

TECHNICAL REPORT ARBRL-TR-02302

TRANSPORT ALGORITHMS FOR PREMIXED,
LAMINAR STEADY STATE FLAMES

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March 1981



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ABERDEEN PROVING GROUND, MARYLAND

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20. ABSTRACT (Cont'd)

nearly independent of the approximation method used. This does not indicate that transport phenomena are unimportant, but rather that the selection of the input values for the individual species transport properties is more important than the selection of the method used to approximate the multispecies transport.

Based on these results we have developed a sixth approximation method that is computationally efficient and which provides results extremely close to the most sophisticated and precise method used.

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I. INTRODUCTION

To determine validated sets of elementary chemical reactions for use in predictive combustion models, we have chosen to simulate the one dimensional, premixed, laminar flame. This approach has the advantage that the predicted temperature and species profiles can in principal be compared with suitable burner experiments of the same flame. The corresponding equations are derived by Bird, Stewart and Lightfoot,¹ and by Williams,² and are given in Appendix A.

Such a simulation requires as input not only the kinetics information (of our immediate interest), but also thermodynamic and transport data. Fortunately the thermodynamics input is by and large well defined.^{3,4} In addition, while some transport coefficients are only well defined through low temperature (< 1000 K) measurements,⁵ the theory is sufficiently developed to allow reasonable estimates to be made at higher temperatures.⁶ A theory has been developed for multicomponent

¹R. B. Bird, W. S. Stewart and E. N. Lightfoot, Transport Phenomena, John Wiley and Sons, NY, (1960).

²F. A. Williams, Combustion Theory, Addison-Wesley, Reading, MA, (1965).

³D. R. Stull and H. Prophet, JANAF Thermochemical Tables, 2nd Edition, NSRDS-NBS-37, June 1971.

⁴S. Gordon and B. J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations", NASA-SP-273, (1971), (1976 program version).

⁵Y. S. Touloukian, P. E. Liley, and S. C. Saxena, Thermophysical Properties of Matter, Vol. 3, Thermal Conductivity (Nonmetallic Liquids and Gases), IFI/Plenum, NY-Washington, (1970).

⁶J. O. Hirshfelder, C. F. Curtiss and R. B. Bird, Molecular Theory of Gases and Liquids, 2nd printing, corrected, with notes, John Wiley and Sons, NY, (1964).

mixtures,⁶⁻¹⁰ but it is computationally cumbersome. To circumvent this, previous workers have generally employed some level of simplification.¹¹⁻²¹

- ⁷C. S. Wang Chang, G. E. Uhlenbeck and J. deBoer, Studies in Statistical Mechanics, Vol. 2, John Wiley and Sons, NY, (1964).
- ⁸L. Monchick, K. S. Yun and E. A. Mason, "Formal Kinetic Theory of Transport Phenomena in Polyatomic Gas Mixtures", *J. Chem. Phys.*, 39, 654-699 (1963).
- ⁹L. Monchick, A. N. G. Pereira and E. A. Mason, "Heat Conductivity in Polyatomic and Polar Gases and Gas Mixtures", *J. Chem. Phys.*, 42, 3241-3256 (1965).
- ¹⁰L. Monchick, R. J. Munn and E. A. Mason, "Thermal Diffusion in Polyatomic Gases: A Generalized Stefan-Maxwell Diffusion Equation", *J. Chem. Phys.*, 45, 3051-3058 (1966).
- ¹¹G. Dixon-Lewis, et al., "Flame Structure and Flame Reaction Kinetics", *Proc. R. Soc., London A* 317, 235-263 (1970); *A* 330, 199-218 (1972); *A* 331, 571-584 (1973); and *A* 346, 261-278 (1975).
- ¹²G. Dixon-Lewis, "Kinetic Mechanism, Structure and Properties of Premixed Flames in Hydrogen-Oxygen-Nitrogen Mixtures", *Phil. Trans. R. Soc., London*, 292, 45-99 (1979).
- ¹³G. Tsatsaronis, "Prediction of Propagating Laminar Flames in Methane, Oxygen, Nitrogen Mixtures", *Combust. and Flame*, 33, 217-239 (1978).
- ¹⁴J. Warnatz, "Calculation of the Structure of Laminar Flat Flames I; Flame Velocity of Freely Propagating Ozone Decomposition Flames", *Ber. Bunsenges Phys. Chem.*, 82, 193-200 (1978).
- ¹⁵D. B. Spalding and P. L. Stephenson, "Laminar Flame Propagation in Hydrogen + Bromine Mixtures", *Proc. R. Soc. London A*, 324, 315-337 (1971).
- ¹⁶P. L. Stephenson and R. G. Taylor, "Laminar Flame Propagation in Hydrogen, Oxygen, Nitrogen Mixtures", *Combust. and Flame* 20, 231-244 (1973).
- ¹⁷L. D. Smoot, W. C. Hecker, and G. A. Williams, "Prediction of Propagating Methane-Air Flames", *Combust. and Flame* 26, 323-342 (1976).
- ¹⁸J. Warnatz, "Calculation of the Structure of Laminar Flat Flames II; Flame Velocity and Structure of Freely Propagating Hydrogen-Oxygen and Hydrogen-Air Flames", *Ber. Bunsenges Phys. Chem.*, 82, 643-649 (1978).
- ¹⁹D. B. Spalding, P. L. Stephenson, and R. G. Taylor, "A Calculation Procedure for the Prediction of Laminar Flame Speeds", *Combust. and Flame* 17, 55-64 (1971).
- ²⁰L. Bledjian, "Computation of Time-Dependent Laminar Flame Structure", *Combust. and Flame*, 20, 5-17 (1973).
- ²¹E. Cramarossa and G. Dixon-Lewis, "Ozone Decomposition in Relation to the Problem of the Existence of Steady-State Flames", *Combust. and Flame* 16, 243-251 (1971).

This paper addresses the question: which of the mathematical approximations to the multicomponent transport properties provides a desirable trade-off between precision and computational effort. Another way of phrasing this question is to ask what loss in precision of predicted flame speeds and profiles occurs as the mathematical approximations to the multicomponent, polyatomic transport expressions are made cruder.

We approach this problem by actually computing the flame properties for a given flame with a fixed set of input conditions. The transport algorithms are varied and the resulting flame speeds and profiles compared. The numerical method is discussed in references 22 and 23. We have selected the H_2 - O_2 - N_2 system as the candidate flame because it has a well characterized set of input parameters. (See Appendix B).

This paper is divided into the following sections. Section II outlines a sequence of five methods for approximating the transport coefficients. Section III shows the numerical results of these approximation methods relative to the most accurate method, and Section IV discusses their relative precision for a set of five flames. Based on these results, we outline in Section V an algorithm which provides a reasonable balance between computational effort and theoretical rigor and includes a crude approximation for the effects of thermal diffusion. There are several appendices that contain sufficient detail to reproduce our computations.

II. APPROXIMATION METHODS

In this section we outline five approximations to the multicomponent, polyatomic formalism, based on the theory of Wang Chang and Uhlenbeck.⁶⁻¹⁰ We start with the most accurate and progressively consider cruder approximations. Method I is the three term Sonine approximation to the formalism. Dixon-Lewis (DL)²⁴ gives a discussion of this approximation, and we will generally follow his approach. Method II involves a level of approximation using smaller matrices. Methods III and IV use

²²T. P. Coffee and J. M. Heimerl, "A Method for Computing the Flame Speed for a Laminar, Premixed, One Dimensional Flame", BRL Technical Report, ARBRL-TR-02212, Jan 80.

²³T. P. Coffee, "A Computer Code for the Solution of the Equations Governing a Laminar, Premixed, One Dimensional Flame", BRL Memorandum Report, to be published.

²⁴G. Dixon-Lewis, "Flame Structure and Flame Reaction Kinetics II. Transport Phenomena in Multicomponent Systems", *Proc. Roy. Soc. A* 307, 111-135 (1968).

non-matrix techniques. Method V discusses the case of constant transport parameters. In each case we need to determine the diffusion velocities V_i , $i = 1, 2, \dots, N$, and the heat flux q .

A. Method I

Following (DL), we can write

$$q = \sum_{i=1}^N \rho Y_i V_i h_i - \lambda_0 \frac{\partial T}{\partial x} - \sum_{i=1}^N \frac{RT D_i^T}{M_i Y_i} \frac{\partial X_i}{\partial x} \quad (1)$$

and

$$V_i = \frac{1}{X_i} \sum_{j=1}^N \frac{Y_j}{X_j} D_{ij} \frac{\partial X_j}{\partial x} - \frac{D_i^T}{\rho Y_i} \frac{\partial}{\partial x} (\ln T), \quad (2a)$$

or

$$V_i = V_i + w_i, \quad (2b)$$

a notation we will later find convenient. The diffusion coefficients can be written in terms of the Sonine expansion coefficients,

$$D_{ij} = X_i \frac{16T}{25p} \frac{\sum_{k=1}^N M_k X_k}{M_j} c_{i00}^{1ji} \quad (3)$$

and

$$D_i^T = \frac{8}{5} \frac{M_i X_i}{R_a} a_{i00}^1. \quad (4)$$

Substituting equations (3) and (4) into equation (2) we find

$$V_i = \frac{16T}{25p} \sum_{j=1}^N (c_{i00}^{1ji} \frac{\partial X_j}{\partial x}) - \frac{8T}{5p} a_{i00}^1 \frac{\partial}{\partial x} (\ln T). \quad (5)$$

Similarly, we can write

$$\lambda_o = \lambda_{o,tr} + \lambda_{o,int} = -4 \sum_{i=1}^N X_i a_{i10}^1 - 4 \sum_{i=1}^N X_i a_{i01}^1 \quad (6)$$

The diffusion velocities and the heat flux are now defined in terms of the a_{i00}^1 , a_{i10}^1 , a_{i01}^1 , and c_{i00}^{1ji} . If we use three terms in the polynomial expansion, these are defined implicitly by the equations

$$\begin{aligned} (L) & (a_{100}^1 \dots a_{N00}^1, a_{110}^1 \dots a_{N10}^1, a_{101}^1 \dots a_{N01}^1)^T \\ & = (0 \dots 0, X_1 \dots X_N, X_1 \dots X_N)^T \end{aligned} \quad (7)$$

and

$$\begin{aligned} (L) & (c_{100}^{1hk} \dots c_{N00}^{1hk}, c_{110}^{1hk} \dots c_{N10}^{1hk}, c_{101}^{1hk} \dots c_{N01}^{1hk})^T \\ & = (\delta_{1h} - \delta_{1k} \dots \delta_{Nh} - \delta_{Nk}, 0 \dots 0, 0 \dots 0) \quad h, k = 1 \dots N. \end{aligned} \quad (8)$$

The elements of the $3N$ by $3N$ matrix (L) are given in Appendix C. The procedures we have used for computing these elements are discussed in Appendix D.

From equation (8), it appears that we must solve N^2 sets of equations to obtain the c_{i00}^{1ji} . In fact, it has been recommended^{6,8,24} that only the a terms be computed using this level of approximation, and that the c terms be computed using a one term expansion (see Method II).

However, this is not necessary if we observe that we are only interested in the V_i 's, and not directly in the c terms. We can convert the c -vector in equation (8) to a vector whose elements are in fact the V_i by multiplying each equation of (8) by $\frac{16T}{25p} \frac{\partial X_h}{\partial x}$ and then summing over h . After some algebra we find

$$(L) (V_1 \dots V_N, \dots)^T = \left(\frac{16T}{25p} \frac{\partial X_1}{\partial x} \dots \frac{16T}{25p} \frac{\partial X_N}{\partial x}, 0 \dots 0, 0 \dots 0 \right)^T. \quad (9)$$

Equation (9) shows that we can solve directly for the required V_i and that the right hand side is not a function of either h or k .

In solving for the transport in our code, we decompose (L) as the product of an upper matrix multiplying a lower matrix. Equations (7) and (9) can then be solved efficiently by back substitution. It is computationally efficient to do this rather than generate another, smaller matrix for the V_i using a one term approximation and solving this new system. To solve these systems of algebraic equations we have used an assembly language algorithm²⁵ which has been found to execute on the BRL CDC 7600 about five times faster than the equivalent FORTRAN coding.

B. Method II

The above formalism is quite complicated to work with, and so further simplifications are almost invariably made.

For diffusion, we can simplify by taking only one term in the Sonine polynomial expansions. This results in

$$(L^{00,00}) (c_{100}^{1hk} \dots c_{N00}^{1hk})^T = (\delta_{1h} - \delta_{1k}, \dots, \delta_{Nh} - \delta_{Nk})^T \quad h, k = 1 \dots N, \quad (10)$$

where the elements of $(L^{00,00})$ are defined in Appendix C. This can be rearranged⁶ to give the Stefan-Maxwell equations, namely,

$$\frac{\partial X_i}{\partial x} = \sum_{j=1}^N \frac{X_j X_i}{D_{ij}} (V_j - V_i), \quad i=1 \dots N. \quad (11)$$

This set of equations is not independent, and the constraint

$$\sum_{i=1}^N Y_i V_i = 0 \quad (12)$$

must be used in place of one of the equations in (11). Then the diffusion velocities can be found by solving a set of N equations in N unknowns. This approach gives zero for the thermal diffusion velocity, W_i .

²⁵ A. C. Hindmarsh, L. J. Sloan, K. W. Fong, and G. H. Rodrigue, "DEC/SOL: Solution of Dense Systems of Linear Algebraic Equations", Lawrence Livermore Laboratory, UCID-30137, 1976.

Thermal conductivity cannot be simplified this easily. However, ignoring internal energy, we can obtain the matrix form

$$L^{10,10} (a_{110}^1 \dots a_{N10}^1)^T = (X_1, \dots X_N)^T, \quad (13)$$

where $\lambda_o = \lambda_{o, \text{tr}} = -4 \sum_{i=1}^N X_i a_{i10}^1$.²⁶ This form will be valid for a mixture of monatomic gases.

To define the heat conductivity for a mixture of polyatomic gases, we adopt Hirshfelder's* Eucken-type relation,^{27,5}

$$\lambda_{\text{mix}}^{\text{poly}} = \lambda_{\text{mix}}^{\text{mon}} + \sum_{i=1}^N \frac{\lambda_i - \lambda_i^{\text{mon}}}{1 + \sum_{j \neq i} \frac{D_{ij}}{D_{ii}} \frac{X_j}{X_i}}. \quad (14)$$

The quantity λ_o in method I is not exactly identical to the usual thermal conductivity $\lambda_{\text{mix}}^{\text{poly}}$, but can be interpreted as the thermal conductivity of a mixture in which the diffusion forces vanish.

If the thermal diffusion coefficients are zero, as they are at this level of approximation, then $\lambda_o = \lambda_{\text{mix}}^{\text{poly}}$.

C. Method III

By making additional assumptions, the Stefan-Maxwell equations (11) can be further simplified. A common assumption is that all but the i th species move with the same velocity V . Then we find that

*The detailed analysis of Monchick, et al.,⁹ shows that the D_{ij} should be $D_{i, \text{int}, j}$. From a practical point of view we have taken $D_{i, \text{int}, j} = D_{ij}$.

²⁶C. Muckenfuss and C. F. Curtiss, "Thermal Conductivity of Multicomponent Gas Mixtures", *J. Chem. Phys.* 29, 1273-1277 (1958).

²⁷J. O. Hirshfelder, "Heat Conductivity in Polyatomic, Electronically Excited, or Chemical Reacting Mixtures. III", *Sixth International Combustion Symposium*, Reinhold Publishing Corporation, NY, 351-366 (1957).

$$\frac{\partial X_i}{\partial x} = X_i (V - V_i) \sum_{j \neq i} \frac{X_j}{D_{ij}} \quad (15)$$

Employing (12) we find

$$V = - \frac{Y_i V_i}{1 - Y_i} \quad (16)$$

which when substituted into (15) yields the formula recommended by Hirshfelder and Curtiss²⁸

$$V_i = - \frac{(1 - Y_i)}{X_i \sum_{j \neq i} \frac{X_j}{D_{ij}}} \frac{\partial X_i}{\partial x} \quad (17)$$

Unfortunately, the expression in (17) does not in general satisfy equation (12). One technique to satisfy this constraint is due to Boris and Oran.²⁹ They note that if a set of diffusion velocities V_i satisfy the Stefan-Maxwell equations (11), then so does the set $(V_i + V_c)$, where V_c is some constant. The value of V_c is chosen such that the constraint (12) is satisfied.*

The heat conductivity formula employed at this level of approximation is taken from Mason and Saxena's^{30,5} simplification of (14), specifically

²⁸J. O. Hirshfelder and C. F. Curtiss, "Theory of Propagation of Flames Part I: General Equations", Third International Combustion Symposium, Williams and Wilkins Co., Baltimore, 121-127 (1949).

²⁹E. S. Oran and J. P. Boris, "Detailed Modeling of Combustion Systems", to appear in Progress in Energy and Combustion Science.

* Boris and Oran also discuss higher order approximations to the Stefan-Maxwell equations that will not be discussed here.

³⁰E. A. Mason and S. C. Saxena, "Approximate Formula for the Thermal Conductivity of Gas Mixtures", Phys. Fluids, 1, 361-369 (1958).

$$\lambda_o = \frac{\sum_{i=1}^N \lambda_i}{1 + \sum_{j \neq i} \phi_{ij} (X_j/X_i)} \quad (18)$$

where

$$\phi_{ij} = \frac{1.065}{8^{1/2}} \left(1 + \frac{M_i}{M_j}\right)^{-1/2} \left[1 + \left(\frac{\eta_i M_j}{\eta_j M_i}\right)^{1/2} \left(\frac{M_i}{M_j}\right)^{1/4}\right]^2. \quad (19)$$

D. Method IV

Equation (17) or some analogous form has often been used to compute diffusion. However, the usual procedure has been to use (17) only to compute $V_1, \dots, V_{N-1}$. Then V_N is computed from (12). This is less accurate than the Boris and Oran procedure, especially for V_N .

Also, an empirical formula for the thermal conductivity,

$$\lambda_o = 0.5 \left[\sum_{i=1}^N X_i \lambda_i + \left\{ \sum_{i=1}^N X_i / \lambda_i \right\}^{-1} \right], \quad (20)$$

is often used.^{31,5}

Method IV is comprised of these common approximations.

E. Method V

In the case of a binary mixture the Stefan-Maxwell equations (11) reduce to Fick's law. Specifically we have,

$$Y_1 V_1 = -D_{12} \frac{\partial Y_1}{\partial x}. \quad (21)$$

³¹J. H. Burgoyne and F. Weinber, "A Method of Analysis of a Plane Combustion Wave", *Fourth Symposium on Combustion*, Williams and Wilkins Co., Baltimore, 294-302 (1953).

A generalization of (21) can be made,¹ and yields

$$Y_i V_i = -D_{im} \frac{\partial Y_i}{\partial x}, \quad (22)$$

where

$$D_{im} = \frac{1 - X_i}{\sum_{j \neq i} \frac{X_j}{D_{ij}}}. \quad (23)$$

In the Lennard-Jones formalism $D_{ij} \propto T^{1.5}/\Omega^{(1,1)*}$, where $\Omega^{(1,1)*}$ is approximately proportional to $T^{-0.17}$.³² Since $\rho \propto T^{-1}$ it is not unreasonable to assume that $\rho^2 D_{ij}$ is approximately independent of temperature. Generalizing, it is often assumed that $(\rho^2 D_{im})$ is constant. Likewise for a monatomic gas $\lambda \propto T^{0.5}/\Omega^{(2,2)*}$, where $\Omega^{(2,2)*} \propto T^{-0.16}$,³² and it is not unreasonable to assume that $(\rho\lambda)$ is approximately independent of temperature. We now outline a procedure that permits an *a priori* selection of these quantities.

For a given flame we know T_u and Y_{iu} , the temperature and the mass fractions of the unburned mixture. We also have a chemical kinetics scheme and a method of computing the specific heats c_{pi} and specific enthalpies h_i . Since enthalpy is conserved, i.e.,

$$\left(\sum_{i=1}^N Y_i h_i \right)_B = \left(\sum_{i=1}^N Y_i h_i \right)_u, \quad (24)$$

we can compute the adiabatic flame temperature T_B . The numerical procedure is to guess a trial burned temperature T_t and, using an ODE package, find the corresponding equilibrium mass fractions Y_{it} . We then compute the enthalpy of the burned mixture and compare with the unburned mixture enthalpy. T_t is iteratively adjusted until the burned and unburned mixture enthalpies agree to within a pre-determined error tolerance. We then accept these values of T_t and Y_{it} as T_B and Y_{iB} .

