N)
0070 READ (5,12,ERR=100) ICH
0071 IF (ICH.EQ.'N') GO TO 140
C

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```

C      --- CIRCULAR LAKE ---
C
0072      SHAPE = 2.1
0073      120      WRITE (6,122)
0074      122      FORMAT (1X,46H GIVE THE RADIUS AND DEPTH OF THE CIRCULAR LAKE,
1              /1X,14H(UNIT : METER))
0075      READ (5,*,ERR=120) R,D
0076      WRITE (1,124) R,D
0077      124      FORMAT (/5X,35H1. THE SPILL IS IN A CIRCULAR LAKE. /
1              /5X,29H2. THE GEOMETRY OF THE LAKE: /
2              8X,12HR = RADIUS = ,E12.5,2X,6HMETERS/
3              8X,11HD = DEPTH = ,E12.5,2X,6HMETERS)

C
C      *****
C      TRANSFER TO STATEMENTS DESCRIBING CURRENT
C      *****
C
0078      GO TO 500

C
0079      140      WRITE (6,142)
0080      142      FORMAT (/1X,29H IS IT A RECTANGULAR LAKE? Y/N)
0081      READ (5,12,ERR=140) ICH
0082      IF (ICH.EQ.'N') GO TO 160

C
C      --- RECTANGULAR LAKE ---
C
0083      SHAPE = 2.2
0084      150      WRITE (6,152)
0085      152      FORMAT (/1X,45H GIVE THE LENGTH (L1), WIDTH (L2) AND DEPTH OF,
1              19H THE LAKE. (METERS)/2X,
2              55H THE POINT X=0,Y=0 IS THE LOWER LEFT CORNER OF THE LAKE.)
0086      READ (5,*,ERR=150) L1,L2,D
0087      WRITE (1,154)
0088      154      FORMAT (/5X,38H1. THE SPILL IS IN A RECTANGULAR LAKE. /
1              /5X,30H2. THE DIMENSION OF THE LAKE : /
2              8X,13HL1 = LENGTH = ,E12.5,2X,6HMETERS/
3              8X,13HL2 = WIDTH = ,E12.5,2X,6HMETERS/
4              8X,13HD = DEPTH = ,E12.5,2X,6HMETERS)

C
C      *****
C      TRANSFER TO STATEMENTS DESCRIBING CURRENT
C      *****
C
0089      GO TO 500

C
C      --- LAKE W/ ARBITRARY SHAPE ---
C
0090      160      CONTINUE
0091      161      WRITE (6,162)
0092      162      FORMAT(/1X,45H THE SPILL IS IN A LAKE WITH ARBITRARY SHAPE. //
*              1X,98H DESCRIBE THE SHAPE WITH 10 PAIRS OF X,Y COORDINA
*              (METERS). (0,0) SHOULD BE NEAR THE SPILL SITE.)
0093      SHAPE = 2.3
0094      WRITE (1,164)
0095      164      FORMAT (/5X,46H1. THE SPILL IS IN AN IRREGULARLY SHAPED LAKE