³²A. A. Westenberg, "Present Status of Information on Transport Properties Applicable to Combustion Research", *Combustion and Flame*, 1, 346-358 (1957).

At this level of approximation we would like to use an appropriate constant (or "global") c_p . So we will assume that $c_{pi} = c_p = \text{constant}$, $i = 1 \dots N$. Then the relation $h_i = h_i^\circ + \int_{T_o}^T c_{pi} dT$ becomes $h_i = h_i^\circ + c_p (T - T_o)$ and the mixture enthalpy is given by

$$\sum_{i=1}^N Y_i h_i = \sum_{i=1}^N Y_i h_i^\circ + c_p (T - T_o) . \quad (25)$$

Substituting (25) into (24) we find

$$c_p = \frac{\sum_{i=1}^N h_i^\circ (Y_{iu} - Y_{iB})}{T_B - T_u} . \quad (26)$$

As a heuristic rule, we select $T = 0.5 (T_B + T_u)$ and $Y_i = 0.5 (Y_{iB} + Y_{iu})$ and then evaluate D_{im} and $\rho\lambda$ by using equations (23) and (20), respectively. Then $\rho^2 D_{im}$, $i = 1, 2, \dots, N-1$, and $\rho\lambda$ are evaluated. The diffusion velocity V_N is found from equation (12).

Others¹⁹⁻²¹ have employed the concept of constant $\rho^2 D_{im}$, $\rho\lambda$ and c_p , but the method of evaluation varies from author to author.

III. NUMERICAL RESULTS

Table 1 shows a summary of the five methods of computing the transport properties used in this paper. Five H_2 - O_2 - N_2 flames were selected and their initial conditions listed in Table 2. The total pressure is fixed at one atmosphere for all flames. The computed flame speed for each flame as a function of transport method is tabulated in Table 3. (The flame speeds for flame A are not corrected to 291 K, as has been done.¹¹ If this were done, the value AI for example would be 12.2 cm/s instead of 14.1 cm/s.) The values of the flame speeds span a large range and for a given flame are essentially independent of the transport method. The largest difference between Method I, the most complete formulation of the transport, and any other method is 16%. (Compare Methods I and III, flame D). Note that even Method V gives results that are quite close to the much more complex Method I.

TABLE 1. SUMMARY OF TRANSPORT METHODS

<u>Method</u>	<u>Remarks</u>
I	3 terms of Sonine polynomial expansion (3 N by 3 N matrix); only method that has non-zero thermal diffusion.
II	For diffusion, 1 term of Sonine polynomial expansion (N by N matrix), Eq. (11) and (12). For thermal conductivity, Hirshfelder-Eucken method (N by N matrix), Eq. (13) and (14).
III	Diffusion velocities computed from simplified Stefan-Maxwell relation, Eq. (17). Each v_i is adjusted by a common factor, V_c , so as to satisfy $\sum_{i=1}^N Y_i V_i = 0$. Thermal conductivity from Mason and Saxena, Eq. (18) and (19).
IV	Diffusion velocities computed from the simplified Stefan-Maxwell relation, Eq. (17), for N-1 species. V_N is computed from Eq. (12). Empirical thermal conductivity formula, Eq. (20).
V	$\rho^2 D_{im} = \text{constant}$; $\rho\lambda = \text{constant}$; $c_p = \text{constant}$; constants are determined <i>a priori</i> .

TABLE 2. INITIAL TEMPERATURE AND MOLE FRACTIONS FOR THE FIVE FLAMES STUDIED

<u>Flame</u>	<u>X_{H2}</u>	<u>X_{O2}</u>	<u>X_{N2}</u>	<u>T_u</u>
A	.1883	.0460	.7657	336
B	.2000	.1680	.6320	298
C	.5000	.1050	.3950	298
D	.9000	.1000	0	298
E	.6000	.4000	0	298

TABLE 3. FLAME SPEEDS CALCULATED USING
THE FIVE TRANSPORT MODELS

<u>Flame</u>	<u>I</u>	<u>II</u>	<u>III</u>	<u>IV</u>	<u>V</u>
A	14.1	14.6	14.9	14.9	16.0
B	98	101	102	103	96
C	292	300	310	308	291
D	378	379	438	402	348
E	892	922	971	969	847

Reproduction of flame speeds is a necessary but not sufficient condition to judge the relative effectiveness of the transport methods. We must also examine the species and temperature profiles of these flames. As examples we consider two sets of profiles that exhibit differences among the five methods that are as large as any observed. Figures 1 and 2 show the OH profiles for flame D. Figures 3 and 4 show the H₂ profiles for flame C. As can be seen these profiles are very similar. Almost all the other species profiles and all temperature profiles show a greater degree of similarity among the five profiles than the examples given.

In general, our results agree with those reported by Warnatz.¹⁸ The exception is flame A, for which Warnatz reported a flame speed of 10.4 cm/sec, referenced to 291K. Our computed flame speed is about twenty percent higher. Based on our results, we infer that Warnatz's use of a transport method slightly different from any of those reported here should not make that large a difference. We do not know the cause of the discrepancy.

As a check of our code, we computed the flame speed for flame A, using the kinetics and transport parameters of Dixon-Lewis¹² and Method I. The resulting flame speed was 9.2 cm/sec, referenced to 291K. This agrees with the computed result reported by Dixon-Lewis and we conclude that our code is functioning properly.

We are comparing the model results produced as we vary the transport algorithm and not comparing the model result with experiment. Thus, the fact that the use of Warnatz' parameters produces a slightly inaccurate flame speed for flame A is of no concern.

IV. DISCUSSION

The numerical results shown in Table 3 demonstrate that reliable results can be obtained for the H₂-O₂-N₂ system even for the case of our *a priori* determined constant transport method. Note that we cannot infer that transport is unimportant! The computed profiles and flame speeds can be sensitive to the choice of transport parameters selected. For the relative tests of the transport methods here, we have employed the same set of species viscosities, thermal conductivities and binary diffusion coefficients in all cases. We have demonstrated that the method used to generate the multicomponent, polyatomic transport coefficients is not critical for the H₂-O₂-N₂ flame. And since this flame is reasonably complex we infer that this result has a high probability of being valid for other flames.

Indeed, we conclude that gross errors detected in comparing the results of different models are more likely to be traceable to differences in input data rather than to the method of approximating multicomponent polyatomic transport properties.

We cannot completely explain the surprising agreement among the

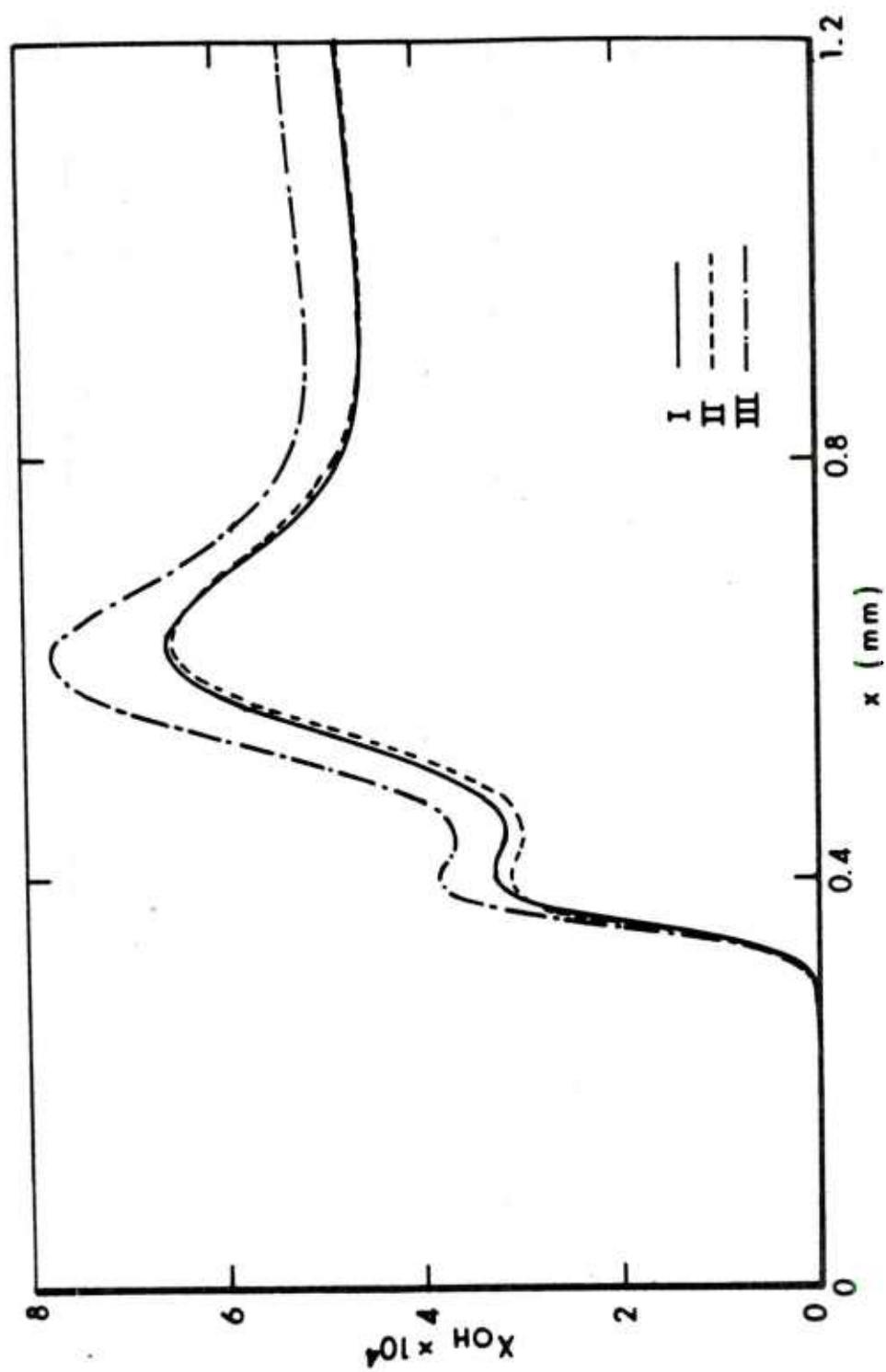


Figure 1. The OH Profile for Flame D.

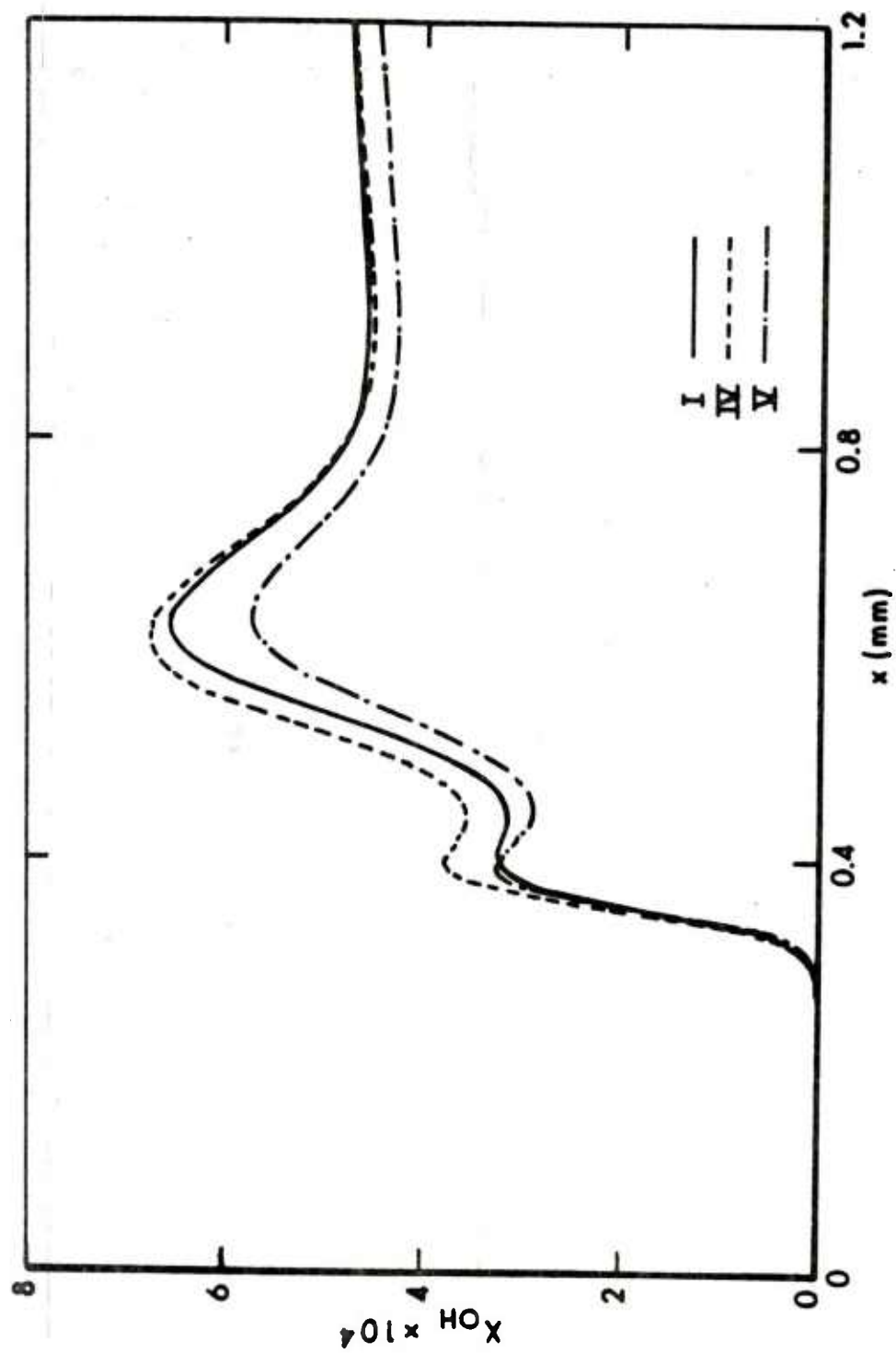


Figure 2. The OH Profile for Flame D.

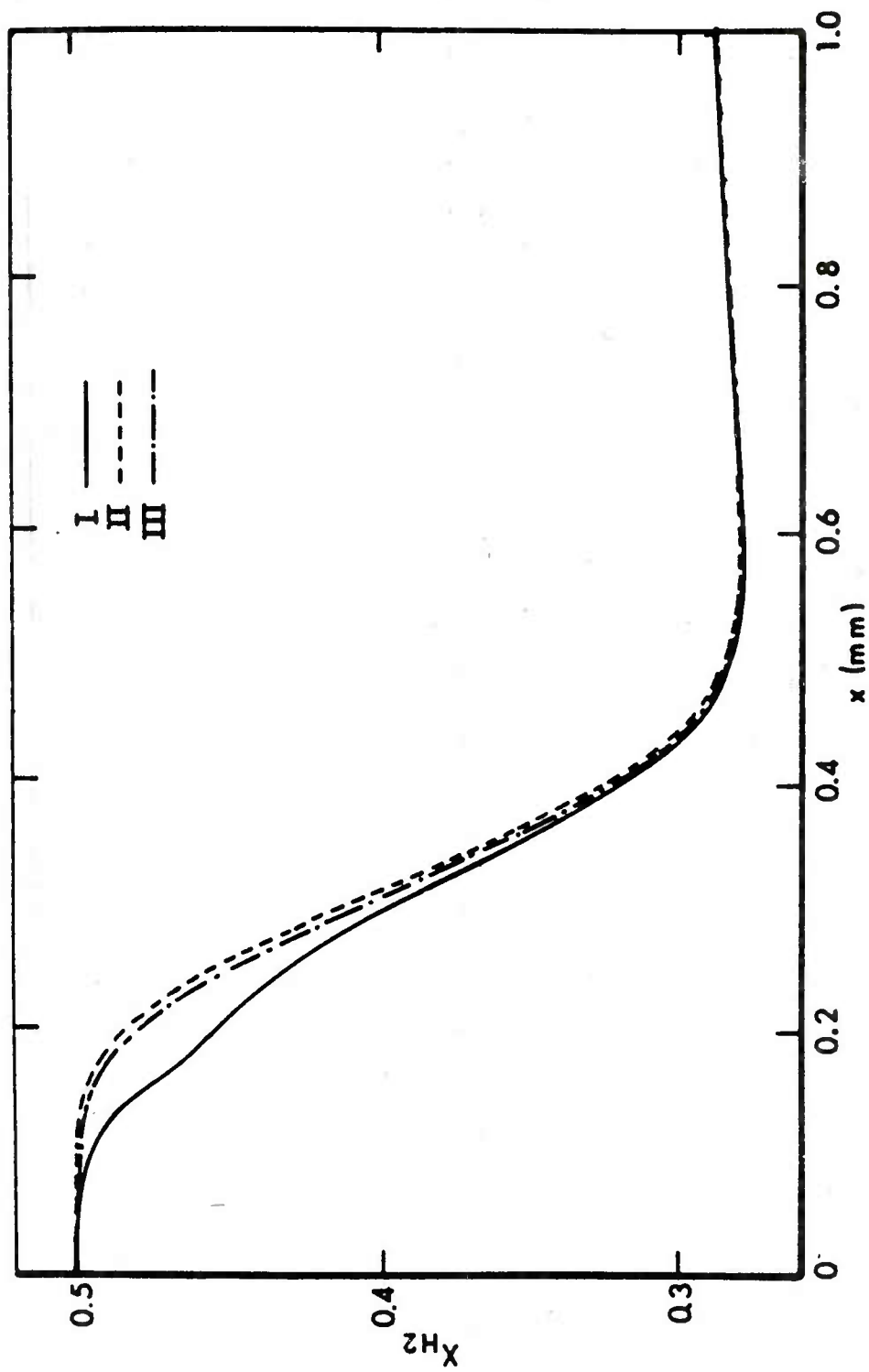


Figure 3. The H_2 Profile for Flame C.

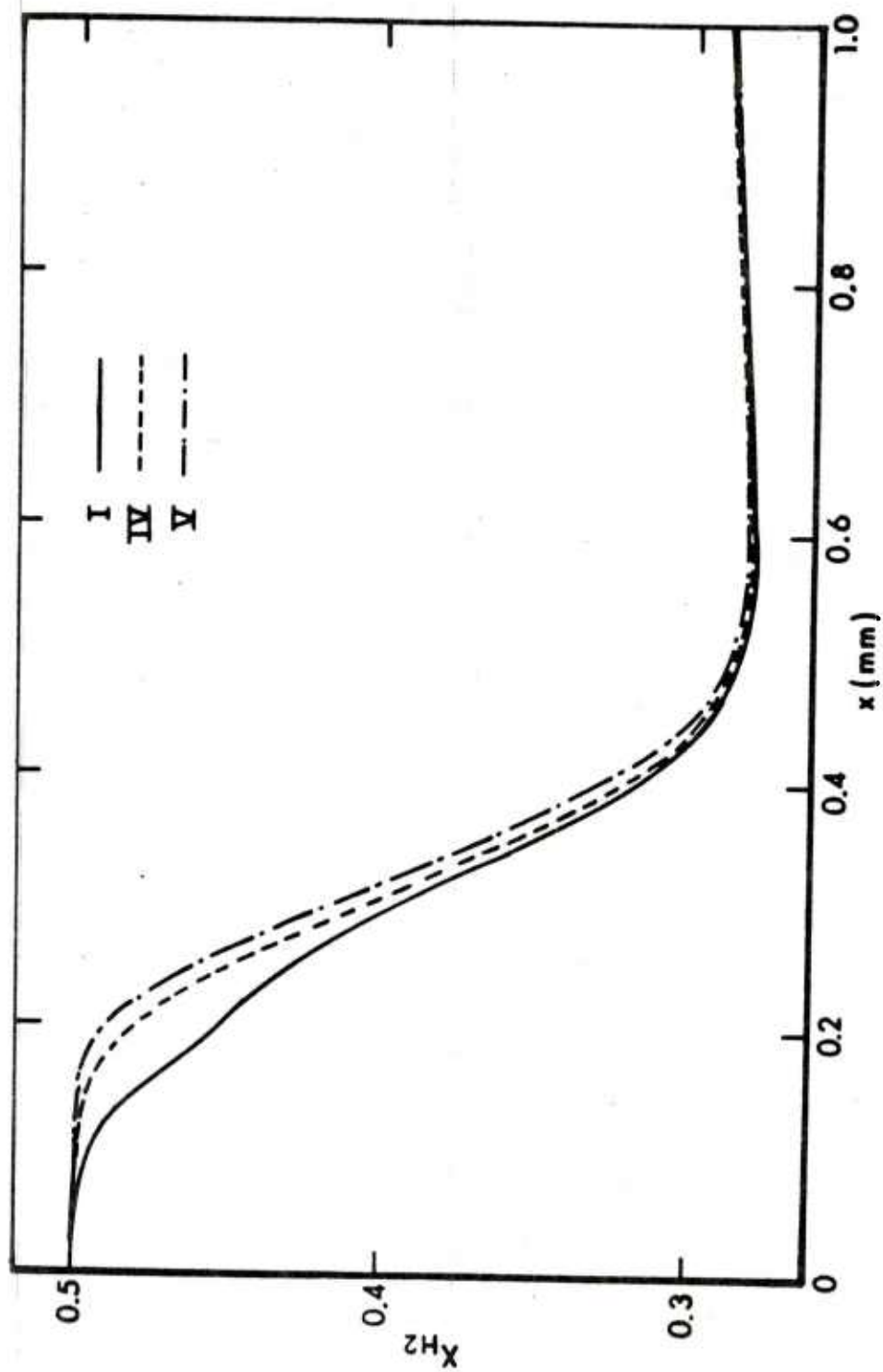


Figure 4. The H_2 Profile for Flame C

various methods. In this section we will show that our results are consistent with the few previous studies of transport algorithms. We will also discuss some additional numerical results that give some indication of the processes involved.

Warnatz¹⁴ essentially compared Methods II and III for an ozone flame and found the differences negligible. However, it was not clear that his observations could be generalized to more complex flames.

In another paper¹⁸ Warnatz included thermal diffusion in a simulation of an H_2 - O_2 - N_2 flame. He used essentially Method IV together with a simple binary formula for thermal diffusion valid only for heavy isotopes.⁶ He found that the effect of thermal diffusion so defined was to lower the flame speed in a rich flame by about 5%. Species and temperature profiles were only slightly changed. He did not discuss the accuracy of this approximation for a mixture.

As noted earlier, Dixon-Lewis²⁴ considered the effect of thermal diffusion. However, he assumed a particular mass flow and simplified chemistry. He found that the thermal diffusion flux of H_2 was quite large and inferred that effects due to thermal diffusion would be important when considering hydrogen atom diffusion in flame systems. This inference is contrary to our findings. Our results also show that, for H and H_2 , the thermal diffusion velocity W_i can be quite large compared to the species diffusion velocity V_i . However, we find that these differences cause only small changes in both the flame speeds and the profiles. This finding supports that of Dixon-Lewis¹² who in a recent paper reported that the inclusion of thermal diffusion for near stoichiometric H_2 -air flames lowers the burning velocity by 5 to 6%.

In an attempt to gain additional insight, we have written an auxiliary code to directly compare the transport properties. The input required for this code are the values of the temperature, the species concentrations, and the temperature and species gradients. Then the thermal conductivity λ_0 and the diffusion velocities V_i are computed using the subroutines written for Methods I through IV, and comparisons among the values for λ_0 and V_i are made. By doing this we avoid the complicated interplay between transport and chemistry that occurs in flames.

The auxiliary code was executed using several hundred sets of input values that were typical of those observed in the flames reported above. These input values were divided into four groups for analysis. Group 1 consisted of small species and temperature gradients, Group 2 of large species and temperature gradients, Group 3 of large species gradients and a zero temperature gradient, and Group 4 of small species gradients and large temperature gradients. By a large gradient we mean a value typical of a flame front.

The values of thermal conductivity computed with the auxiliary code showed little variation, regardless of the input group or approximation

method used. Specifically, the differences between Methods I and II, I and III, and I and IV averaged 2, 3 and 5%, respectively. In general, the thermal conductivities of the individual species are not this well known either theoretically or experimentally. So despite the widely different levels of complexity, the four methods produced equivalent values for λ_0 .

The results of the comparisons for diffusion velocities are more difficult to summarize. Differences varied from less than 1% up to several hundred percent, depending on the particular input values and the particular species considered. Differences of 30 to 40% were common and in general were larger for the major species than for the minor species.

We could not establish why there was a high degree of similarity in the flame speeds and profiles even though these were large differences in the V_i in the auxiliary code. We speculate that part of the reason for this is due to the constraint $\sum_{i=1}^N Y_i V_i = 0$, which is satisfied by all of our methods. Another constraint on the diffusion velocities in the flame code is the fixed chemistry employed. How the non-linear feedback between the chemistry and the transport affects the similarity in the flame speeds and profiles is unknown.

Nevertheless, some interesting conclusions can be drawn from these comparisons. For instance, it is often assumed that thermal diffusion is negligible. This assumption corresponds to that made in Group 3. (If the temperature gradient is zero, the thermal diffusion velocities w_i will also be zero).

For this group, we find that the values of the diffusion velocities computed by Methods I and II agree to about 1%. In contrast, the values of the diffusion velocities computed by Methods III and IV differ from those computed by Method I by much more (typical differences are around 40%). This comparison implies that Method II (i.e., the Stefan-Maxwell equations) is much more accurate in determining the values for the diffusion velocities than the non-matrix methods. Note that this conclusion is valid only for the case of zero temperature gradient.

For the other three groups of input to our auxiliary code, we find that the diffusion velocities computed by Method III are usually in better agreement with those computed by Method I than those computed by Method II! This situation can occur because in Method III the errors in ignoring thermal diffusion and in approximating the molecular diffusion velocities are generally of opposite sign. We conclude that it is a waste of effort to use a matrix method (such as the Stefan-Maxwell equations) to compute diffusion velocities unless thermal diffusion is also considered.

Method III is generally more accurate than Method IV. Method IV can be extremely inaccurate in computing the diffusion velocity for the

Nth species. In the cases considered we have found that the values computed by Method IV for N_2 differ, on the average, more than 100% from the values found by Method I. This is due to the procedure used to obtain the diffusion velocity for the Nth species. This procedure tends to associate cumulative errors caused by neglect of the constraint, Eq. (12), with the Nth species, here N_2 . We have found that Method III (the Boris and Oran procedure) is at least as accurate and in some cases substantially more accurate than the traditional Method IV for computing the V_i . Furthermore the Boris and Oran procedure involves very little additional computational effort.

V. A NEW TRANSPORT METHOD

For flames more complicated than H_2 - O_2 - N_2 we require a transport algorithm that is computationally efficient and relatively precise. The most exact procedure considered, Method I, can become prohibitively expensive for a large number of species. Method V is computationally efficient, but we feel caution is necessary in using such a simplified model. There does not seem to be a great deal to choose from among Methods II, III, and IV and so we have assembled a new method, Method VI.

As with Methods II-V we require expressions for λ_0 and for the $V_i (= V_i + W_i)$. For the thermal conductivity we use the simplest formula (20), since the exact choice does not appear to be important. For the molecular diffusion velocities V_i we use the expression in equation (17).

For problems with light species and steep temperature gradients, the neglect of thermal diffusion is often as important as the differences between the computational methods. So below we generate a technique that approximates the thermal diffusion contribution to the diffusion velocity, W_i . We shall first derive an expression for W_i of a binary mixture and then generalize the results.

For a binary mixture equation (2a) can be written

$$V_1 = - \frac{(1-Y_1)}{X_1 X_2} D_{12} \frac{\partial X_1}{\partial x} - \frac{D_1^T}{\rho Y_1} \frac{\partial \ln T}{\partial x} \quad (27)$$

from which we identify

$$W_1 = - \frac{D_1^T}{\rho Y_1} \frac{\partial \ln T}{\partial x} \quad (28)$$

Since, from Eq. (17),

$$v_1 = - \frac{(1-Y_1)}{X_1 X_2} D_{12} \frac{\partial X_1}{\partial x} \quad (29)$$

and since the thermal diffusion ratio is defined by reference 6

$$k_{12} = \frac{X_1 X_2}{\rho Y_1 Y_2} \frac{D_1^T}{D_{12}} \quad (30)$$

we can write, after some algebra,

$$w_1 = k_{12} v_1 \frac{\partial}{\partial x} (\ln T) / \frac{\partial X_1}{\partial x} \quad (31)$$

Theoretical expressions for k_{12} have been derived and even in the first approximation the expressions are quite complicated.⁶ For the special case of heavy isotopes, however, the first approximation simplifies to⁶

$$k_{12} = \frac{15(2A^* + 5)(6C^* - 5)(M_1 - M_2)}{2A^*(16A^* - 12B^* + 55)(M_1 + M_2)} X_1 X_2 \quad (32)$$

Fortunately Eq. (32) reproduces H₂-N₂ thermal diffusion ratios to within 30%, and so we use it as a simple but reasonable approximation for k_{12} . Equation (31) can now be evaluated (in the code).

Generalizing Eq. (31) we define

$$w_i = k_{im} v_i \frac{\partial}{\partial x} (\ln T) / \frac{\partial X_i}{\partial x} \quad (33)$$

If an expression for k_{im} can be obtained, then w_i of Eq. (33) can be evaluated. Chapman and Cowling³³ have derived an approximation for k_{im} ,

³³S. Chapman and T.G. Cowling, The Mathematical Theory of Non-Uniform Gases, Third Edition, Cambridge University Press (1970).

specifically

$$k_{im} = \sum_{\substack{j=1 \\ i \neq j}}^N k_{ij} \quad (34)$$

where k_{ij} is given by an expression analogous to Eq. (32).

From Eq. (32) we can see that the influence of ω_i will be the greater the larger the mass differences. Normally the thermal diffusion ratio does not exceed 0.1 and for the H_2 - O_2 - N_2 system, we have computed ω_i only for the species H and H_2 . The resulting diffusion velocities $V_i = V_i + \omega_i$ do not satisfy the constraint $\sum_{i=1}^N Y_i V_i = 0$. We use the Boris and Oran procedure discussed in Section II to obtain this condition.

Computationally, the quantity $15(2A^* + 5)/(2A^*(16A^* - 12B^* + 55))$ can be fitted very accurately by a function of the form: $a \exp(c/T^*)$. The quantity $(6C^* - 5)$ varies over the range zero to one and could not be fitted accurately by a simple expression. The fit for C^* given in Appendix D is used instead.

This new method for approximating multispecies transport has been exercised in our test flames. Table 4 compares the flame speeds for Methods I and VI. The results are so close that we infer that some of the errors made in the approximations involved in Method VI are cancelling.

Figure 5 compares the OH profiles for flame D and figure 6 compares the H_2 profiles for flame C. In general, for the minor species, the accuracy of Method VI is comparable to Methods II or III. However, in almost every profile involving a major species, the accuracy was improved.

VI. ADDENDUM

A few additional comparisons have recently been made. In the spirit of approximation exemplified in the discussion of Method V, the further assumption is sometimes made that all the Lewis numbers ($Le_i = \lambda/c_p \rho D_{im}$) are equal to unity. Given values for $\rho\lambda$ and c_p , this assumption defines the diffusion coefficients and removes the requirement of supplying independent information for them. We tested how well this additional level of simplification fared by applying it in the code using flame C. The computed flame speed was about 40% lower than for Method I. While the major species profiles were still reasonably close to those of Method I, they were noticeably less accurate than Method V. The minor species profiles showed large differences: the peak concentrations of O, HO_2 , and H_2O_2 were lower than those of Method I by about a factor of two.

In an effort to substantiate our earlier inference concerning the transfer of these results to other (hydrocarbon) flames we performed some checks on the stoichiometric methane-air flame. For this flame we used the input parameters listed by Tsatsaronis,¹³ the kinetics scheme was used as listed, and we made no attempt to critically evaluate it. The flame speeds computed for Methods I, V, and VI are in the ratio 1.00 to 0.88 to 0.94, respectively. The profiles for Method VI are more accurate than those produced by Method V. These results follow the same trend as in the $H_2-O_2-N_2$ flames reported above.

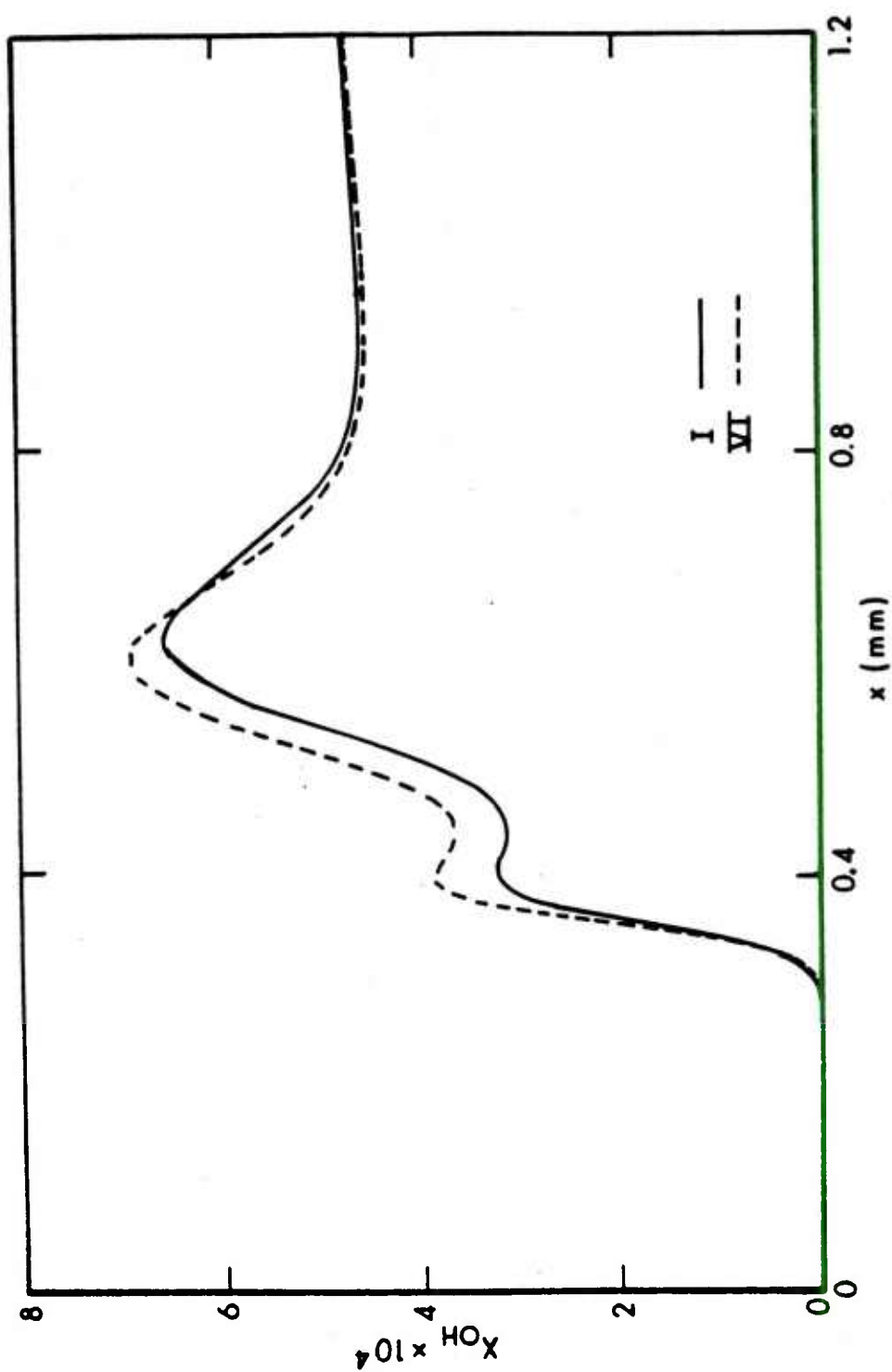


Figure 5. The OH Profile for Flame D.

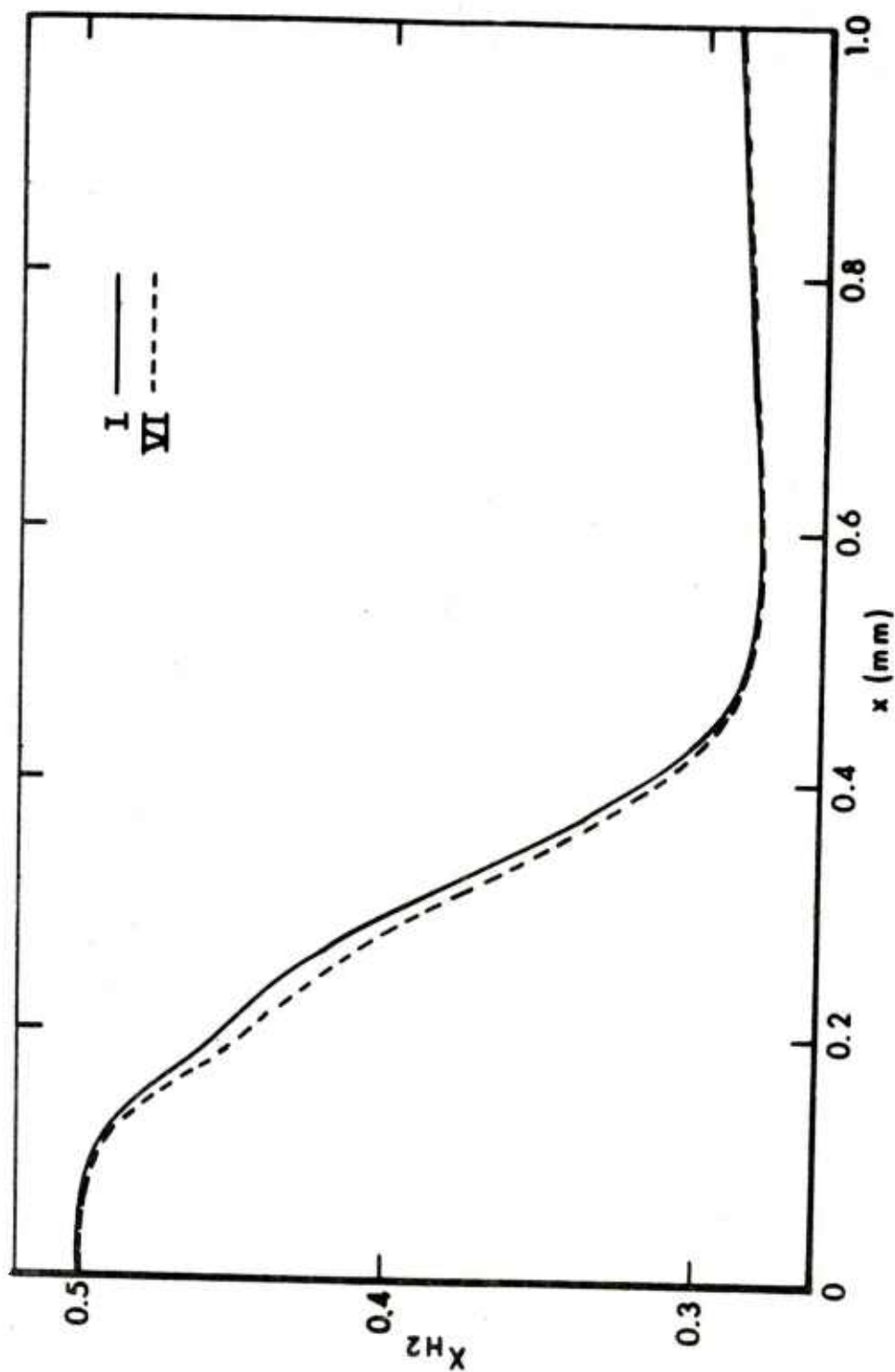


Figure 6. The H₂ Profile for Flame C.

TABLE 4. FLAME SPEEDS CALCULATED USING TWO TRANSPORT MODELS

<u>Flame</u>	<u>I</u>	<u>VI</u>
A	14.1	14.0
B	98	97
C	292	292
D	378	402
E	892	894

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APPENDIX A. THE FLAME EQUATIONS

We are interested in the equations that describe a one-dimensional, laminar, premixed flame that propagates in an unbounded ideal gas. The effects of radiation, viscosity, and body forces are ignored. Since the burning velocity is small compared with the local speed of sound, the pressure is taken to be constant. The resulting equations (see for example reference 2 of text) are:

Overall Continuity:

$$\rho \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \quad . \quad (A-1)$$

Continuity of Species:

$$\rho \frac{\partial Y_i}{\partial t} + \rho u \frac{\partial Y_i}{\partial x} = - \frac{\partial}{\partial x} (\rho Y_i V_i) + R_i M_i, \quad i = 1, \dots, N \quad . \quad (A-2)$$

and Conservation of Energy:

$$\rho c_p \frac{\partial T}{\partial t} + \rho u c_p \frac{\partial T}{\partial x} = - \frac{\partial q}{\partial x} + \sum_{i=1}^N h_i \left[\frac{\partial (\rho Y_i V_i)}{\partial x} - R_i M_i \right] \quad . \quad (A-3)$$

The boundary conditions are the following ($t \geq 0$). For $x = -\infty$;

$$T = T_u \quad \text{and} \quad Y_i = Y_{iu} \quad (i=1, \dots, N) \quad , \quad (A-4)$$

and for $x = \infty$;

$$\frac{\partial T}{\partial x} = \frac{\partial Y_i}{\partial x} = 0 \quad (i=1, \dots, N) \quad . \quad (A-5)$$

The transport properties that we are interested in are the diffusion velocities V_i and the heat flux q .