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1          5X, 47H2. THE FOLLOWING POINTS SPECIFY THE BOUNDARY OF,
2          10H THE LAKE. )
C
C          *****
C          TRANSFER TO STATEMENTS DESCRIBING IRREGULAR SHAPE
C          *****
0096      GO TO 300
C
C          ---- SPILL MUST BE IN COASTAL WATER ----
C
C          FOR A COAST:
C          D = DEPTH, M
C          X(1),Y(1),X(2),Y(2) = TWO COORDINATES DESCRIBING A STRAIGHT
C          COAST LINE, M
C          X(I),Y(I) = COORDINATES DESCRIBING AN IRREGULAR COAST LINE, I
C
0097      200      CONTINUE
0098      WRITE (6,202)
0099      202      FORMAT (/1X,31HSPILL MUST BE IN COASTAL WATER.)
0100      203      WRITE (6,204)
0101      204      FORMAT (/1X,23HIS COAST STRAIGHT ? Y/N)
0102      READ (5,12,ERR=203) ICH
0103      IF (ICH.EQ. 'N') GO TO 220
C
C          ---- STRAIGHT COAST LINE ----
C
0104      SHAPE = 3.1
0105      WRITE (1,210)
0106      210      FORMAT (/5X,42H1. THE SPILL OCCURS IN COASTAL WATER WITH ,
1              20HSTRAIGHT COAST LINE. )
0107      211      WRITE (6,212)
0108      212      FORMAT (/1X,36HGIVE THE DEPTH OF THE COASTAL WATER. )
0109      READ (5,*,ERR=211) D
0110      214      WRITE (6,215)
0111      215      FORMAT(/1X,62HGIVE 2 (X,Y) COORDINATES OF THE STRAIGHT COAST L
*E IN METERS. )
0112      READ (5,*,ERR=214) X(1), Y(1), X(2), Y(2)
0113      WRITE (1,218) D, X(1), Y(1), X(2), Y(2)
0114      218      FORMAT (/5X,36H2. THE DEPTH OF THE COASTAL WATER IS,
1              E12. 5, 2X, 6HMETERS/8X, 31HTHE COAST LINE IS GIVEN BY THE
2              19HFOLLOWING 2 POINTS. /
3              20X, 1HX, 17X, 1HY/10X, 1H1, 3X, E12. 5, 5X, E12. 5/
4              10X, 1H2, 3X, E12. 5, 5X, E12. 5)
C
C          *****
C          TRANSFER TO STATEMENTS DESCRIBING CURRENT
C          *****
0115      GO TO 500
C
C          ---- IRREGULAR COAST LINE ----
C
0116      220      CONTINUE
0117      SHAPE = 3.2

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0118      223      WRITE (1,222)
0119      222      FORMAT (//5X,42H1. THE SPILL OCCURS IN COASTAL WATER WITH ,
1              20HIRREGULAR COAST LINE//,5X,
2              48H2. THE FOLLOWING POINTS SPECIFY THE BOUNDARY OF ,
3              11HCOAST LINE.)
0120      WRITE (6,224)
0121      224      FORMAT (/1X,48HTHE SPILL OCCURS IN COASTAL WATER WITH IRREGULA
1              11H COAST LINE/
*              1X,107HDESCRIBE THE COAST LINE WITH 10 PAIRS OF (X,Y)
*ORDINATES (METERS). (0,0) SHOULD BE NEAR THE SPILL ORIGIN.)

C
C      *****
C      STATEMENTS 300-324 INPUT IRREGULAR LAKE AND COAST SHAPES
C      *****
0122      300      CONTINUE
0123      DO 301 I=1,10
0124      READ(5,*,ERR=223)X(I),Y(I)
0125      301      CONTINUE
0126      WRITE (1,302)
0127      WRITE (6,302)
0128      302      FORMAT (/15X,1HX,15X,1HY)
0129      DO 309 I=1,10
0130      WRITE (1,306) I,X(I),Y(I)
0131      WRITE (6,306) I,X(I),Y(I)
0132      306      FORMAT (10X,I2,2X,E12.5,5X,E12.5)
0133      309      CONTINUE
0134      310      CONTINUE
0135      320      WRITE (6,321)
0136      321      FORMAT (/1X,17HINPUT WATER DEPTH)
0137      READ (5,*,ERR=320) D
0138      WRITE (1,324) D
0139      324      FORMAT (10X,18HTHE WATER DEPTH IS,E12.5,2X,6HMETERS)

C
C      *****
C      STATEMENTS 500-600 INPUT CURRENTS
C      *****
0140      500      CONTINUE
0141      501      WRITE (6,502)
0142      502      FORMAT (/1X,21HIS THERE CURRENT? Y/N)
0143      READ (5,12,ERR=501) ICH
0144      IF (ICH.EQ. 'Y') GO TO 510
0145      WRITE (1,504)
0146      504      FORMAT (//5X,23H3. THERE IS NO CURRENT.)
0147      GO TO 600

C
0148      510      CONTINUE
C
C      ---- THERE IS CURRENT ----
C
0149      511      WRITE (6,512)
0150      512      FORMAT (/1X,24HIS CURRENT CONSTANT? Y/N)
0151      READ (5,12,ERR=511) ICH
0152      IF (ICH.EQ. 'N') GO TO 517

```

```

C
C      ---- CONSTANT CURRENT IN OPEN WATER (STATEMENTS 513-516) ----
C      FOR A CONSTANT CURRENT, UX(1,1) = X-COMPONENT,
C      UY(1,1) = Y-COMPONENT, M/SEC
C
0153 513 WRITE (6,514)
0154      IC=1
0155 514 FORMAT (/1X,40HINPUT CONSTANT CURRENT SPEED UCX AND UCY,
1      /1X,18H(UNIT : METER/SEC))
0156      READ (5,*,ERR=513) UX(1,1),UY(1,1)
0157      WRITE (1,516) UX(1,1),UY(1,1)
0158 516 FORMAT (/5X,41H3. THE CURRENT IS CONSTANT WITH MAGNITUDE, /
1      8X,5HUCX =,F12.2,2X,9H METER/SEC, /
2      8X,5HUCY =,F12.2,2X,9H METER/SEC)
0159      GO TO 600
0160 517 WRITE (6,518)
0161 518 FORMAT(/1X,35HIS CURRENT A FUNCTION OF TIME ? Y/N)
0162      READ (5,12,ERR=517) ICH
0163      IF(ICH.EQ.'Y') GO TO 520
C
C      --- CURRENT IS A FUNCTION OF LOCATION ONLY ---
C      (TRANSFERS TO 532 FOR INPUT AFTER PRINTING OUT LEGEND)
C
0164      IC=2
0165      WRITE(1,519)
0166 519 FORMAT(/5X,40H3. THE CURRENT IS NOT A FUNCTION OF TIME/
1      8X,44HHOWEVER IT DOES CHANGE WITH SURFACE POSITION)
0167      GO TO 532
0168 520 WRITE(6,1001)
0169 1001 FORMAT(/1X,40HIS CURRENT A FUNCTION OF TIME ONLY ? Y/N)
0170      READ(5,12,ERR=520) ICH
0171      IF (ICH.EQ.'Y') GO TO 1020
C
C      *****
C      GO TO 1020 WHEN CURRENT = F(TIME AND SPACE)
C      *****
C
0172      IC=4
0173      WRITE(1,1005)
0174 1005 FORMAT(/5X,41H3. THE CURRENT IS A FUNCTION OF BOTH TIME,
1      /8X,13H AND LOCATION)
0175      GO TO 532
0176 1020 IC=3
0177      WRITE(1,1025)
0178 1025 FORMAT(/5X,39HTHE CURRENT IS A FUNCTION OF TIME ONLY.)
C
C      ---- CURRENT SPEED VARIED WITH TIME AND/OR LOCATION ----
C
C      *****
C      WHEN CURRENT = F(TIME) ONLY, THE CURRENTS ARE:
C      UX(1,I) = X-COMPONENT AT TIME T(I), M/SEC
C      UY(1,I) = Y-COMPONENT AT TIME T(I), M/SEC
C      TI(I) = SPECIFIED TIMES (10), SEC
C      *****
C