APPENDIX B. $\text{H}_2\text{-O}_2\text{-N}_2$ INPUT PARAMETERS

The required input data for the $\text{H}_2\text{-O}_2\text{-N}_2$ flames are for the most part taken from Warnatz (see reference 18 of text).

The kinetic scheme consists of thirty reactions and has been taken in toto from Warnatz' Table 3, which for the most part was taken from the Leeds review.¹ Our interest here is a study of the effects of using different transport algorithms, and not a critical evaluation of the kinetics. So we have uncritically used Warnatz' mechanism. This mechanism is in reasonable agreement with experimental data.

The enthalpies and heat capacities are evaluated using the sixth order polynomial fits of Gordon and McBride (see reference 4 of text). These reproduce the JANNAF (see reference 3 of text) values to within a few parts per thousand over the temperature range 300K-3000K.

The transport parameters are given in Table B-2. These are from Warnatz except for ξ_{ii}^∞ for OH, which is from Dixon-Lewis (see reference 12 of text). The values for σ and ϵ/k are obtained from viscosity measurements.

The manipulation of these parameters is discussed in Appendix D.

^{B1}D. L. Baulch, D. D. Drysdale, D. G. Horne, and A. C. Lloyd, Evaluated Kinetic Data for High Temperature Reactions, Vol. 1, Butterworths, London 1972.

TABLE B-1. REACTIONS IN THE $H_2-O_2-N_2$ SYSTEM

NO	REACTION	A*	B	C
1	$OH + H_2 \rightarrow H_2O + H$	$2.2E13^{**}$	0	- 2590
2	$H + H_2O \rightarrow OH + H_2$	$9.3E13$	0	-10250
3	$H + O_2 \rightarrow OH + O$	$2.2E14$	0	- 8450
4	$O + OH \rightarrow H + O_2$	$1.0E13$	0	0
5	$O + H_2 \rightarrow OH + H$	$1.8E10$	1	- 4480
6	$H + OH \rightarrow O + H_2$	$8.3E09$	1	- 3500
7	$OH + OH \rightarrow H_2O + O$	$6.3E12$	0	- 550
8	$O + H_2O \rightarrow OH + OH$	$6.8E13$	0	- 9240
9	$H + H + M' \rightarrow H_2 + M'$	$9.0E17$	-1	0
10	$H + OH + M' \rightarrow H_2O + M'$	$2.2E22$	-2	0
11	$H + O_2 + M' \rightarrow HO_2 + M'$	$5.0E15$	0	500
12	$H + HO_2 \rightarrow OH + OH$	$2.5E14$	0	- 950
13	$H + HO_2 \rightarrow H_2 + O_2$	$2.5E13$	0	- 350
14	$H + HO_2 \rightarrow H_2O + O$	$1.5E13$	0	- 500
15	$OH + HO_2 \rightarrow H_2O + O_2$	$5.0E13$	0	- 500
16	$O + HO_2 \rightarrow OH + O_2$	$5.0E12$	0	- 500
17	$OH + OH + M \rightarrow H_2O_2 + M$	$9.1E14$	0	2550
18	$H + H_2O_2 \rightarrow H_2O + OH$	$3.2E14$	0	- 4500
19	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$8.5E12$	0	- 500
20	$H_2 + M' \rightarrow H + H + M'$	$8.8E14$	0	-48300
21	$O + O + M \rightarrow O_2 + M$	$7.0E13$	0	900
22	$HO_2 + M' \rightarrow H + O_2 + M'$	$7.0E15$	0	-23000
23	$OH + OH \rightarrow HO_2 + H$	$1.2E13$	0	-20200

TABLE B-1. REACTIONS IN THE $H_2-O_2-N_2$ SYSTEM (Cont'd)

<u>NO</u>	<u>REACTION</u>	<u>A*</u>	<u>B</u>	<u>C</u>
24	$HO_2 + H_2 \rightarrow H_2O_2 + H$	7.3E11	0	- 9400
25	$H + H_2O_2 \rightarrow H_2 + HO_2$	1.7E12	0	- 1900
26	$H_2O_2 + M \rightarrow OH + OH + M$	1.2E17	0	-22900
27	$O + H_2O_2 \rightarrow OH + HO_2$	2.8E13	0	- 3200
28	$O + H_2O_2 \rightarrow H_2O + O_2$	2.8E13	0	- 3200
29	$OH + H_2O_2 \rightarrow H_2O + HO_2$	1.0E13	0	- 910
30	$HO_2 + H_2O \rightarrow H_2O_2 + OH$	2.8E13	0	-16500

[M] = total concentration

[M'] = 6.0 $[H_2O]$ + 1.0 $[H_2]$ + 0.4 $[O_2]$ + 0.4 $[N_2]$

* A is in units of $cm^3/mole\text{-}sec$ or $cm^6/mole^2\text{-}sec$, $k = AT^B \exp (C/T)$.

** $2.2E13 = 2.2 \times 10^{13}$.

TABLE B-2. MOLECULAR PARAMETERS USED FOR
THE DETERMINATION OF TRANSPORT PROPERTIES

<u>Species</u>	$\sigma [\text{\AA}]$	$\frac{\epsilon}{k} [\text{K}]$	$\mu [\text{Debye}]$	$\alpha [\text{\AA}^3]$	ξ_{ii}^∞
O	2.75	80	0	0	
O ₂	3.46	107	0	1.60	14.4
H	2.05	145	0	0	
H ₂	2.92	38	0	0.79	280
OH	2.75	80	0	0	4.5
H ₂ O	2.60	572	1.844	0	4.0
N ₂	3.62	97.5	0	0	15.7

HO₂, H₂O₂ like O₂

APPENDIX C. DEFINITION OF THE MATRIX L

The matrix L can be partitioned into nine N by N matrices

$$L = \begin{pmatrix} L^{00,00} & L^{00,10} & L^{00,01} \\ L^{10,00} & L^{10,10} & L^{10,01} \\ L^{01,00} & L^{01,10} & L^{01,01} \end{pmatrix} \quad (C-1)$$

where

$$L_{ii}^{00,00} = 0, \quad (C-2)$$

$$L_{ij}^{00,00} = \frac{16}{25} \frac{T}{P} \left[\frac{X_i X_j}{D_{ij}} + \sum_{k \neq i} \frac{M_j}{M_i} \frac{X_k X_j}{D_{ik}} \right], \quad i \neq j, \quad (C-3)$$

$$L_{ij}^{00,10} = - \frac{8T}{5P} \frac{M_j (1.2 C_{ij}^* - 1) X_i X_j}{(M_i + M_j) D_{ij}}, \quad i \neq j, \quad (C-4)$$

$$L_{ii}^{00,10} = - \sum_{j \neq i} L_{ji}^{00,10}, \quad (C-5)$$

$$L_{ij}^{10,00} = L_{ji}^{00,10}, \quad (C-6)$$

$$L_{ij}^{01,00} = L_{ij}^{00,01} = 0 \quad (C-7)$$

$$L_{ii}^{10,10} = - \frac{16}{15} \frac{M_i}{R} \frac{X_i^2}{\eta_i} \left(1 + \frac{10}{3\pi} \frac{C_{i, \text{rot}}}{R \xi_{ii}} \right) - \frac{16T}{25P} \sum_{k \neq i} \left\{ \frac{X_i X_k}{(M_i + M_k)^2 D_{ik}} \times \right.$$

$$\left[\frac{15}{2} M_i^2 + \frac{25}{4} M_k^2 - 3 M_k^2 B_{ik}^* + 4 M_i M_k A_{ik}^* \left(1 + \frac{5}{3\pi} \left\{ \frac{C_{i, \text{rot}}}{R \xi_{ik}} + \frac{C_{k, \text{rot}}}{R \xi_{ik}} \right\} \right) \right] \left. \right\}, \quad (C-8)$$

$$L_{ij}^{10,10} = \frac{16T}{25P} \frac{M_i M_j X_i X_j}{(M_i + M_j)^2 D_{ij}}$$

$$\left\{ \frac{55}{4} - 3 B_{ij}^* - 4 A_{ij}^* \left[1 + \frac{5}{3\pi} \left(\frac{C_{i, \text{rot}}}{R \xi_{ij}} + \frac{C_{j, \text{rot}}}{R \xi_{ji}} \right) \right] \right\}, \quad i \neq j \quad (C-9)$$

$$L_{ii}^{10,01} = \frac{16M_i X_i^2 C_{i, \text{rot}}}{3\pi R \eta_i C_{i, \text{int}} \xi_{ii}}$$

$$+ \frac{32 T}{5\pi p C_{i, \text{int}}} \sum_{k=i} \frac{M_i A_{ik}^* X_i X_k C_{i, \text{rot}}}{(M_i + M_k) D_{ik} \xi_{ik}}, \quad (C-10)$$

$$L_{ij}^{10,01} = \frac{32 T M_j A_{ij}^* X_i X_j C_{j, \text{rot}}}{5 p \pi C_{j, \text{int}} (M_i + M_j) D_{ji} \xi_{ji}} \quad (C-11)$$

$$L_{ij}^{01,10} = L_{ji}^{10,01}, \quad (C-12)$$

$$L_{ij}^{01,10} = 0, \quad i \neq j \quad (C-13)$$

and

$$L_{ii}^{01,01} = - \frac{8M_i X_i^2 C_{i, \text{rot}}}{\pi \eta_i \xi_{ii} C_{i, \text{int}}^2}$$

$$- \frac{4RT}{p C_{i, \text{int}}} \left\{ \sum_k \frac{X_i X_k}{D_{i, \text{int}, k}} \right.$$

$$\left. + \sum_{k \neq i} \frac{12 M_i A_{ik}^* X_i X_k C_{i, \text{rot}}}{5\pi M_k D_{ik} C_{i, \text{int}} \xi_{ik}} \right\}. \quad (C-14)$$

When solving equations (7) and (6) for the thermal conductivity, λ_0 will turn out to have the units $\text{cm}^2\text{-atm-s}^{-1}\text{-K}^{-1}$. To convert to the more usual units of $\text{cal-cm}^{-1}\text{-s}^{-1}\text{-K}^{-1}$, we multiply by $R/R_a = 1.9872/82.05$.

APPENDIX D. MANIPULATION OF TRANSPORT DATA

The quantities required to compute the elements of the matrix L used in Method I can be calculated from the transport parameters (Table B-2) and the heat capacities (see reference 4 of text). We shall discuss the procedures in this appendix.

The viscosity η_i and the binary diffusion coefficients D_{ij} can be obtained from Lennard-Jones (non-polar) or Stockmayer (polar) parameters σ_k and ϵ_k/k . For polar molecules (here only H_2O) we also need the dipole moment μ_i . For the binary diffusion coefficient of a polar and a non-polar species, we also need the polarizability α_i of the non-polar species. Then η_i and D_{ij} are calculated using tabulated values of the collision integrals^{1,2} (see also reference 6 of text).

The quantities A^*_{ij} , B^*_{ij} , and C^*_{ij} do not have exactly their standard meanings (see reference 9 of text). However, they can be closely approximated by the usual quotients of collision integrals. For Lennard-Jones parameters, these are tabulated in reference 6 of text. For simplicity, we will assume that at most one of the species is polar (in our case H_2O). Since a polar molecule interacting with a non-polar molecule can be represented by a Lennard-Jones potential, all the quantities A^*_{ij} , B^*_{ij} , and C^*_{ij} can be cast into the Lennard-Jones formalism. They are functions only of $T^*_{ij} = T/(\epsilon_{ij}/k)$, where ϵ_{ij} is obtained from ϵ_i and ϵ_j by standard combining rules¹ (see also reference 6 of text).

The collision numbers ξ_{ij} for rotational relaxation of species i on colliding with species j are difficult to obtain, particularly if $i \neq j$. Fortunately, these values are not critical. For simplicity, we will assume that $\xi_{ij} = \xi_{ii}$. Parker³ has calculated values for ξ_{ii} for homonuclear diatomic molecules, as well as the temperature relation

$$\xi_{ii} = \xi_{ii}^{\infty} \left[1 + \frac{\pi^{3/2}}{2(T_i^*)^{1/2}} + \left(\frac{\pi^2}{4} + \pi \right) \frac{1}{T_i^*} \right]^{-1} \quad (D-1)$$

We use his values for O_2 and N_2 . For other types of molecules, we must look for experimental values. In this paper, we take these other ξ_{ii} 's to be constant. The values for ξ_{ii} are taken from Warnatz (see reference 14 of text) except the value of ξ_{ii} for OH (see reference 12 of text).

^{D1} R. C. Reid and T. K. Sherwood, *The Properties of Gases and Liquids*, 2nd Edition, McGraw-Hill, NY, (1966).

^{D2} L. Monchick and E. A. Mason, "Transport Properties of Polar Gases", *J. Chem. Phys.*, 33, 1676-1697 (1961).

The quantities $\mathcal{D}_{i,int,j}$ refer to the diffusion of internal energy, which is approximated by $\mathcal{D}_{ij}$. More accurate values are very difficult to calculate, and there is no known way of determining them experimentally (see reference 9 of text).

To obtain the $C_{i,rot}$ and $C_{i,int}$, we need to properly partition $C_{i,v}$, the heat capacity at constant volume. $C_{i,v}$ can be calculated from the Gordon and McBride polynomial fits (see reference 4 of text). It can be partitioned as

$$C_{i,v} = C_{i,tr} + C_{i,int}, \quad (D-2)$$

where $C_{i,tr} = 1.5 R$. The internal energy can be further partitioned into rotational and vibrational energy. $C_{i,rot} = 0$ for a monatomic molecule, $C_{i,rot} = R$ for a linear molecule, and $C_{i,rot} = 1.5 R$ for a polyatomic molecule.

For Method I, we do not need to directly compute the separate species thermal conductivities λ_i . These values are required for the other methods, so we will discuss them here.

For monatomic gases,

$$\lambda_i^{mon} = \frac{15}{4} \frac{R}{M_i} \eta_i, \quad (D-3)$$

where a hard sphere model has been assumed¹ (see also reference 6 of text).

For polyatomic gases, there are many procedures. We will follow the analysis of Mason and Monchick,^{1,4} and write

$$\frac{\lambda_i M_i}{\eta_i} = f_{tr} C_{i,tr} + f_{int} C_{i,int} \quad (D-4)$$

where

^{D3} J. G. Parker, "Rotational and Vibrational Relaxation in Diatomic Gases", *Phys. Fluids*, 2, 449-462 (1959).

^{D4} E. A. Mason and L. Monchick, "Heat Conductivity of Polyatomic and Polar Gases", *J. Chem. Phys.*, 36, 1622-1639 (1962).

$$f_{tr} = \frac{5}{2} \left[1 - \frac{10}{3\pi} \left(1 - \frac{2}{5} \frac{M_i \rho \mathcal{D}_{i,int,i}}{\eta_i} \right) \left(\frac{C_{i,rot}}{R \xi_{ii}(rot)} + \frac{C_{i,vib}}{R \xi_{ii}(vib)} \right) \right], \quad (D-5)$$

$$f_{int} = \frac{M_i \rho \mathcal{D}_{i,int,i}}{\eta_i} \left[1 + \frac{5}{\pi} \left(1 - \frac{2}{5} \frac{M_i \rho \mathcal{D}_{i,int,i}}{\eta_i} \right) \left(\frac{C_{i,rot}}{C_{i,int} \xi_{ii}(rot)} + \frac{C_{i,vib}}{C_{i,int} \xi_{ii}(vib)} \right) \right]. \quad (D-6)$$

Normally, $\xi_{ii}(vib) \gg \xi_{ii}(rot)$, so we will ignore the vibrational term. We then refer to $\xi_{ii}(rot)$ just as ξ_{ii} . As usual, we approximate $\mathcal{D}_{i,int,i}$ by the self diffusion coefficient $\mathcal{D}_{ii}$.

Using either Lennard-Jones or Stockmayer collision integrals,

$$\frac{M_i \rho \mathcal{D}_{ii}}{\eta_i} = 1.1999 A^* \approx 1.32. \quad (D-7)$$

Equation (D-4) then simplifies to

$$\frac{\lambda_i M_i}{\eta_i} = 1.32 C_{i,v} + 1.77R - .886 \frac{C_{i,rot}}{\xi_{ii}}. \quad (D-8)$$

As before, the exact value of ξ_{ii} is not critical in the computation.

For actual use in the code, a fit to the η_i , λ_i , and $\mathcal{D}_{ij}$ is made of the form aT^b over an appropriate temperature range, using the logarithmic method with proper transformation of weights.⁵ The resulting fits are accurate within two percent.

^{D5} R. J. Cvetanovic and D. L. Singleton, *Internat. J. Chem. Kinet.*, 9, 481-488, 1977; R. J. Cvetanovic and D. L. Singleton, *Internat. J. Chem. Kinet.*, 1007-1009, 1977.

The quantities A^* , B^* , and C^* are fit over a range $1.0 \leq T^* \leq 400$. This covers the range likely to occur in a flame. If the fit is extended to values of $T^* < 1$, the accuracy suffers. A^* can be fit very accurately by a function of the form: $a(T^*)^b$. To fit B^* and C^* accurately, we need to use the functional form: $a \exp(c/T^*)$ (see Table D-1).

Given the above information, we have developed software to write the actual transport subroutine used in the code.

TABLE D-1. FITS TO THE FUNCTIONS A^* , B^* , C^*
($a(T^*)^b$ or $a \exp(c/T^*)$)

Function	a	b	c
A^*	1.0885	9.0557E-3	0
B^*	1.0786	0	8.5001E-2
C^*	.95426	0	- .14357

APPENDIX E. PROGRAM LISTINGS

We have included here the FORTRAN programs for writing the transport subroutines, as well as examples of the subroutines themselves. Some of these routines are very long for the H_2 - O_2 - N_2 system (over 3500 lines for Method I). So as an example we have considered a binary mixture of H_2 and N_2 . This shows the main features of the programs while conserving space.

A copy of the actual flame code used is given in reference 23 of the text. Method V (constant transport) is included in this code as the default. The appropriate constant transport values for a given flame must be read in, but the subroutine itself is not rewritten.

For our other transport methods, the subroutine is written specifically for a given set of chemical species. The procedure is straightforward. We attach to TAPE15 the coefficients for computing the thermodynamic quantities. We attach to TAPE9 the least squares fits for the viscosities, thermal conductivities, and binary diffusion coefficients. There are computed in another program using the methods discussed in this article. The program also requires the appropriate Lennard-Jones (Stockmayer) parameters, the pressure, and for some methods the least squares fits for A^* , B^* , and C^* . The flame code actually works with non-dimensional forms of the flame equations, so appropriate normalization terms for the space coordinate, time coordinate, and temperature must also be supplied.

The transport statements are written onto TAPE3. This tape is read and attached to a standard set of initial statements. The corresponding FORTRAN subroutine F can then be attached to the flame code.

Given the mass fractions, the non-dimensional temperature, and their first and second space derivatives, F computes the corresponding time derivatives. The needed chemistry terms are found by calling the subroutine RT. This subroutine is also written by a FORTRAN program (see reference 22 of text).

For details on the actual form of the equations used and the connections between F and the rest of the flame code, see reference 23 of the text.