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0179      521      WRITE(6,522)
0180      522      FORMAT(/,5X,41H GIVE TIME AND X,Y CURRENT AT 10 INSTANTS. /,5X,
*           50H THE MAXIMUM TIME MUST BE AT LEAST AS GREAT AS LAST/5X
*           25H PRINT-OUT TIME REQUESTED. ,26H TIME SHOULD BE IN MINUTE)
0181      DO 525 I=1,10
0182      READ(5,*,ERR=520) TI(I),UX(1,I),UY(1,I)
0183      DO 524 J=2,10
0184      UX(J,I)=UX(1,I)
0185      UY(J,I)=UY(1,I)
0186      524      CONTINUE
0187      525      CONTINUE
0188      WRITE(1,526)
0189      526      FORMAT(/,10X,9H TIME(MIN),11X,9H UX(M/SEC),6X,9H UY(M/SEC))
0190      DO 530 I=1,10
0191      WRITE(1,528) TI(I),UX(1,I),UY(1,I)
0192      528      FORMAT(10X,E15.1,5X,F10.5,5X,F10.5)
0193      TI(I)=TI(I)*60.
0194      530      CONTINUE
0195      GOTO 600

C
C
C *****
C STATEMENTS 532-600 GIVE INPUT WHEN CURRENT = F(SPACE). IF
C CURRENT IS ALSO A FUNCTION OF TIME, A DO-LOOP IS SET UP TO
C GIVE INPUT AT 10 TIME INSTANTS.
C *****
C
0196      532      WRITE(6,533)
0197      533      FORMAT(/,5X,50H IF A LAKE, THE X,Y CURRENT MUST BE GIVEN AT CEI
$R/5X,50H OF 9 RECTANGULAR BOXES (3X3 GRID) THAT COVER LAKE. /5X,
$49H IF A COAST, THE X,Y CURRENT MUST BE GIVEN FOR THE/5X,71H 9 Y-
$CES THAT EXTEND OUT FROM THE 10 X,Y POINTS DESCRIBING THE COAST
0198      IF(SHAPE.GE.3.0) GOTO 547
0199      534      WRITE(6,535)
0200      535      FORMAT(/5X,46H GIVE THE 4 X-COORDINATES (METERS) THAT SPECIFY/
*           44H THE HORIZONTAL GRID. THE FIRST AND LAST MUST/5X,
*           37H COINCIDE WITH THE LENGTH OF THE LAKE. )

C
C *****
C STATEMENTS FROM HERE TO 555 ARE DO-LOOPS TO SPECIFY THE GRID
C FOR THE CURRENTS. XU(I) AND YU(I) ARE THE GRID FOR A LAKE BE
C
C YU(4) 0 * 0 * 0 * 0
C        * 7 * 8 * 9 *
C        0 * 0 * 0 * 0
C        * 4 * 5 * 6 *
C        0 * 0 * 0 * 0
C        * 1 * 2 * 3 *
C YU(1) 0 * 0 * 0 * 0
C        XU(1)      XU(4)
C
C
C FOR A COAST THE GRID IS:
C
C      *   *   *   *
C      *   *   *   *

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C          * 1 * 2 * 3 * AND SO ON
C          *   *   *   *
C          *   *   *   0
C          *   *   0**XU(4)
C          *   0**   YU(4)
C          0**
C          XU(1)
C          YU(1)
C          *****
C
0201      DO 537 I=1,4
0202      READ(5,*,ERR=534) XU(I)
0203      537 CONTINUE
0204      WRITE(6,538)
0205      538 FORMAT(/5X,38HNOW GIVE THE 4 Y-COORDINATES (METERS). /5X,
*          60HTHE FIRST AND LAST MUST COINCIDE WITH THE WIDTH OF THE LAKE.
0206      DO 540 I=1,4
0207      READ(5,*,ERR=534) YU(I)
0208      540 CONTINUE
0209      WRITE(1,542)(XU(I), I=1,4)
0210      542 FORMAT(/5X,43HX-COORDINATES OF HORIZONTAL GRID IN METERS: //1X,
1          4(E12.5,2X))
0211      WRITE(1,543)(YU(I), I=1,4)
0212      543 FORMAT(/5X,41HY-COORDINATES OF VERTICAL GRID IN METERS: //1X,
1          5(E12.5,2X))
0213      GOTO 551
0214      547 WRITE(6,548)
0215      548 FORMAT(/5X,47HGIVE THE 10 X-COORDINATES (METERS) THAT SPECIFY/
*          5X,51HTHE 9 SLICES. THE FIRST AND LAST MUST COINCIDE WITH/5X,
*          24HTHE LENGTH OF THE COAST. )
0216      DO 550 I=1,10
0217      READ(5,*,ERR=547) XU(I)
0218      550 CONTINUE
0219      WRITE(1,552)(XU(I), I=1,10)
0220      552 FORMAT(5X,
1          47HX-COORDINATES THAT FORM THE 9 SLICES IN METERS: //1X,
2          5(E12.5,2X)/1X,5(E12.5,2X))
0221      551 WRITE(6,555)
0222      555 FORMAT(/5X,49HINPUT UX AND UY CURRENTS(M/SEC) FOR EACH OF THE 9
*          /5X,49HBOXES OR SLICES. BOXES ARE NUMBERED LEFT-TO-RIGHT/
*          5X,51H1,2,3 IN BOTTOM ROW, 4,5,6 IN MIDDLE ROW, AND 7,8,9/
*          5X,51HIN TOP ROW. SLICES FOR A COAST ARE NUMBERED 1 TO 9,/
*          5X,51HLEFT-TO-RIGHT. IF THE CURRENTS ALSO DEPEND ON TIME,/
*          5X,47HYOU WILL BE ASKED FOR 10 SUCH SETS OF CURRENTS. )
0223      I=1
0224      IF(1C.EQ.2) GOTO 563
0225      560 WRITE(6,561)I
0226      561 FORMAT(/5X,21HCURRENTS FOR NUMBER ,I3,1X,5HTIME. )
C
C          *****
C          THIS IS THE DO-LOOP WHEN CURRENT IS ALSO A FUNCTION OF TIME.
C          TI(I) = TIME INSTANTS (10). CURRENTS ARE:
C
C          UX(J,I) = X-COMPONENT, M/SEC
C          UY(J,I) = Y-COMPONENT, M/SEC

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C          J = BOX OR SLICE NO.
C          I = TIME NO.
C          *****
C
0227 563 DO 564 J=1,9
0228 READ(5,*,ERR=551) UX(J,I),UY(J,I)
0229 564 CONTINUE
0230 IF(IC.EQ.2) GOTO 580
0231 I=I+1
0232 IF(I.EQ.11) GOTO 570
0233 GOTO 560
0234 570 WRITE(6,571)
0235 571 FORMAT(/5X,42HNOW GIVE THE TEN TIME INSTANTS IN MINUTES.)
0236 572 DO 575 I=1,10
0237 READ(5,*,ERR=570) TI(I)
0238 575 CONTINUE
0239 580 I=1
0240 IF(IC.EQ.2) GOTO 590
0241 582 WRITE(6,585) TI(I)
0242 583 WRITE(1,585) TI(I)
0243 585 FORMAT(/20X,5HTIME=,E12.5,1X,7HMINUTES)
0244 TI(I)=TI(I)*60.
0245 590 WRITE(6,593)
0246 591 WRITE(1,593)
0247 593 FORMAT(/20X,52HUX(M/SEC) AND UY(M/SEC) IN THE NINE BOXES OR SL
*ES.)
0248 WRITE(6,594)
0249 WRITE(1,594)
0250 594 FORMAT(10X,1H1,7X,1H2,7X,1H3,7X,1H4,7X,1H5,7X,1H6,7X,1H7,7X,1H8
* 7X,1H9)
0251 WRITE(6,595)(UX(J,I),J=1,9)
0252 WRITE(1,595)(UX(J,I),J=1,9)
0253 WRITE(6,596)(UY(J,I),J=1,9)
0254 WRITE(1,596)(UY(J,I),J=1,9)
0255 595 FORMAT(1X,2HUX,2X,9(3X,F5.2))
0256 596 FORMAT(1X,2HUY,2X,9(3X,F5.2))
0257 IF(IC.EQ.2)GOTO 600
0258 I=I+1
0259 IF(I.EQ.11)GOTO 600
0260 GOTO 582
0261 600 CONTINUE
0262 602 WRITE (6,605)
0263 605 FORMAT (/1X,31HIS THERE WIND IN THE AREA ? Y/N)
0264 READ (5,12,ERR=602) ICH
0265 IF (ICH.EQ.'Y') GO TO 700
0266 WRITE (1,610)
0267 610 FORMAT(/5X,32H4. THERE IS NO WIND IN THE AREA.)
0268 GO TO 800
0269 700 CONTINUE
C
C ----- CALL SUBROUTINE TO CALCULATE TRANSPORT
C VELOCITY DUE TO WIND
C
0270 CALL WIND
0271 GO TO 999