The listing that follows gives the FORTRAN program (MAIN) and the corresponding transport subroutines for a binary mixture of H_2 and N_2 (F) for Methods I, II, III, IV and VI.

```

1  PROGRAM LOADF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
2  * TAPE3,TAPE9,TAPE15)
3  C LOADF CREATES THE SUBROUTINE F IN PDECOL-FLCT.
4  DIMENSION II(72)
5  DIMENSION LH(25),W(25),AU(7,25),AL(7,25)
6  DIMENSION ALD(25),BLD(25),ABD(25,25),HBD(25,25)
7  DIMENSION LBPR(25)
8  DIMENSION III(44)
9  DIMENSION LBROT(25),SGA(25),ESK(25),UM(25),ALP(25),ZROT(25),DF(25)
10 DIMENSION LD(25),LDV(25)
11 DIMENSION AV(25),BV(25)
12 DIMENSION E(25,25)
13 WRITE(3,1000)
14
15 I000 FORMAT(1HC,2X,34HWE WANT TO AVOID DIVISION BY ZERO. )
16 WRITE(3,1012)
17 I012 FORMAT(6X,14HDO 5 K=1,NPDEM)
18 WRITE(3,1014)
19 I014 FORMAT(6X,32HIF(ABS(U(K)),LT.SMALL)U(K)=SMALL )
20 I016 FORMAT(1X,1H5,4X,36HIF(ABS(UPH(K)),LT.SMALL)UPH(K)=SMALL )
21 READ(5,12)NLINE
22 I2 FORMAT(1014)
23 C NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
24 DO 20 K=1,NLINE
25 READ(5,22)I1
26 WRITE(3,22)I1
27 CONTINUE
28 I20 FORMAT(72A1)
29 I24 FORMAT(1X,72A1/)
30 READ(5,12)NSPC
31 NM=NSPC-1
32 LBM=IH-
33 LBU=2HU(
34 LBP=IH)
35 WRITE(3,1020)((LHM,LBU,K,LBP),K=1,NM)
36 I020 FORMAT(6X,6HYN=1.0,8(A1,42,12,A1),A1,2(/5X,1H*,1X,
37 * 8(A2,12,A1,A1)) )
38 WRITE(3,1025)
39 I025 FORMAT(6X,33HCALL RT(U,YN,R,NPOE,KPDE,IC,KSKR) )
40 WRITE(3,18)NSPC
41 I8 FORMAT(6X,4HIST=12,7H*(IC-I) )
42 C ASSUME AT MOST ONE POLAR SPECIES. (DIPOLE MOMENT NON-ZERO).
43 C THEN A* AND B* CAN BE APPROXIMATED BY LENNAK-JONES COLLISION
44 C INTEGRALS, EVEN IF THE INPUT PARAMETERS ARE STUCKMAYER.
45 DO 30 K=1,NSPC
46 HEAD(5,32) LR(K),W(K),DF(K),SGA(K),ESK(K),UM(K),ALP(K),ZROT(K),
47 * LBROT(K)
48 WRITE(6,34)K,LR(K),W(K),DF(K),SGA(K),ESK(K),UM(K),ALP(K),ZROT(K),
49 * LBROT(K)
50 HEAD(15,36)(AU(L,K),L=1,5),(III(L),L=1,5)
51 WRITE(6,36)(AU(L,K),L=1,5),(III(L),L=1,5)
52 READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
53 WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
54 HEAD(15,37)(AL(L,K),L=4,7),(III(L),L=1,20)
55 WRITE(6,37)(AL(L,K),L=4,7),(III(L),L=1,20)
56 CONTINUE
57 I30 HEAD(5,232)TPN,PHN,TMN
58

```

```

232 FORMAT(IP3E12.4)
C THE ROWS AND COLUMNS CORRESPONDING TO INTERNAL EFFECTS FOR MONATOMICS
C ARE SKIPPED. LD KEEPS TRACK OF WHICH ROW OR COLUMN IS BEING
C WORKED ON.
LD(I)=1
IF (DF(1).EQ.0.0)LD(1)=0
DO 38 L=2,NSPC
LM=L-1
LD(L)=LD(LM)+1
IF (DF(L).EQ.0.0)LD(L)=LD(L)-1
CONTINUE
38
32 FORMAT(A5,7F7.0,A5)
34 FORMAT(/2X,14,4X,A5,4X,7F8.2,4X,A5/)
36 FORMAT(5E15.8,5A1)
37 FORMAT(4E15.8,20A1)
WRITE(3,1100)IPN
FORMAT(6X,13HDT=UPH(NPDE)*,IPE14.6)
WRITE(3,27)
FORMAT(6X,22HIF(KSK1.GT.1)GO TO 100)
WRITE(3,28)
FORMAT(6X,22HIF(KSKR.GT.1)GO TO 125 )
READ(5,12)NLINE
DO 40 K=1,NLINE
READ(5,22)11
WRITE(3,22)11
40 CONTINUE
C *****
C ENTHALPIES AND HEAT CAPACITIES.
C *****
WRITE(3,42)
FORMAT(6X,24HIF(T.GT.1000.)GO TO 2000)
DO 50 K=1,NSPC
WRITE(3,52)K,AL(1,K),AL(2,K)
WRITE(3,54)(AL(L,K),L=3,5)
A=AL(2,K)
B=AL(3,K)*2.0
C=AL(4,K)*3.0
D=AL(5,K)*4.0
WRITE(3,1112)K,A,B,C,D
1112 * 2(4H+T*(,1PE16.8,7H)))*DT )
FORMAT(6X,24HDC,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8,5X,1H*,1X,
* 2(4H+T*(,1PE16.8,7H)))*DT )
WRITE(3,62)K,AL(6,K),AL(1,K)
WRITE(3,64)AL(2,K),AL(3,K)
WRITE(3,66)AL(4,K),AL(5,K)
CONTINUE
50
52 FORMAT(6X,1HC,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
54 FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8,5H))))
WRITE(3,56)
FORMAT(6X,10HGO TO 3000)
WRITE(3,58)
58
FORMAT(4H2000,2X,8HCONTINUE)
DO 60 K=1,NSPC
WRITE(3,52)K,AU(1,K),AU(2,K)
WRITE(3,54)(AU(L,K),L=3,5)
A=AU(2,K)
B=AU(3,K)*2.0
C=AU(4,K)*3.0

```

```

115      D=AU(5,K)*4.0
        WHITE(3,I1I2)K,A+B,C,D
        WHITE(3,62)K,AU(6,K),AU(1,K)
        WHITE(3,64)AU(2,K),AU(3,K)
        WHITE(3,66)AU(4,K),AU(5,K)
120      CONTINUE
        60      FORMAT(6X,I1H,I2,9H=1.9872*(,IPEI6.8,4H+T*(,IPEI6.8)
        62      FORMAT(5X,IH*,IX,4H+1*(,IPEI6.8,4H/2.0,4H+1*(,IPEI6.8,4H/3.0)
        64      FORMAT(5X,IH*,IX,4H+1*(,IPEI6.8,4H/4.0,4H+1*(,IPEI6.8,
        66      * 4H/5.0,4H))))))
125      WHITE(3,68)
        FORMAT(4H3000.2X,8HCONTINUE)
        68      WHITE(3,I34)
        134      FORMAT(1HC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES. )
        DO 140 K=1,NSPC
        130      WRITE(3,I42)K,K,W(K)
        1116     FORMAT(6X,7HDC(1ST+,I2,4H)=DC,I2,IH,F6.2)
        140      WRITE(3,I44)K,K,W(K)
        140      CONTINUE
        142      FORMAT(6X,6HC(1ST+,I2,3H)=C,I2,IH,F6.2)
        144      FORMAT(6X,6HH(1ST+,I2,3H)=H,I2,IH,F6.2)
        146      WRITE(3,I46)
        146      FORMAT(1X,3HI25.2X,8HCONTINUE)
        C *****
        C THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
        C READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
        C COEFFICIENTS FROM A FILE CREATED BY VALUES, CY=5.
        C *****
        145      READ(5,I2)NLINE
        DO 72 K=1,NLINE
        145      READ(5,22)I1
        WRITE(3,22)I1
        72      CONTINUE
        78      FORMAT(1HC,5X,IHV,I2,IH=,IPEI4.6,5H*(I**,IPEI4.6,IH) )
        READ(5,I2)NLINE
        DO 70 K=1,NLINE
        150      READ(5,22)I1
        WRITE(3,22)I1
        70      CONTINUE
        DO 80 K=1,NSPC
        155      READ(9,82)AV(K),BV(K),I1I
        WRITE(6,84)K,LB(K),AV(K),BV(K),I1I
        READ(9,82)ALD(K),BLD(K),I1I
        WRITE(6,84)K,LB(K),ALD(K),BLD(K),I1I
        160      CONTINUE
        80      FORMAT(1P2EI4.6,44A1)
        82      FORMAT(1/2X,I4,4X,A4,4X,IP2EI4.6,44A1/)
        84      DO 76 K=1,NSPC
        165      WRITE(3,78)K,AV(K),BV(K)
        76      DO 90 K=1,NSPC
        90      WRITE(3,92)K,ALD(K),BLD(K)
        92      CONTINUE
        90      FORMAT(1HC,5X,2HVL,I2,IH=,IPEI4.6,5H*(I**,IPEI4.6,IH) )
        READ(5,I2)NLINE
        DO 100 K=1,NLINE
        170      READ(5,22)I1

```

04/15/80 14.17.09

FTN 4.8+498

PROGRAM LOADF 76/76 OPT=1 ROUND=**/ 1*ACE

```

175      100      WRITE(3,22)111
              CONTINUE
              NM=NSPC-1
              DO 110 I=1,NSPC
                DO 110 J=1,NSPC
                  READ(9,82)ABD(1,J),HBD(1,J),111
                  WRITE(6,112)1,J,LB(1),LB(J),ABD(1,J),HBD(1,J),111
                CONTINUE
              110  FORMAT(/2X,14,4X,14,4X,A4,4X,A4,4X,1P2E14.6,44A1/)
              112  HEAD(S,114)PRESS
              114  FORMAT(F6.0)
              WRITE(3,116)PRESS
              116  WRITE(6,116)PRESS
              FORMAT(1HC,2X,7HPRESS =,F6.2)
              DO 120 I=1,NSPC
                DO 120 J=1,NSPC
                  ABD(1,J)=ABD(1,J)/PRESS
                  WRITE(3,122)1,J,ABD(1,J),HBD(1,J)
                CONTINUE
              120  FORMAT(1HC,5X,1HD,212,1H=,1PE14.6,5SH*(T**,1PE14.6,1H) )
              122  C *****
              C  SPACE DERIVATIVES.
              C *****
              195  LHPL=1H+
              WRITE(3,148)
              148  FORMAT(1HC,2X,42HDEFINE USEFUL COMBINATIONS AND DERIVATIVES )
              NS=NSPC+1
              WRITE(3,149)NS
              149  FORMAT(6X,4HYS=Y,12)
              DO 150 K=1,NSPC
                WRITE(3,152)K,K
              150  CONTINUE
              152  FORMAT(6X,1HX,12,2H=Y,12,3H/Y5)
              DO 160 K=1,NM
                WRITE(3,162)K,K
                WRITE(3,164)K,K
                WRITE(3,166)K,K
              160  CONTINUE
              162  FORMAT(6X,1HU,12,3H=U(,12,1H) )
              164  FORMAT(6X,2HUU,12,5H=UPH(,12,1H) )
              166  FORMAT(6X,3HUUU,12,6H=UPH2(,12,1H) )
              LBU=1HU
              172  WRITE(3,172)NSPC,((LBM,LBU,K),K=1,NM)
              215  FORMAT(6X,1HU,12,4H=1.0,8(A1,A1,12),A1,2(/5X,1H*,1X,
                * 8(A1,12,A1) ) )
              LBUU=2HUU
              174  WRITE(3,174)NSPC,((LBM,LBUU,K),K=1,NM)
              220  FORMAT(6X,2HUU,12,1H=,8(A1,A2,12),A1,2(/5X,1H*,1X,
                * 8(A2,12,A1) ) )
              LBUUU=3HUUU
              176  WRITE(3,176)NSPC,((LBM,LBUUU,K),K=1,NM)
              225  FORMAT(6X,3HUUU,12,1H=,8(A1,A3,12),A1,2(/5X,1H*,1X,
                * 8(A3,12,A1) ) )
              DO 180 K=1,NSPC
                WRITE(3,182)K,K,w(K)
              180  CONTINUE
              182  FORMAT(6X,2HDY,12,3H=1HU,12,1H/err,2)

```

```

230      LBDY=2HDY
      WRITE(3,186)((LPL,LBDY,K),K=1,NSPC)
      FORMAT(6X,4HDYS=,8(A1,A2,I2),A1,2(/5X,IH*,IX,8(A2,I2,A1)) )
      DO 190 K=1,NSPC
      WRITE(3,188)K,K,W(K)
      FORMAT(6X,3HDY,I2,4H=000,I2,1H/,F6.2)
      CONTINUE
      LBDY=3HDY
      WRITE(3,192)((LPL,LBDY,K),K=1,NSPC)
      FORMAT(6X,5HDYS=,5(A1,A3,I2),A1,2(/5X,IH*,IX,5(A3,I2,A1)) )
      PSK=PRESS/82.05
      WRITE(3,234)TPN,PHN,TMN
      WRITE(6,234)TPN,PHN,TMN
      * 5HTMN =,IPEI2.4)
      WRITE(3,242)PSR
      FORMAT(6X,5HDSH=,IPE20.12,2IH*(DT/T+DYS/YS)/(T*YS) )
      WRITE(3,1202)
      FORMAT(6X,I6HDYS=DYS/(YS*YS) )
      WRITE(3,194)
      DO 1250 K=1,NSPC
      WRITE(3,1204)K,K,K
      FORMAT(6X,2HDX,I2,3H=DY,I2,5H/YS-Y,I2,5H*UDYSY )
      WRITE(3,196)K,K,K,K,K
      FORMAT(6X,3HDDX,I2,5H=(DDY,I2,7H-2.0*DY,I2,13H*UDYS/YS,2.0*Y,I2,
      * 9H*UDYSQ-Y,I2,12H*UDYS/YS)/YS )
      C ZROT HAS BEEN READ IN AT T = INFINITY.
      C IF LBROT = 5H CNST, THEN TREAT ZROT AS A CONSTANT.
      C IF LBROT = 5H VAR, THEN USE THE FORMULA OF PARKER FOR THE
      C TEMPERATURE DEPENDENCE.
      PI=2.0*ACOS(0.0)
      LBVR=5H VAR
      LBCN=5H CNST
      IF (DF(K).EQ.0.0)GO TO 1210
      B=SQRT(PI*PI*PI*ESK(K))/2.0
      C=(PI*PI/4.0*PI)*ESK(K)
      A=DF(K)/(2.0*ZROT(K))
      B=A*B
      C=A*C
      C WRITE CROT/ZROT
      IF (LBROT(K).EQ.LBVR)WRITE(3,1206)K,A,B,C
      1206 * 8HSQRT(T)+,IPE20.12,IH*,IPE20.12,IH/,5X,IH*,IX,
      IF (LBROT(K).EQ.LBCN)WRITE(3,1207)K,A
      1207 FORMAT(6X,4HCSZR,I2,IH=,IPE20.12)
      B=B/2.0
      IF (LBROT(K).EQ.LBVR)WRITE(3,1120)K,B,C
      1120 FORMAT(6X,5HDCSZR,I2,3H=-,IPE14.12,9H/SQRT(T)+,
      * IPE19.12,RH/T)*DT/I )
      IF (LBROT(K).EQ.LBCN)WRITE(3,1121)K
      1121 FORMAT(6X,5HDCSZR,I2,4H=0.0 )
      A=10.0/(3.0*PI)
      WRITE(3,1274)K,K,A,K
      WRITE(3,1134)K,K,A,K
      C WRITE C INTERNAL.
      A=W(K)/1.9872

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FTN 4.8+49H

76/76 OPT=1 ROUND=**/ TRACE

PROGRAM LOADF

```

1212 WRITE(3,I2I2)K,K,A
      FORMAT(6X,4HCINT,I2,7H=C(IST+,I2,2H)*,IPE20,I2,4H-2.5)
1124 WRITE(3,I124)K,K,A
      FORMAT(6X,5HDCINT,I2,8H=DC(IST+,I2,2H)*,IPE20,I2)
1216 WRITE(3,I216)K,K,K
      FORMAT(6X,3HCSC,I2,5H=CSZR,I2,5H/CINT,I2)
1128 WRITE(3,I128)K,K,K,K
      FORMAT(6X,4HOCSC,I2,7H=(DCSZR,I2,5H-CSZR,I2,6H*DCINT,I2,
* 5H/CINT,I2,6H)/CINT,I2 )
      GO TO 1250
1210 CONTINUE
      WRITE(3,I272)K,K
      WRITE(3,I132)K,K
1250 CONTINUE
      DO 1300 I=1,NSPC
      DO 1300 J=1,NSPC
1254 WRITE(3,I254)I,J,I,J
      FORMAT(6X,IHX,2I2,2H=X,I2,2H*X,I2)
1256 WRITE(3,I256)I,J,I,J,I,J
      FORMAT(6X,2HDX,2I2,3H=DX,I2,2H*X,I2,2H*X,I2,3H*DX,I2)
      A=1.0/ABD(I,J)
      B=-BRO(I,J)
C WRITE THE RECIPROCAL OF THE BINARY DIFFUSION COEFFICIENT.
1258 WRITE(3,I258)I,J,A,B
      FORMAT(6X,2HVD,2I2,IH=,IPE20,I2,6H*(I***(,IPE14,6,2H) )
      A=A*B
      B=B-I.0
1262 WRITE(3,I262)I,J,A,B
      FORMAT(6X,3HVD,2I2,IH=,IPE20,I2,6H*(I***(,IPE14,6,5H))*DT )
1266 WRITE(3,I266)I,J,I,J,I,J
      FORMAT(6X,3HXS,2I2,2H=X,I2,2H*X,I2,3H*VD,2I2)
1270 WRITE(3,I270)I,I,J,I,I,J,I,I,J
      FORMAT(6X,4HXS,2I2,3H=DX,2I2,3H=DX,2I2,3H*VD,2I2,2H*X,I2,2H*VD,2I2)
      IF (I.EQ.J) GO TO 1300
      A=5.0/(3.0*PI)
      IF (OF(I).EQ.0.0.AND.UF(J).EQ.0.0) WRITE(3,I272)I,J
      IF (OF(I).EQ.0.0.AND.UF(J).EQ.0.0) WRITE(3,I132)I,J
1132 FORMAT(6X,3HDCZ,2I2,4H=0.0)
1272 IF (OF(I).NE.0.0.AND.UF(J).EQ.0.0) WRITE(3,I274)I,J,A,I
      IF (OF(I).NE.0.0.AND.UF(J).EQ.0.0) WRITE(3,I134)I,J,A,I
1134 FORMAT(6X,3HOCZ,2I2,IH=,IPE20,I2,7H*(DCSZR,I2,IH) )
1274 IF (OF(I).EQ.0.0.AND.UF(J).NE.0.0) WRITE(3,I274)I,J,A,J
      IF (OF(I).EQ.0.0.AND.UF(J).NE.0.0) WRITE(3,I134)I,J,A,J
      IF (OF(I).EQ.0.0.AND.UF(J).NE.0.0) WRITE(3,I276)I,J,A,I,J
      IF (OF(I).NE.0.0.AND.UF(J).NE.0.0) WRITE(3,I136)I,J,A,I,J
1136 FORMAT(6X,3HOCZ,2I2,IH=,IPE20,I2,7H*(DCSZR,I2,IH) )
1276 IF (OF(I).EQ.0.0.AND.UF(J).EQ.0.0) WRITE(3,I276)I,J,A,I,J
1300 CONTINUE
      LHX=IHX
      LHVU=3H*VD
      K=1
1304 WRITE(3,I304)K,((L*PL*LBX,L*LBVU,K,L),L=2,NSPC)
      FORMAT(6X,4HXS,2I2,IH=5(2A1,I,A3,2I2),A1,3(/5X,IH*,I*,
* 5(A1,I2,A3,2I2,A1) )
      LHX=PHDX

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345      LBVDV=4H*DVD
      WRITE(3,1308)K,((LBPL,LBDX,L,LBVD,L,K,L,LBPL,LBX,L,LBVDV,K,L)
      *L=2,NSPC)
1308      * 9/(5X,1H*,1X,2(A2,12,A3,2I2,2A1,12,A4,2I2),A1,
      DO 1310 K=2,NM
      KM=K-1
      KP=K+1
      WRITE(3,1304)K,((LBPL,LBX,L,LBVD,L,K),L=1,KM),
      * ((LBPL,LBX,L,LBVD,K,L),L=KP,NSPC)
      WRITE(3,1308)K,((LBPL,LBDX,L,LBVD,L,K,LBPL,LBX,L,LBVDV,K,L),
      *L=1,KM),((LBPL,LBDX,L,LBVD,K,L,LBPL,LBX,L,LBVDV,K,L),L=KP,NSPC)
1310      CONTINUE
      K=NSPC
      WRITE(3,1304)K,((LBPL,LBX,L,LBVD,L,K),L=1,NM)
      WRITE(3,1308)K,((LBPL,LBDX,L,LBVD,L,K,LBPL,LBX,L,LBVDV,K,L),
      *L=1,NM)
      DO 1325 K=1,NSPC
      A=1.0/AV(K)
      B=-BV(K)-1.0
      C WRITE THE RECIPROCAL OF THE VISCOSITY TIMES THE TEMPERATURE.
      WRITE(3,1312)K,A,B
1312      FORMAT(6X,3HSTV,12,1H=,1PE20.12,6H*(T**,(1PE14.6,2H)) )
      A=A*B
      B=B-1.0
      WRITE(3,1314)K,A,B
1314      FORMAT(6X,4HSTV,12,1H=,1PE20.12,6H*(T**,(1PE14.6,5H))*DT)
1316      WRITE(3,1316)K,K,K,K
      WRITE(3,1320)K,K,K,K,K
1320      FORMAT(6X,5HSTV,12,3H=DX,2I2,4H*STV,12,2H=X,2I2,5H*STV,12)
1325      CONTINUE
      C *****
      C SPECIFIC HEAT OF THE MIXTURE.
      C *****
      WRITE(3,124)
124      FORMAT(1HC,2X,44HSPECIFIC HEAT OF THE MIXTURE. NTIS FORMULA. )
      LBC=6HC(1ST+
      LBU=3H)*U
      WRITE(3,132)((LBPL,LBC,K,LBU,K),K=1,NSPC)
132      FORMAT(6X,7HCM(IC)=,4(A1,A6,12,A3,12),A1,
      * 4(/5X,1H*,1X,4(A6,12,A3,12,A1)) )
      C *****
      C THERMAL CONDUCTIVITY AND DIFFUSION.
      C *****
      C HOLTZMAN CONSTANT.
      RK=1.38054E-16
      C GAS CONSTANT.
      RG=1.9872
      WRITE(3,272)
      WRITE(3,274)
272      FORMAT(1HC,2X,24HDIFFUSION AND HEAT FLUX. )
274      FORMAT(1HC,2X,16HSEE DIXON-LEWIS. )
      WRITE(3,276)
276      FORMAT(1HC,2X,60H11. TRANSPORT PHENOMENA IN MULTICOMPONENT SYSTEM
      *S.
      READ(5,279)AAST,HAS1,I11

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FTN 4.8*498

PROGRAM LOAUF 76/76 OPT=1 MOUND=+*/* TRACE

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400      279      FORMAT(IP2E14.6,44A1)
        WRITE(6,123)AAS,BAS1,111
123      FORMAT(1/2X,IP2E14.6,44A1)
        READ(5,279)ABST,CBST,111
        WRITE(6,123)ABST,CHST,111
        READ(5,279)ACST,CCST,111
        WRITE(6,123)ACST,CCST,111
C      LM 00.00
        WRITE(3,301)
301      FORMAT(1HC,2X,8HLM 00.00)
        DO 305 K=1,NSPC
        WRITE(3,302)K,K
305      CONTINUE
302      FORMAT(6X,2HZ(,12,1H,12,SH)=0.0 )
        DO 310 I=1,NSPC
        DO 310 J=1,NSPC
        IF(1.EQ.J)GO TO 310
        A =W(J)/W(I)
        IMIN=MIN0(1,J)
        IMAX=MAX0(1,J)
        WRITE(3,308)I,J,IMIN,IMAX,A,J,I
308      * 5H*XSXD*12)
        WRITE(3,312)I,J,IMIN,IMAX,A,J,I,J,I
312      * 5H*XSXD,12,2H*X,12,6H*DSXD,12,1H) )
        FORMAT(6X,2HZ(,12,1H,12,SH)=XSU,212,1H*,1PE20.12,2H*X,12,
        * 5H*XSXD*12)
310      CONTINUE
C      FIND THE SIGMA FOR EACH PAIR OF SPECIES.
C      ASSUME THAT ONLY ONE SPECIES IS POLAR.
        DO 320 I=1,NSPC
        DO 320 J=1,NSPC
        IF(1.EQ.J)GO TO 320
        E(I,J)=SQRT(ESK(I)*ESK(J))
        IF(UM(I).EQ.0.0.AND.UM(J).EQ.0.0)GO TO 320
C      COMBINING RULE. P. 528, REID AND SHERWOOD.
        IF(UM(I).NE.0.0)LP=1
        IF(UM(J).NE.0.0)LP=J
        IF(LP.EQ.I)LNP=J
        IF(LP.EQ.J)LNP=I
        UMP=UM(LP)*1.0E-1H
        SGC=SGA(LP)*1.0E-8
        TPSTAR=UMP*UMP/(ESK(LP)*RK*SGC*SGC*SQRT(H*0))
        FC=1.0+(1.0/SQRT(2.0))*(ALP(LNP)*TPSTAR/(SGA(LNP)**3))*
        * SQRT(ESK(LP)/ESK(LNP))
        WRITE(6,1234)I,J,LP,LNP,FC
1234      FORMAT(414,1PE12.4)
        E(I,J)=E(I,J)*FC*FC
320      CONTINUE
C      FIND T*, A*, R*, AND C*.
        WRITE(3,1350)
1350      FORMAT(1HC,2X,24HFIND T*, A*, R*, AND C*. )
        DO 1360 I=1,NM
        IP=I+1
        DO 1360 J=IP,NSPC
        WRITE(3,1354)E(I,J)
1354      FORMAT(6X,5HTS=T*,1PE14.6)
        WRITE(3,1364)E(I,J)

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1364 FURMAT(6X,7HDTSDT/,IPE14.6)
      WRITE(3,1356)I,J,AAST,ABST
1356 FURMAT(6X,3HAST,2I2,1H=,IPE14.6,7H*(TS**((,IPE14.6,2H)) )
      A=AAST*ABST
      B=ABST-1.0
      WRITE(3,1366)I,J,A,B
1366 FURMAT(6X,4HDAST,2I2,1H=,IPE20.12,11H*DTSDT*(TS**((,IPE14.6,2H)) )
      WRITE(3,1365)CBST
1365 FURMAT(6X,7HEX=EXP(,IPE14.6,4H/TS) )
      LBB=3HBST
      WRITE(3,1358)LBB,I,J,ABST
1358 FURMAT(6X,A3,2I2,1H=,IPE14.6,3H*EX)
      LHUB=4HDBST
      A=-ABST*CBST
      WRITE(3,1368)LBUB,I,J,A
1368 FURMAT(6X,A4,2I2,1H=,IPE14.6,15H*DTSDT*EX/(TS*TS) )
      WRITE(3,1365)CCST
      LBC=3HCST
      WRITE(3,1358)LBC,I,J,ACST
      LBUC=4HDCST
      A=-ACST*CCST
      WRITE(3,1368)LBDC,I,J,A
1360 CONTINUE
      C LM 00,10 AND LM 10,00
      WRITE(3,321)
321 FURMAT(1HC,2X,21HLM 00,10 AND LM 10,00 )
      DO 330 IS=1,NSPC
      DO 330 JS=1,NSPC
      IF(15.EQ.JS)GO TO 330
      I=IS
      J=JS*NSPC
      A=-2.5*W(1S)/(W(1S)+W(JS))
      IMIN=MIN0(1S,JS)
      IMAX=MAX0(1S,JS)
      WRITE(3,326)A,IMIN,IMAX
326 FURMAT(6X,3HCT=,IPE20.12,9H*(1.2*CT,2I2,5H-1.0) )
      A=A*1.2
      WRITE(3,1140)A,IMIN,IMAX
1140 FURMAT(6X,4HDCI=,IPE20.12,5H*UCSI,2I2)
      IMIN=MIN0(1S,JS)
      IMAX=MAX0(1S,JS)
      WRITE(3,328)I,J,IMIN,IMAX
328 FURMAT(6X,2HZ(,12,1H=,12,8H)=CT*XSD,2I2)
      WRITE(3,1144)I,J,IMIN,IMAX,IMIN,IMAX
1144 FURMAT(6X,2HDZ,12,1H=,12,8H=CT*I,ASD,2I2,8H*DCI*XSD,2I2)
330 CONTINUE
      I1=1
      I2=1+NSPC
      LBZ=2HZ(
      LBC=1H,
      LBP=1H,
      LHM=1H-
      WRITE(3,336)I1,I2,((LBM,LBZ,K,LHC,12,LHP),K=2,NSPC)
336 FURMAT(6X,2HZ(,12,1H=,12,2H)=,5(A1,A2,12,A1,12,A1),A1,
      * 3(,5X,1H*,1X,5(A2,12,A1,12,2A1)) )
      LBWZ=2HDZ
      LBSP=1HS

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FIN 4.8*498

PROGRAM LOADF 76/76 OPT=I ROUNDED=**/ TRACE

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515      WRITE(3,338)I,I,I2,((LBM,LBZ,K,LHC,I2,LBP),K=1,IM),
516      FORMAT(6X,2HDZ,I2,IHS,I2,IH=4(A1,A2,I2,A1,I2),A1,
517      * 2(/5X,IH*,IX,7(A2,I2,A1,I2,A1)) )
518      DO 340 I=2,NM
519      IM=I-1
520      IP=I+1
521      I1=I
522      I2=I+NSPC
523      WRITE(3,336)I,I,I2,((LBM,LBZ,K,LHC,I2,LBP),K=1,IM),
524      * ((LBM,LBZ,K,LBP),K=IP,NSPC)
525      WRITE(3,338)I,I,I2,((LBM,LBZ,K,LHC,I2,LBP),K=1,IM),
526      * ((LBM,LBZ,K,LHC,I2,LBP),K=IP,NSPC)
527      CONTINUE
528      I1=NSPC
529      I2=NSPC+NSPC
530      WRITE(3,336)I,I,I2,((LBM,LBZ,K,LHC,I2,LBP),K=1,NM),
531      WRITE(3,338)I,I,I2,((LBM,LBZ,K,LBP),K=1,NM)
532      DO 350 IS=1,NSPC
533      DO 350 JS=1,NSPC
534      IN=IS+NSPC
535      JN=JS
536      WRITE(3,342)IN,JN,JN,IN
537      WRITE(3,346)IN,JN,JN,IN
538      FORMAT(6X,2HZ(I2,IH,I2,4H)=Z(I2,IH,I2,IH) )
539      FORMAT(6X,2HDZ,I2,IHS,I2,3H=OZ,I2,IHS,I2)
540      CONTINUE
541      C LM 01.00 AND LM 00.01
542      C ROWS OF LM 01.00 AND COLUMNS OF LM 00.01 CORRESPONDING TO
543      C MONATOMICS ARE DELETED.
544      WRITE(3,351)
545      FORMAT(1HC,2X,2IHLM 01.00 AND LM 00.01 )
546      DO 360 IS=1,NSPC
547      DO 360 JS=1,NSPC
548      IF (OF(IS).EQ.0.0)GO TO 360
549      I=LD(IS)+2*NSPC
550      J=JS
551      WRITE(3,362)I,J
552      FORMAT(6X,2HZ(I2,IH,I2,5H)=0.0)
553      CONTINUE
554      DO 363 IS=1,NSPC
555      DO 363 JS=1,NSPC
556      IF (OF(JS).EQ.0.0)GO TO 363
557      I=IS
558      J=LD(JS)+2*NSPC
559      WRITE(3,362)I,J
560      CONTINUE
561      C LM 10.10 SYMMETRIC.
562      WRITE(3,361)
563      FORMAT(1HC,2X,8HLM 10.10 )
564      DO 370 IS=1,NM
565      IP=IS+1
566      DO 370 JS=IP,NSPC
567      I=IS+NSPC
568      J=JS+NSPC
569      A=W(IS)*W(JS)/(W(IS)+W(JS))*2)
570      WRITE(3,372)A,IS,JS,IS,JS
571      FORMAT(6X,3HCT=,1PE20.12,15H*(13.75-3.0*AS I,212,

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575      * 8H-4.0*AST,2I2,3H*CZ,2I2,1H) )
      WRITE(3,1146)A,IS,JS,IS,JS,IS,JS,IS,JS,IS,JS,IS,JS,IS,JS
      FORMAT(6X,5H*DCI=-,IPE20,12,10H*(3.0*DBST,2I2,9H*4.0*(AST,
576      * 2I2,4H*DCZ,2I2,5X,1H*,1X,5H*DBST,2I2,3H*CZ,2I2,2H) ) )
      WRITE(3,376)I,J,IS,JS
      FORMAT(6X,2H*Z(,I2,1H,,I2,8H)=CI*XSD,2I2)
577      WRITE(3,377)J,I,I,J
      FORMAT(6X,2H*Z(,I2,1H,,I2,4H)=Z(,I2,1H,,I2,1H) )
578      WRITE(3,380)I,J,IS,JS,IS,JS
      FORMAT(6X,2H*Z(,I2,1H,,I2,8H)=CI*UXSD,2I2,8H*DCI*XSD,2I2)
579      WRITE(3,379)J,I,I,J
      FORMAT(6X,2H*Z(,I2,1H,,I2,3H=DZ,12,1H*,I2)
580      CONTINUE
      DO 400 IS=1,NSPC
      I=IS+NSPC
      RGA=82.05
      C USE THE GAS CONSTANT IN UNITS OF CM**3-ATM/MOLE-K SO ALL THE
      C ELEMENTS OF Z ARE IN THE SAME UNITS.
      A=-5.0*PRESS*W(IS)/(3.0*RGA)
      WRITE(3,382)A,IS,IS
      FORMAT(6X,3H*CI=,IPE20,12,3H*CZ,2I2)
581      WRITE(3,383)A,IS,IS
      FORMAT(6X,4H*DCI=,IPE20,12,4H*DCZ,2I2)
582      DO 390 KS=1,NSPC
      IF (KS.EQ.15) GO TO 390
      IMIN=MIN0(15,KS)
      IMAX=MAX0(15,KS)
      A=7.5*W(IS)*W(IS)+6.25*W(KS)*W(KS)
      B=3.0*W(KS)*W(KS)
      C=4.0*W(IS)*W(KS)
      RMT=1.0/((W(IS)+W(KS))*2)
      A=A*RMT
      B=B*RMT
      C=C*RMT
      WRITE(3,386)KS,C,IMIN,IMAX,IMIN,IMAX
      FORMAT(6X,2H*CI,12,1H=,IPE20,12,4H*AST,2I2,3H*CZ,2I2)
583      WRITE(3,1150)KS,C,((IMIN,IMAX),L=1,4)
      FORMAT(6X,3H*DCI,12,1H=,IPE20,12,6H*(DAST,2I2,3H*CZ,2I2,
584      * 4H*AST,2I2,4H*DCZ,2I2,1H) )
      WRITE(3,388)KS,A,B,IMIN,IMAX,KS
      FORMAT(6X,2H*CI,12,1H=,IPE20,12,1H=,IPE20,12,4H*DBST,2I2,3H*CI,12)
585      WRITE(3,1154)KS,B,IMIN,IMAX,KS
      FORMAT(6X,3H*DCI,12,2H=-,IPE20,12,5H*DBST,2I2,4H*DCI,12)
      CONTINUE
      LHXSD=3H*XS0
      LHDXS0=4H*XS0
      LBCT=3H*CT
      LHDCI=4H*DCI
      IF (IS.GT.1) GO TO 393
      WRITE(3,392)I,I,IS,((LBM,LBXS0,IS,KS,LHCT,KS),KS=2,NSPC)
      FORMAT(6X,2H*Z(,I2,1H,,I2,9H)=CI*XSTV,I2,
586      * 2(AI,A3,2I2,A3,I2),AI,5(/5X,1H*,IX,4(A3,2I2,A3,I2,AI)) )
      WRITE(3,394)I,I,IS,IS,((LBM,LBXS0,IS,KS,LBCT,KS,LBM,LHXSD,IS,
587      * KS,LHDCI,KS),KS=2,NSPC)
      FORMAT(6X,2H*Z(,I2,1H,,I2,9H)=CI*UXSTV,I2,9H*DCI*XSTV,I2,AI,A4,
588      * 2I2,A3,I2,AI,A3,2I2,A4,I2,AI,1(/5X,1H*,IX,2(A4,2I2,A3,I2,AI,A3,
589      * 2I2,A4,I2,AI)) )

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620 GO TO 400
621 IF (IS.LT.NSPC) GO TO 396
622 WRITE(3,392) I, I, IS, ((LBM,LBXSD,KS,IS,LBCT,KS),KS=I,NM)
623 WRITE(3,394) I, I, IS, IS, ((LBM,LBUXSD,KS,IS,LBCT,KS,LBM,LBXSD,
624 * KS,IS,LBDCI,KS),KS=I,NM)
625 GO TO 400
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685 430 CONTINUE
      LHCT=2HCT
      LBDCT=3HDCI
      LBXSD=4H*XSD
      LBUXSD=5H*DXSD
      IF (IS.GT.1) GO TO 433
      WRITE(3,432)I,J,IS,((LBPL,LBCT,KS,LBXSD,IS,KS),KS=2,NSPC)
      FORMAT(6X,2H2I,12,1H,12,9H)=CT*XSTV,I2,3(A1,A2,I2,A4,2I2),A1,
      * 5(/5X,1H*,1X,4(A2,I2,A4,2I2,A1))
      WRITE(3,434)I,J,IS,IS,((LBPL,LBCT,KS,LBXSD,IS,KS,LBPL,LBDCT,
      * KS,LBXSD,IS,KS),KS=2,NSPC)
      FORMAT(6X,2H2I,12,1H,12,9H)=CT*UXSTV,I2,9H*DCI*XSTV,I2,
      * A1,A2,I2,A5,2I2,A1,A3,I2,A4,2I2,A1,10(/5X,1H*,1X,
      * 2(A2,I2,A5,2I2,A1,A3,I2,A4,2I2,A1))
      GO TO 440
700 433 IF (IS.LT.NSPC) GO TO 436
      WRITE(3,432)I,J,IS,((LBPL,LBCT,KS,LBXSD,KS,IS),KS=I,NM)
      WRITE(3,434)I,J,IS,IS,((LBPL,LBCT,KS,LBXSD,KS,IS,LBPL,LBDCT,
      * KS,LBXSD,KS,IS),KS=I,NM)
      GO TO 440
705 436 CONTINUE
      IM=IS-I
      IP=IS+I
      WRITE(3,432)I,J,IS,((LBPL,LBCT,KS,LBXSD,KS,IS),KS=I,IM),
      * ((LBPL,LBCT,KS,LBXSD,IS,KS),KS=IP,NSPC)
      WRITE(3,434)I,J,IS,IS,((LBPL,LBCT,KS,LBXSD,KS,IS,LBPL,LBDCT,
      * KS,LBXSD,KS,IS),KS=I,IM),((LBPL,LBCT,KS,LBXSD,IS,KS,LBPL,LBDCT,
      * KS,LBXSD,IS,KS),KS=IP,NSPC)
      CONTINUE
440 CONTINUE
450 DO 418 IS=I,NSPC
      DO 418 JS=I,NSPC
      IF (DF(15).EQ.0.0) GO TO 418
      I=LD(15)+2*NSPC
      J=JS+NSPC
      WRITE(3,412)I,J,J,I
      FORMAT(6X,2H2I,12,1H,12,4H)=Z(I,I2,1H,12,1H)
      WRITE(3,416)I,J,J,I
      FORMAT(6X,2H2I,12,1H,12,3H)=DZ(I2,1H,12)
412 416 CONTINUE
      C LM 01,01
      C ROWS AND COLUMNS OF LM 01,01 CORRESPONDING TO MONATOMICS ARE DELETED.
451 WRITE(3,451)
      FORMAT(1HC,2X,BHLM 01,01)
      DO 460 IS=I,NSPC
      DO 460 JS=I,NSPC
      IF (IS.EQ.JS) GO TO 460
      IF (DF(15).EQ.0.0) (OF(JS).EQ.0.0) GO TO 460
      I=LD(15)+2*NSPC
      J=LD(JS)+2*NSPC
      WRITE(3,362)I,J
      CONTINUE
      LHL=IH
      LHP=IH)
      DO 490 IS=I,NSPC
      IF (DF(15).EQ.0.0) GO TO 490
      I=LD(15)+2*NSPC