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CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C          SUBROUTINE WIND
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C          THIS SUBROUTINE INPUTS THE WIND VELOCITY AND WAVE HEIGHT. IT
C          IS CALLED BY SUBROUTINE "WBS". IT SETS UP THE FOLLOWING CODE:
C
C          IW = 0 : NO WIND
C          IW = 1 : CONSTANT WIND
C          IW = 2 : WIND = F(TIME)
C
0001          SUBROUTINE WIND
0002          COMMON/CONTOUR/SHAPE, X(10), Y(10), XC, YC, IC, IW, ISP, XO, YO
0003          COMMON/ENVOR/PV, VISA, DENA, TDC
0004          COMMON/TRANSIT/UX(10, 10), UY(10, 10), VWX(10),
1              VWY(10), THETA(10), TI(10), ID, IT, IV,
2              XU(10), YU(10), TT(10)
0005          COMMON/CONSTAT/UC, VW, UTBAR, UO, U1, WT, ALPH, THETA1
0006          COMMON/SIZE/R, D, WW, L1, L2, H, RO
C
0007          PI=ACOS(-1.)
0008          I = SHAPE
0009          1 WRITE (6, 10)
0010          10 FORMAT (/1X, 27HIS WIND SPEED CONSTANT? Y/N)
0011          READ (5, 12, ERR=1) ICH
0012          12 FORMAT(A1)
0013          IF (ICH.EQ. 'N') GO TO 40
0014          IW = 1
0015          14 WRITE (6, 15)
C
C          *****
C          CONSTANT WIND ----
C          VW = WIND SPEED, M/SEC
C          THETA1 = WIND ANGLE WITH RESPECT TO X-AXIS OR
C                   CHANNEL AXIS, RADIANS
C          VWX(1) = X-COMPONENT OF VW
C          VWY(1) = Y-COMPONENT OF VW
C          *****
0016          15 FORMAT (/1X, 42HINPUT WIND SPEED (METER/SEC) AND DIRECTION,
1              /1X, 15HANGLE (DEGREES))
0017          READ (5, *, ERR=14) VW, THETA1
0018          WRITE (1, 21) VW, THETA1
0019          21 FORMAT (//5X, 35H4. THE WIND IS STEADY WITH SPEED OF, F12. 2, 2X,
1              9HMETER/SEC, /8X, 13H AND ANGLE OF, F12. 2, 2X, 7HDEGREES)
0020          THETA1=THETA1*PI/180.
0021          IF (I.EQ. 1) GO TO 150
0022          VWX(1) = VW * COS(THETA1)
0023          VWY(1) = VW * SIN(THETA1)
0024          TWIND = VW
0025          GO TO 150
C
C          *****

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C      ---- WIND SPEED VARIES WITH TIME ----
C      *****
C
0026  40  CONTINUE
0027      IW = 2
0028      I = SHAPE
0029      GO TO (50,60,60) I

C      *****
C      I = 1 : RIVER
C      I = 2 OR 3 : LAKE OR COAST
C      *****
0030  50  CONTINUE

C      ---- IN RIVER OR CHANNEL ----
C
0031  51  WRITE (6,52)
0032  52  FORMAT(1X,40HWIND SPEED OVER CHANNEL DEPENDS ON TIME./1X,
* 68HINPUT TIME (MIN), WIND SPEED (M/SEC), AND DIRECTION ANGLE (DI
*GREES)./1X,52HUSE 10 TIME INSTANTS, AND LAST TIME MUST BE AT LEAS
*/1X,35HAS GREAT AS MAXIMUM PRINT-OUT TIME.)