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462 WRITE(3,462) IS
    FORMAT(6X,I4HCTM=-6.25/CINT,I2)
    WRITE(3,1166) IS,IS
745 FORMAT(6X,I5HDCIM=6.25*DCINT,I2,6H/(CINT,I2,5H*CINT,I2,IH) )
    A=2.0*PRESS*W(I5)/(PI*GA)
    WRITE(3,466) A,IS
748
749
750 FORMAT(6X,3HCT=,IPE20,I2,4H*CSC,I2)
    WRITE(3,1170) A,IS
751
752 FORMAT(6X,4HDCI=,IPE20,I2,5H*DCSC,I2)
    DO 470 KS=1,NSPC
753 IF (IS.EQ.KS) GO TO 470
754 A=I2.0*W(I5)/(5.0*PI*W(KS))
755 IMIN=MIN0(IS,KS)
    IMAX=MAX0(IS,KS)
    WRITE(3,472) KS,A,IMIN,IMAX,IS
756
757 FORMAT(6X,2HCT,I2,5H=I.0,*,IPE20,I2,4H*AST,I2,4H*CSC,I2)
758
759 WRITE(3,1172) KS,A,IMIN,IMAX,IS,IMIN,IMAX,IS
760
761 FORMAT(6X,3HDCI,I2,IH=,IPE20,I2,6H*(DAST,I2,4H*CSC,I2,
    * 4H*AST,I2,5H*DCSC,I2,IH) )
762
763 CONTINUE
    IF (IS.GT.1) GO TO 475
    WRITE(3,1176) IS,IS,IS,((LBPL,LBCT,KS,LBXSD,IS,KS),KS=2,NSPC)
764
765 FORMAT(6X,4HSUM=,7HCT*XSTV,I2,4H*XSD,I2,2(AI,A2,I2,A4,2I2),AI,
    * 5(/5X,IH*,IX,4(A2,I2,A4,2I2,AI)) )
766
767 WRITE(3,1180) IS,IS,IS,((LBPL,LBCT,KS,LBXSD,IS,KS,LBPL,LBDCI,
    * KS,LBXSD,IS,KS),KS=2,NSPC)
768
769 FORMAT(6X,5HOSUM=,8HDCI*XSTV,I2,9H*CT*DXSTV,I2,5H*DXSD,I2,
    * AI,A2,I2,A5,2I2,AI,A3,I2,A4,2I2,AI,I0(/5X,IH*,IX,
    * 2(A2,I2,A5,2I2,AI,A3,I2,A4,2I2,AI)) )
770
771 WRITE(3,476) I,I
    FORMAT(6X,2HZ(I2,IH,*,I2,9H)=CTM*SUM)
772
773 WRITE(3,478) I,I
    FORMAT(6X,2HDZ,I2,IH,I2,I8H=DCIM*SUM*CTM*DSUM )
774
775 GO TO 490
    IF (IS.LT.NSPC) GO TO 480
    WRITE(3,1176) IS,IS,IS,((LBPL,LBCT,KS,LBXSD,KS,IS),KS=1,NM)
776
777 WRITE(3,1180) IS,IS,IS,((LBPL,LBCT,KS,LBXSD,KS,IS,LBPL,LBDCI,
    * KS,LBXSD,KS,IS),KS=1,NM)
778
779 WRITE(3,476) I,I
    WRITE(3,478) I,I
780
781 GO TO 490
    IM=IS-I
    IP=IS+I
782
783 WRITE(3,1176) IS,IS,IS,((LBPL,LBCT,KS,LBXSD,KS,IS),KS=I,IM),
    * ((LBPL,LBCT,KS,LBXSD,IS,KS),KS=IP,NSPC)
784
785 WRITE(3,1180) IS,IS,IS,((LBPL,LBCT,KS,LBXSD,KS,IS,LBPL,LBDCI,
    * KS,LBXSD,KS,IS),KS=I,IM),((LBPL,LBCT,KS,LBXSD,KS,IS,LBPL,LBDCI,
    * KS,LBXSD,IS,KS),KS=IP,NSPC)
786
787 WRITE(3,476) I,I
    WRITE(3,478) I,I
788
789 CONTINUE
790
791 C SOLVE FOR DIFF VELOCITIES AND ENERGY FLUX.
    WRITE(3,498)
792
793 FORMAT(1HC,2X,47HSOLVE FOR DIFFUSION VELOCITIES AND ENERGY FLUX. )
794
795 NMT=L0(NSPC)+2*NSPC
    NDI=30
    WRITE(3,500) NMT,NDI
796
797
798
799

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800      500      FORMAT(6X,9HCALL DEC(,I2,1H,,I2,11H,Z,1PS,IER) )
      DO 495 K=1,NSPC
      WRITE(3,492)K,K,PHN
      492      FORMAT(6X,2HV(,I2,7H)=RH*DX,I2,1H/,IPEI4.6)
      WRITE(3,702)K,K,K,PHN
      702      FORMAT(6X,2HDV,I2,8H=(URH*DX,I2,7H+RH*DDX,I2,2H)/,IPEI4.6)
      805      CONTINUE
      DO 515 I=1,NSPC
      IP=I*NSPC
      WRITE(3,512)IP
      512      FORMAT(6X,2HV(,I2,5H)=0.0)
      WRITE(3,712)IP
      712      FDRMAT(6X,2HDV,I2,4H=0.0)
      515      CONTINUE
      DO 517 I=1,NSPC
      IF (DF(I).EQ.0.0)GO TO 517
      IP=LD(I)+2*NSPC
      WRITE(3,512)IP
      WRITE(3,712)IP
      517      CONTINUE
      WRITE(3,520)NMT,NDIM
      820      FORMAT(6X,9HCALL SOL(,I2,1H,,I2,14H,Z,V,IPS) )
      CALL UR(NSPC,NMT,NDIM)
      DO 525 I=1,NSPC
      WRITE(3,522)I,I
      522      FORMAT(6X,2HVX,I2,3H=V(,I2,1H) )
      WRITE(3,722)I,I
      722      FORMAT(6X,3HDVX,I2,4H=DV(,I2,1H) )
      525      CONTINUE
      DO 528 I=1,NSPC
      WRITE(3,512)I
      WRITE(3,712)I
      528      CONTINUE
      DO 530 I=1,NSPC
      IP=I*NSPC
      WRITE(3,532)IP,I
      WRITE(3,714)IP,I
      714      FORMAT(6X,2HDV,I2,3H=DX,I2)
      530      CONTINUE
      532      FORMAT(6X,2HV(,I2,3H)=X,I2)
      DO 535 I=1,NSPC
      IF (DF(I).EQ.0.0)GO TO 535
      IP=LD(I)+2*NSPC
      WRITE(3,532)IP,I
      WRITE(3,714)IP,I
      535      CONTINUE
      WRITE(3,520)NMT,NDIM
      CALL DR(NSPC,NMT,NDIM)
      LHV=2HV(
      LHP=1H)
      DO 540 I=1,NSPC
      WRITE(3,538)I,I,PHN
      840      538      FORMAT(6X,2HVT,I2,14H=-2.5*RH*DT*V(,I2,5H)/(T*,IPEI4.6,1H) )
      540      CONTINUE
      WRITE(3,726)IPN
      845      726      FORMAT(6X,1SHDT=UPH2(NPUE)*,1P,14.6)
      DO 730 K=1,NSPC
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860      WRITE(3,728)K,K,K,K,K,PHN
      FORMAT(6X,3H0VT,I2,I6H=-2.5*(URH*DT*V(,I2,
      * IH)+RH*DDT*V(,I2,I1H)+RH*DT*UV(,I2,I0H)-RH*DT*V(,I2,2H)*,
      * /5X,IH*,IX,9H0T/T)/(T*,IPEI4.6,IH) )
861      CONTINUE
862      DO 545 I=1,NSPC
863      WRITE(3,542)I,I,I,I
864      FORMAT(6X,2HUV,I2,2H=U,I2,4H*(VX,I2,3H+VT,I2,IH) )
865      CONTINUE
866      DO 745 I=1,NSPC
867      WRITE(3,742)I,I,I,I,I,I,I
868      FORMAT(6X,3H0UV,I2,3H=DU,I2,4H*(VX,I2,3H+VT,I2,IH)*,
869      * 2H+U,I2,5H*(DVX,I2,4H+UVT,I2,IH) )
870      CONTINUE
871      DO 550 I=1,NSPC
872      WRITE(3,548)I,I,I
873      FORMAT(6X,9HRHUV(I1T+,I2,7H)=RH*UV,I2)
874      CONTINUE
875      DO 750 I=1,NSPC
876      WRITE(3,748)I,I,I,I
877      FORMAT(6X,10HRHUV(I1T+,I2,8H)=URH*UV,I2,7H+RH*DUV,I2)
878      CONTINUE
879      C CONVERT FROM CM**3-ATM/SEC-CM-K TO CAL/SEC-CM-K.
880      A=-25.0*PRESS*I.9872/(4.0*82.05)
881      LBX=IHX
882      LBV=3H*V(
883      LBTRS=5HRLTRS
884      WRITE(3,556)((LBPL*LBX,K,LBV,K*NSPC*LBP),K=I,NSPC)
885      FORMAT(6X,4HSUM=,5(2AI,I2,A3,I2,A1),AI,3(/5X,IH*,IX,
      * 5(AI,I2,A3,I2,2AI)) )
886      LBDX=2HDX
887      LBV=4H*DV(
888      WRITE(3,756)((LBPL*LBDX,K,LBV,K*NSPC*LBP,LBX,K*LBV,
      * K*NSPC*LBP),K=1,NSPC)
889      FORMAT(6X,5HDSUM=,2(AI,A2,I2,A3,I2,3AI,I2,A4,I2,A1),AI,
      * 6(/5X,IH*,3(A2,I2,A3,I2,3AI,I2,A4,I2,2AI)) )
890      WRITE(3,557)LBTRS,A
891      FORMAT(6X,A5,IH=,IPEI4.6,6H*SUM/T)
892      LBDRS=6HDLRLTRS
893      WRITE(3,757)LBDRS,A
894      FORMAT(6X,A6,IH=,IPEI4.6,18H*(DSUM-SUM*DT/T)/T )
895      LBINT=5HPLINT
896      DO 553 I=1,NSPC
897      IF (DF(I).EQ.0.0)GO TO 553
898      J=LD(I)
899      LOV(J)=I
900      CONTINUE
901      NT=LD(NSPC)
902      IF (NT.EQ.0)GO TO 554
903      WRITE(3,556)((LBPL*LBX,LDV(K),L+V,K+2*NSPC*LBP),K=1,NT)
904      WRITE(3,756)((LBPL*LBX,LDV(K),L+V,K+2*NSPC*LBP,LBX,LDV(K)*,
905      * LHV,K+2*NSPC*LBP),K=1,NT)
906      WRITE(3,557)LBINT,A
907      LBINT=6HDLRLINT
908      WRITE(3,757)LBINT,A
909      CONTINUE
910      WRITE(3,562)

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562  FORMAT(6X,15HRLM=RLTKS+RLINT )
      WRITE(3,762)
915  FORMAT(6X,18HDLRLM=DRLTRS+DRLINT)
      WRITE(3,766)
566  FORMAT(6X,15HRLM(IC)=RH*RLM)
      WRITE(3,766)
920  FORMAT(6X,25HDLRLM(IC)=DRH*RLM+RH*DLRLM )
      LBDX=2HDX
      WRITE(3,570)((LHPL,LBDX,L,LBV,L,LBP),L=1,NSPC)
570  FORMAT(6X,4HSUM=,5(A1,A2,I2,A3,I2,A1),A1,3(/5X,IH*,IX,
      * 5(A2,I2,A3,I2,2A1)) )
      LBDX=3HDX
      WRITE(3,770)((LHPL,LBDX,L,LBV,L,LBP,LHPL,LBDX,L,LBP),
      * L=1,NSPC)
925  FORMAT(6X,5HDSUM=,2(A1,A3,I2,A3,I2,2A1,A2,I2,A4,I2,A1),A1,
      * 9(/5X,IH*,IX,2(A3,I2,A3,I2,2A1,A2,I2,A4,I2,2A1)) )
930  A=-2.5*I.9872*PRESS/(82.05*PHN)
      WRITE(3,572)A
572  FORMAT(6X,3HDX=,IPE20,I2,7H*RH*SUM)
      WRITE(3,772)A
935  C *****
772  FDRMAT(6X,RHDX(IC)=,IPE20,I2,IH*(DRH*SUM+RH*DSUM))
      C *****
      C FIND THE TIME DERIVATIVES.
      C *****
      WRITE(3,612)
612  FORMAT(1HC,2X,26HFINU THE TIME DERIVATIVES.)
      WRITE(3,622)
622  FDRMAT(6X,15HSP=ASP+BSPTIME)
      TMSPH2=TMN/(PHN*PHN)
      WRITE(3,628)
628  FORMAT(1X,3H100,2X,8HCONTINUE)
      WRITE(3,632)
632  FDRMAT(6X,25HIF(KPDE.EQ.NPDE)GO TO I50)
      WRITE(3,636)TMN
636  FORMAT(6X,3HRY=,IPE20,I0,8H*(KPDE) )
      TMSPH=TMN/PHN
      WRITE(3,638)TMSPH
638  FORMAT(6X,4HXY=,IPE20,I0,I6H*DRHUV(IST+KPDE) )
      WRITE(3,642)
642  FDRMAT(6X,23HVAL=SP*UPH(KPDE)*(IY+RY)
      WRITE(3,646)
646  FORMAT(6X,6HRETURN)
      WRITE(3,648)
648  FORMAT(1X,3H150,2X,8HCONTINUE)
      WRITE(3,662)TMSPH2
662  FORMAT(6X,3HIL=,IPE20,I0,IH*)
      WRITE(3,664)
664  FORMAT(5X,IH*,IX,4IH(DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE)) )
      LBL=IH
      LHC=6HC(IST+
      LHRHUV=10H)*RHUV(IST
      WRITE(3,668)TMSPH,((LHBL,LHPL,LHLC,K,LHHRUV,LHPL,K,LRP),K=1,NSPC)
      * ,LRP
945  FDRMAT(6X,4HTD=,IPE20,I0,I2H*UPH(NPDE)*(I2A1+A6,I2,A10,A1,I2,3A1,
      * 10(/5X,IH*,IX,2(A6,I2,A10,A1,I2,3A1)) )
      TMSPT=TMN/TPN
      LHR=2HR(

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04/15/80 14.17.09

FTN 4.8+498

PROGRAM LOADF 76/76 OPT=1 ROUND=-**/ IHACE

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970      LBH=8H)*H(IST+
        WRITE(3,672)TMSTP,((LB8L,LBPL,LHM,K,LBH,K,LBP),K=1,NSPC),LBP
672      * 9(/5X,IH*,IX,2(A2,I2,A8,I2,3A1))
        A=-TMN/(TPN*PHN)
        WRITE(3,674)A
975      * 674      FORMAT(6X,3HTX=,IPE20,I2,8H*DUX(IC) )
        WRITE(3,676)
676      * 676      FORMAT(6X,38HF VAL=SP*UPH(NPOE)+ (IL*TR+ID*TX)/CM(IC) )
        STOP
        END
980
971      MAIN
972      MAIN
973      MAIN
974      MAIN
975      MAIN
976      MAIN
977      MAIN
978      MAIN
979      MAIN
980      MAIN
981      MAIN