C      *****
C      FOR WIND = F(TIME) :
C      VWX(I) = X-COMPONENT AT TIME T(I), M/SEC
C      VWY(I) = Y-COMPONENT AT TIME T(I), M/SEC
C      TT(I) = TIME INSTANT (10), SEC
C      THETA(I) = WIND ANGLE WITH RESPECT TO X-AXIS OR
C      CHANNEL AXIS, RADIAN
C
C      NOTE: IN THE INPUT, VWX(I) IS USED TEMPORARILY TO INPUT
C      THE WIND SPEED, THEN X AND Y COMPONENTS ARE CALCULATED
C      INTERNALLY.
C      *****
C
0033      DO 54 I=1,10
0034      READ(5,*,ERR=51) TT(I),VWX(I),THETA(I)
0035      THETA(I)=THETA(I)*PI/180.
0036      VW=VWX(I)
0037      THETA1=THETA(I)
0038      VWY(I)=VWX(I)*SIN(THETA(I))
0039      VWX(I)=VWX(I)*COS(THETA(I))
0040  54  CONTINUE
0041      GOTO 100

C      ---- IN OPEN WATER ----
C
0042  60  WRITE(6,62)
0043  62  FORMAT(1X,45HWIND SPEED OVER LAKE OR COAST DEPENDS ON TIME/1X,
* 55HBUT IS CONSTANT OVER ENTIRE AREA. USE 10 TIME INSTANTS./
* 1X,50HAND LAST TIME MUST BE AT LEAST AS GREAT AS MAXIMUM/1X,
* 53HPRINT-OUT TIME. INPUT TIME (MIN), WIND SPEED (M/SEC)./1X,
* 30HAND DIRECTION ANGLE (DEGREES).)
0044      DO 64 I=1,10

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0045      READ(5,*,ERR=60) TT(I), VWX(I), THETA(I)
0046      THETA(I)=THETA(I)*PI/180.
0047      VW=VWX(I)
0048      THETA1=THETA(I)
0049      VWY(I)=VWX(I)*SIN(THETA(I))
0050      VWX(I)=VWX(I)*COS(THETA(I))
0051      64
      C
0052      100      WRITE (1,102)
0053      102      FORMAT (//5X,35H4. WIND SPEED IS A FUNCTION OF TIME//
      1          8X,4HTIME,10X,10HWIND SPEED,10X,9WDIRECTION)
0054      DO 110 I = 1,10
0055      THETA(I)=THETA(I)*180./PI
0056      TWIND=SGRT(VWX(I)**2. + VWY(I)**2.)
0057      WRITE(1,105)TT(I), TWIND, THETA(I)
0058      105      FORMAT (5X,F10.2,7X,F10.5,9X,F10.5)
0059      THETA(I)=THETA(I)*PI/180.
0060      TT(I)=TT(I)*60.
0061      110      CONTINUE
      C
0062      150      CONTINUE
      C
0063      GOTO(299,199,199), I
0064      199      WRITE(6,200)
0065      200      FORMAT (/1X,30HINPUT MEAN WAVE HEIGHT. (METER)/
      * 1X,45HDEFAULT VALUE (EQ. (III.32) OF REPORT) IS USED/1X,
      * 16HBY INPUTTING -1.)
0066      READ (5,*,ERR=199) H
0067      IF(H.LT.0.) H=0.01384*TWIND
0068      WRITE(1,210) H
0069      210      FORMAT(/8X,19HMEAN WAVE HEIGHT IS,F6.2,2X,6HMETERS)
0070      299      RETURN
0071      END

```