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1      SUBROUTINE DR(NSPC,NMT,NDIM)
C      FIND THE DERIVATIVES OF THE SOLUTIONS V.
      LHDZ=2HDZ
      LKSP=IHS
      LHM=IH-
      LHV=3H*V(
      LBP=IH)
      I=1
      NTOP=2*NSPC
      WRITE(3,10)I,1,((LHM,LBDZ,1,LBSP,J,LBV,J,LBP),J=2,NTOP)
10      FORMAT(6X,3HDV(,12,4H)=DV,12,3(A1,A2,12,A1,12,A3,12,A1),A1,
      * 7(/5X,1H*,1X,4(A2,12,A1,12,A3,12,2A1)) )
      NM=NSPC-1
      DO 15 I=2,NM
15      IM=I-1
      IP=I+1
      NST=NSPC+1
      WRITE(3,10)I,1,((LBM,LBDZ,1,LBSP,J,LBV,J,LBP),J=1,IM),
      * ((LBM,LBDZ,1,LBSP,J,LBV,J,LBP),J=1P,NSPC),
      * ((LBM,LBDZ,1,LBSP,J,LBV,J,LBP),J=NST,NTOP)
20      CONTINUE
15      I=NSPC
      WRITE(3,10)I,1,((LHM,LBDZ,1,LBSP,J,LBV,J,LBP),J=1,NM),
      * ((LBM,LBDZ,1,LBSP,J,LBV,J,LBP),J=NST,NTOP)
      DO 25 I=1,NSPC
      IP=I+NSPC
      WRITE(3,10)IP,1P,((LBM,LBDZ,1P,LBSP,J,LBV,J,LBP),J=1,NMT)
25      CONTINUE
      ITOP=NMT-2.0*NSPC
      DO 30 I=1,ITOP
      IP=1.2*NSPC
      WRITE(3,10)IP,1P,((LHM,LBDZ,1P,LBSP,J,LBV,J,LBP),J=NST,NTOP),
      * LHM,LBDZ,1P,LBSP,1P,LBV,1P,LBP
30      CONTINUE
      WRITE(3,32)NMT,NDIM
32      FORMAT(6X,9HCALL SOL(,12,1H,,12,10H,Z,DV,1PS) )
      RETURN
      END

```

BLOCK	ADDRESS	LENGTH	FILE
LOADF	110	17367	LGO
DR	17477	401	LGO
/STP.END/	20100	1	SL-FTNL18
/FCL.C./	20101	30	SL-FTNL18
/QB.10./	20131	144	SL-FTNL18
Q2NTRY=	20275	4	SL-FTNL18
COMIO=	20301	10	SL-FTNL18
FECMSK=	20311	41	SL-FTNL18
FEIFST=	20352	3	SL-FTNL18
FLTN=	20355	156	SL-FTNL18
FLTOUT=	20533	315	SL-FTNL18
FMTP=	21050	377	SL-FTNL18
FORSYS=	21447	300	SL-FTNL18
FORUTL=	21747	45	SL-FTNL18
GETFIT=	22014	54	SL-FTNL18
INCOM=	22070	144	SL-FTNL18
INPC=	22234	173	SL-FTNL18
KODER=	22427	476	SL-FTNL18
KRAKER=	23125	454	SL-FTNL18
OUTC=	23601	155	SL-FTNL18
OUTCOM=	23756	204	SL-FTNL18
SPA=	24162	11	SL-FTNL18
ERRCAP=	24173	317	SL-FTNL18
FERCAP=	24512	171	SL-FTNL18
ACUS	24703	6	SL-FTNL18
ACOSIN.	24711	63	SL-FTNL18
EXP.MSG	24774	16	SL-FTNL18
SQRT	25012	6	SL-FTNL18
SQRT.	25020	32	SL-FTNL18
SYSID=	25052	1	SL-FTNL18
SYS=1ST	25053	65	SL-FTNL18

1	H2	2.00	2.00	2.92	38.00	0.00	.79	280.00	CNST
.31001901E+01	.51119464E-03	.52644210E-07	-.34909973E-10	.36945345E-14	H2				
-.87738042E+03	-.19629421E+01	.30574451E+01	.26765200E-02	-.58099162E-05	H2				
.55210391E-08	-.18122739E-11	-.98890474E+03	-.22997056E+01		H2				
2	N2	28.00	2.00	3.62	97.50	0.00	0.00	15.70	VAR
.28963194E+01	.15154866E-02	-.57235277E-06	.99807393E-10	-.65223555E-14	N2				
-.90586184E+03	.61615148E+01	.36748261E+01	-.12081500E-02	.23240102E-05	N2				
-.63217559E-09	-.22577253E-12	-.10611588E+04	.23580424E+01		N2				

1	H2	2.188700E-06	6.502900E-01	H2	VISCOSITY.
1	H2	6.357900E-06	7.383300E-01	H2	THERMAL CONDUCTIVITY.
2	N2	4.266700E-06	6.613600E-01	N2	VISCOSITY.
2	N2	6.407700E-07	7.999600E-01	N2	THERMAL CONDUCTIVITY.

1	1	H2	H2	1.119300E-04	1.661400E+00	H2	H2	BINARY DIFFUSION.
1	2	H2	N2	5.951700E-05	1.663800E+00	H2	N2	BINARY DIFFUSION.
2	2	N2	N2	1.537400E-05	1.672900E+00	N2	N2	BINARY DIFFUSION.

PRESS = 1.00

TPN = 1.0000E+03

PHN = 5.0000E-05 TMN = 1.0000E-03

1.088500E+00 9.055700E-03 A* HCB FIT A*TS**8

1.078600E+00 8.500100E-02 B* HCB FIT A*EXP(C/T)

9.542600E-01 -1.435700E-01 C* HCB FIT A*EXP(C/T)

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1  SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPDE,IC,KSKT,KSKR)
2  DIMENSION Z(30,30),IPS(30)
3  DIMENSION V(30),DV(30)
4  DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
5  COMMON/TABAB/ASP,ASP,TPN,PHN,TM,SPH,TMSPH2,TMSTP,TPENT
6  COMMON/TABP/PRESS,PSK,NPOEM
7  COMMON/TABSM/SMALL
8  COMMON/TABAM/YAB,WAB
9  DIMENSION R(20)
10 DIMENSION C(1000),H(1000),RHL M(100),ORHLM(100),CM(100)
11 DIMENSION OC(1000)
12 DIMENSION DQX(100)
13 COMMON/TABCT/RL,CPMA,H0(20),R2D(20),R2DM(20)
14 COMMON/TARMF/RHUV(IU00),ORHUV(IU00)
15 COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
16 AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.
17 C WE WANT TO AVOID DIVISION BY ZERO.
18 DO 5 K=1,NPDEM
19 IF (ABS(U(K)).LT.SMALL)U(K)=SMALL
20 IF (ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL
21 C TEST CASE. BINARY MIX OF H2 AND N2. TRANSPORT WARNATZ PAR.
22 C U = MASS FRACTIONS. Y = MASS FRACTIONS / MOLECULAR WEIGHTS.
23 YN=1.0-U( 1)
24 CALL RT(U,YN,R,NPDE,KPDE,IC,KSKR)
25 IST= 2*(IC-1)
26 OT=UPH(NPDE)* 1.000000E+03
27 IF (KSKT.GT.1)GO TO 100
28 IF (KSKR.GT.1)GO TO 125
29 C NTIS ENTHALPIES AND HEAT CAPACITIES.
30 IF (T.GT.1000.)GO TO 2000
31 C 1=1.9872*( 3.05744S10E+00+T*( 2.67652000E-03
32 *+T*( -S.80991620E-06+T*( S.52103910E-09+T*( -1.81227390E-12))))
33 OC 1=1.9872*( 2.67652000E-03+T*( -1.16198324E-05
34 *+T*( 1.65631173E-08+T*( -7.24909560E-12))))*OT
35 H 1=1.9872*( -9.88904740E+02+T*( 3.05744S10E+00
36 *+T*( 2.67652000E-03+T*( -5.80991620E-06+T*(
37 *+T*( S.52103910E-09+T*( -1.81227390E-12/S.0))))))
38 C 2=1.9872*( 3.67482610E+00+T*( -1.20815000E-03
39 *+T*( 2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13))))
40 UC 2=1.9872*( -1.20815000E-03+T*( 4.64802040E-06
41 *+T*( -1.89652677E-09+T*( -9.03090120E-13))))*OT
42 H 2=1.9872*( -1.06115880E+03+T*( 3.67482610E+00
43 *+T*( -1.20815000E-03+T*( 2.32401020E-06+T*(
44 *+T*( -6.32175590E-10+T*( -2.25772530E-13/S.0))))))
45 GO TO 3000
46 CONTINUE
47 C 1=1.9872*( 3.10019010E+00+T*( S.11194640E-04
48 *+T*( S.26442100E-08+T*( -3.4909730E-11+T*( 3.694534S0E-15))))
49 OC 1=1.9872*( 5.11194640E-04+T*( 1.05288420E-07
50 *+T*( -1.04729919E-10+T*( 1.4771380E-14))))*OT
51 H 1=1.9872*( -8.77380420E+02+T*( 3.10019010E+00
52 *+T*( S.11194640E-04+T*( 5.26442100E-08+T*(
53 *+T*( -3.4909730E-11+T*( 3.694534S0E-15/S.0))))))
54 C 2=1.9872*( 2.89631940E+00+T*( 1.51548660E-03
55 *+T*( -S.72352770E-07+T*( 9.98113930E-11+T*( -6.52233550E-15))))
56 OC 2=1.9872*( 1.51548660E-03+T*( -1.14470554E-06
57 *+T*( 2.99422179E-10+T*( -2.50444220E-14))))*OT
58

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      H 2=1.9872*(-9.05861840E+02+T*( 2.89631940E+00
      * +T*( 1.51548660E-03/2.0+T*( -5.72352770E-07/3.0
      * +T*( 9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))
      3000 CONTINUE
      C SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
      C(IST+1)=C 1/ 2.00
      DC(IST+1)=DC 1/ 2.00
      H(IST+1)=H 1/ 2.00
      C(IST+2)=C 2/ 28.00
      DC(IST+2)=DC 2/ 28.00
      H(IST+2)=H 2/ 28.00
      125 CONTINUE
      C VISCOSITY FROM WARNATZ ST PAR.
      C LEAST SQUARES FIT, T=300,2000.
      C THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
      C LEAST SQUARES FIT, T=300,2000.
      C V 1= 2.188700E-06*(T** 6.502900E-01)
      C V 2= 4.266700E-06*(T** 6.613600E-01)
      C RL 1= 6.357900E-06*(T** 7.383300E-01)
      C RL 2= 6.407700E-07*(T** 7.999600E-01)
      C BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
      C LEAST SQUARES FIT, T=300,2000.
      C PRESS = 1.00
      C D 1 1= 1.119300E-04*(T** 1.661400E+00)
      C D 1 2= 5.951700E-05*(T** 1.663800E+00)
      C D 2 2= 1.537400E-05*(T** 1.672900E+00)
      C DEFINE USEFUL COMBINATIONS AND DERIVATIVES
      YS=Y 3
      X 1=Y 1/Y
      X 2=Y 2/Y
      U 1=U( 1)
      DU 1=UPH( 1)
      DUU 1=UPH2( 1)
      U 2=1.0-U 1
      DU 2=-DU 1
      DUU 2=-DUU 1
      DY 1=DU 1/ 2.00
      DY 2=DU 2/ 28.00
      DYS=+DY 1+DY 2
      DDY 1=DUU 1/ 2.00
      DDY 2=DUU 2/ 28.00
      DDYS=+DDY 1+DDY 2
      C TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03
      DRH=- 1.218769043266E-02*(DT/T+DYS/YS)/(T*YS)
      DYS=DYS/(YS*YS)
      DYSYS0=(DYS/YS)**2
      DX 1=DY 1/Y-YS 1*DY
      DX 2=(DDY 1-2.0*DY 1*DYS/YS+2.0*Y 1*DDYS/YS)/YS
      CSZR 1= 3.571428571429E-03
      UCSZR 1=0.0
      CZ 1 1=1.0+ 1.061032953946E+00*(CSZR 1)
      DCZ 1 1= 1.061032953946E+00*(UCSZR 1)
      CINT 1=C(IST+1)* 1.006441223833E+00-2.5
      DCINT 1=DC(IST+1)* 1.006441223833E+00
      CSC 1=CSZR 1/CINT 1
      DCSC 1=(DCSZR 1-CSZR 1*DCINT 1)/CINT 1
      DX 2=DY 2/Y-YS 2*DY

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04/15/80 14.18.15

FTN 4.8*498

76/76 OPT=1 ROUNDED=+*/ TRACE

SUBROUTINE F

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115 DUX 2=10DY 2-2.0*UY 2*UDYS/YS+2.0*Y 2*UDYSQ-Y 2*UDYS/YS)/YS
    CSZR 2= 6.369426751592E-02+ 1.751045651893E+00/
    * SURT(T)+ 3.483292299373E+01/T
    DCZR 2=- ( 8.755228259466E-01/SURT(T)+ 3.483292299373E+01/T)*DT/T
    CZ 2 2=1.0+ 1.061032953946E+00*(CSZR 2)
    DCZ 2 2= 1.061032953946E+00*(DCZR 2)
    CINT 2=C(IST+ 2)* 1.409017713366E+01-2.5
    UCINT 2=DC(IST+ 2)* 1.409017713366E+01
    CSC 2=CSZR 2/CINT 2
    DCSC 2=(DCZR 2-CSZR 2*DCINT 2/CINT 2)/CINT 2
    X 1 1=X 1*X 1
    UX 1 1=DX 1*X 1*X 1*UX 1
    VU 1 1= 8.934155275619E+03*(T**(-1.661400E+00))
    DVU 1 1= -1.484320557491E+04*(T**(-2.661400E+00))*DT
    XSD 1 1=X 1 1*VD 1 1
    UXSD 1 1=DX 1 1*VD 1 1*X 1 1*VDV 1 1
    X 1 2=X 1*X 2
    UX 1 2=DX 1*X 2*X 1*UX 2
    VD 1 2= 1.680192213989E+04*(T**(-1.663800E+00))
    VVD 1 2= -2.795503805635E+04*(T**(-2.663800E+00))*DT
    XSD 1 2=X 1 2*VD 1 2
    UXSD 1 2=DX 1 2*VD 1 2*X 1 2*VDV 1 2
    CZ 1 2=1.0+ 5.305164769730E-01*(CSZR 1+CSZR 2)
    UCZ 1 2= 5.305164769730E-01*(DCSZR 1+DCSZR 2)
    X 2 2=X 2*X 2
    UX 2 2=DX 2*X 2*X 2*UX 2
    VD 2 2= 6.504488096787E+04*(T**(-1.672900E+00))
    DVD 2 2= -1.088135813711E+05*(T**(-2.672900E+00))*DT
    XSD 2 2=X 2 2*VD 2 2
    UXSD 2 2=DX 2 2*VD 2 2*X 2 2*VDV 2 2
    SXSD 1=X 2*VD 1 2
    USXSD 1=DX 2*VD 1 2*X 2*VDV 1 2
    SXSD 2=X 1*VD 1 2*X 3*VD 2 3
    DSXSD 2=DX 1*VD 1 2*X 1*VDV 1 2*DX 3*VD 2 3*X 3*VDV 2 3
    SXSD 2=X 1*VD 1 2
    USXSD 2=DX 1*VD 1 2*X 1*VDV 1 2
    STV 1= 4.568922191255E+05*(T**(-1.650290E+00))
    USTV 1= -7.540046603006E+05*(T**(-2.650290E+00))*DT
    XSTV 1=X 1 1*STV 1
    UXSTV 1=DX 1 1*STV 1*X 1 1*VDV 1 1
    STV 2= 2.343731689596E+05*(T**(-1.661360E+00))
    USTV 2= -3.893782079828E+05*(T**(-2.661360E+00))*DT
    XSTV 2=X 2 2*STV 2
    UXSTV 2=DX 2 2*STV 2*X 2 2*VDV 2 2
    C SPECIFIC HEAT OF THE MIXTURE. THIS FORMULA.
    CM(TIC)=C(IST+ 1)*U 1+C(IST+ 2)*U 2
    C DIFFUSION AND HEAT FLUX.
    C SEE DIXON-LEWIS.
    C 11. TRANSPORT PHENOMENA IN MULTICOMPONENT SYSTEMS.
    C LM 00+00
    Z( 1, 1)=0.0
    Z( 2, 2)=0.0
    Z( 1, 2)=XSD 1 2+ 1.400000000000E+01*X 2*XSD 1
    Z( 2, 1)=XSD 1 2+ 1.400000000000E+01*(UX 2*XSD 1+X 2*USXSD 1)
    Z( 2, 1)=XSD 1 2+ 7.142857142857E-02*X 1*XSD 2
    Z( 2, 1)=XSD 1 2+ 7.142857142857E-02*(UX 1*XSD 2+X 1*USXSD 2)
    C FIND T*, A*, R*, AND C*.

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175      TS=1/ 6.086871E+01
        DT=DT/ 6.086871E+01
        AST 1 2= 1.088500E+00*(TS**(-9.055700E-03))
        DAST 1 2= 9.857129450000E-03*DT*(TS**(-9.909443E-01))
        EX=EXP( 8.500100E-02/TS)
        BST 1 2= 1.078600E+00*EX
        DBST 1 2= -9.168208E-02*DT*EX/(TS*TS)
        EX=EXP(-1.435700E-01/TS)
        CST 1 2= 9.542600E-01*EX
        DCST 1 2= 1.370031E-01*DT*EX/(TS*TS)
C      LM 00,10 AND LM 10,00
        CT= -1.66666666667E-01*(1.2*CT 1 2-1.0)
        DCT= -2.000000000000E-01*DCST 1 2
        Z( 1, 4)=CT*XSD 1 2
        DZ 1S 4=CT*DXSD 1 2+DCT*XSD 1 2
        CT= -2.333333333333E+00*(1.2*CT 1 2-1.0)
        DCT= -2.800000000000E+00*DCST 1 2
        Z( 2, 3)=CT*XSD 1 2
        DZ 2S 3=CT*DXSD 1 2+DCT*XSD 1 2
        Z( 1, 3)=-Z( 2, 3)
        DZ 1S 3=-DZ 2S 3
        Z( 2, 4)=-Z( 1, 4)-Z( 3, 4)
        DZ 2S 4=-DZ 1S 4-DZ 3S 4
        Z( 2, 4)=-Z( 1, 4)
        DZ 2S 4=-DZ 1S 4
        Z( 3, 1)=Z( 1, 3)
        DZ 3S 1=DZ 1S 3
        Z( 3, 2)=Z( 2, 3)
        DZ 3S 2=DZ 2S 3
        Z( 4, 1)=Z( 1, 4)
        DZ 4S 1=DZ 1S 4
        Z( 4, 2)=Z( 2, 4)
        DZ 4S 2=DZ 2S 4
C      LM 01,00 AND LM 00,01
        Z( 5, 1)=0.0
        Z( 5, 2)=0.0
        Z( 6, 1)=0.0
        Z( 6, 2)=0.0
        Z( 1, 5)=0.0
        Z( 1, 6)=0.0
        Z( 2, 5)=0.0
        Z( 2, 6)=0.0
C      LM 10,10
        CT= 6.22222222222E-02*(13.75-3.0*BST 1 2-4.0*AST 1 2+CT 1 2)
        DCT=- 6.22222222222E-02*(3.0*DT*ST 1 2+4.0*(AST 1 2+DCT 1 2
          *+DAST 1 2+CT 1 2))
        Z( 3, 4)=CT*XSD 1 2
        DZ 3S 4=CT*DXSD 1 2+DCT*XSD 1 2
        Z( 4, 3)=Z( 3, 4)
        DZ 4S 3=DZ 3S 4
        CT= -4.062563477554E-02*CT 1 1
        DCT= -4.062563477554E-02*DCZ 1 1
        CT 2= 2.488888888889E-01*AST 1 2*CT 1 2
        DCT 2= 2.488888888889E-01*(DAST 1 2+CT 1 2+AST 1 2+DCT 1 2)
        CT 2= 5.47777777777E+00- 2.61333333333E+00*HST 1 2+CT 2
        DCT 2=- 2.61333333333E+00*DHST 1 2+DCT 2
        Z( 3, 3)=CT*XSTV 1-XSD 1 2*CT 2

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04/15/80 14.18.15

FTN 4.8+498

76/76 OPT=1 ROUND=+*/ THACE

SUBROUTINE F

```
230      DZ 3S 3=CT*DXSTV 1+DCT*XSTV 1-DXSD 1 2*CT 2-XSD 1 2*DCST 2
      CT= -5.687588868576E-01*CZ 2 2
      DCT= -5.687588868576E-01*UCZ 2 2
      CT 1= 2.4888888888889E-01*AST 1 2*CT 1 2
      DCT 1= 2.4888888888889E-01*(DAST 1 2*CT 1 2+AST 1 2*DCST 1 2)
      CT 1= 6.4561111111111E+00- 1.3333333333333E-02*BST 1 2*CT 1
      DCT 1= 1.3333333333333E-02*BST 1 2*DCST 1
      DZ 4S 4=CT*DXSTV 2-XSD 1 2*CT 1
      DZ 4S 4=CT*DXSTV 2+DCT*XSTV 2-DXSD 1 2*CT 1-XSD 1 2*DCST 1
      C LM 10*01 AND LM 01*10
      CT= 2.970892271049E+00*AST 1 2*DCSC 2
      DCT= 2.970892271049E+00*(DAST 1 2*DCSC 2+AST 1 2*DCSC 2)
      Z( 3, 6)=XSD 1 2*CT
      DZ 3S 6=DXSD 1 2*CT+XSD 1 2*DCST
      CT= 2.122065907892E-01*AST 1 2*DCSC 1
      DCT= 2.122065907892E-01*(DAST 1 2*DCSC 1+AST 1 2*DCSC 1)
      Z( 4, 5)=XSD 1 2*CT
      DZ 4S 5=DXSD 1 2*CT+XSD 1 2*DCST
      CT= 6.465770590774E-02*DCSC 1
      DCT= 6.465770590774E-02*DCSC 1
      CT 2= 2.122065907892E-01*AST 1 2*DCSC 1
      DCT 2= 2.122065907892E-01*(DAST 1 2*DCSC 1+AST 1 2*DCSC 1)
      Z( 3, 5)=CT*XSTV 1+CT 2*XSD 1 2
      DZ 3S 5=CT*DXSTV 1+DCT*XSTV 1+CT 2*DXSD 1 2+DCT 2*XSD 1 2
      CT= 9.052078827083E-01*DCSC 2
      DCT= 9.052078827083E-01*DCSC 2
      CT 1= 2.970892271049E+00*AST 1 2*DCSC 2
      DCT 1= 2.970892271049E+00*(DAST 1 2*DCSC 2+AST 1 2*DCSC 2)
      Z( 4, 6)=CT*XSTV 2+CT 1*XSD 1 2
      DZ 4S 6=CT*DXSTV 2+DCT*XSTV 2+CT 1*DXSD 1 2+DCT 1*XSD 1 2
      Z( 5, 3)=Z( 3, 5)
      DZ 5S 3=DZ 3S 5
      Z( 5, 4)=Z( 4, 5)
      DZ 5S 4=DZ 4S 5
      Z( 6, 3)=Z( 3, 6)
      DZ 6S 3=DZ 3S 6
      Z( 6, 4)=Z( 4, 6)
      DZ 6S 4=DZ 4S 6
      C LM 01*01
      Z( 5, 6)=0.0
      Z( 6, 5)=0.0
      CTM=-6.25/CINT 1
      DCTM=6.25*DCINT 1/(CINT 1*CINT 1)
      CT= 1.551784941786E-02*DCSC 1
      DCT= 1.551784941786E-02*DCSC 1
      CT 2=1.0+ 5.456740906008E-02*AST 1 2*DCSC 1
      DCT 2= 5.456740906008E-02*(DAST 1 2*DCSC 1+AST 1 2*DCSC 1)
      SUM=CT*XSTV 1+XSD 1 1+CT 2*XSD 1 2
      USUM=DCT*XSTV 1+CT*DXSTV 1+DXSD 1 1+CT 2*DXSD 1 2+DCT 2*XSD 1 2
      Z( 5, 5)=CTM*SUM
      DZ 5S 5=DCTM*SUM+CTM*DSUM
      CTM=-6.25/CINT 2
      DCTM=6.25*DCINT 2/(CINT 2*CINT 2)
      CT= 2.172498918500E-01*DCSC 2
      DCT= 2.172498918500E-01*DCSC 2
      CT 1=1.0+ 1.069521217578E+01*AST 1 2*DCSC 2
      DCT 1= 1.069521217578E+01*(DAST 1 2*DCSC 2+AST 1 2*DCSC 2)
      Z( 5, 4)=1.069521217578E+01*AST 1 2*DCSC 2
      DCT 1= 1.069521217578E+01*(DAST 1 2*DCSC 2+AST 1 2*DCSC 2)
```

```

SUM=CT*XSTV 2*XSD 2 2*CT 1*XSD 1 2
DSUM=DT*XSTV 2*CT*UXSTV 2*DXSD 2 2*CT 1*DXSD 1 2+DCT 1*XSD 1 2
Z( 6, 6)=CTM*SUM
DZ 6S 6=DCTM*SUM+CTM*DSUM
C SOLVE FOR DIFFUSION VELOCITIES AND ENERGY FLUX.
CALL DEC( 6,30,Z,V,IER)
V( 1)=RH*DX 1/ S.0000000E-05
V( 1)=(DRH*DX 1+RH*DX 1)/ S.0000000E-05
V( 2)=RH*DX 2/ S.0000000E-05
V( 2)=(DRH*DX 2+RH*DX 2)/ S.0000000E-05
V( 3)=0.0
DV 3=0.0
V( 4)=0.0
DV 4=0.0
V( 5)=0.0
DV 5=0.0
V( 6)=0.0
DV 6=0.0
CALL SOL( 6,30,Z,V,1PS)
DV( 1)=DV 1-DZ 1S 2*V( 2)-DZ 1S 3*V( 3)-DZ 1S 4*V( 4)
DV( 2)=DV 2-DZ 2S 1*V( 1)-DZ 2S 3*V( 3)-DZ 2S 3*V( 3)-
* DZ 2S 4*V( 4)
DV( 2)=DV 2-DZ 2S 1*V( 1)-DZ 2S 3*V( 3)-DZ 2S 4*V( 4)
DV( 3)=DV 3-DZ 3S 1*V( 1)-DZ 3S 2*V( 2)-DZ 3S 3*V( 3)-
* DZ 3S 4*V( 4)-DZ 3S 5*V( 5)-DZ 3S 6*V( 6)
DV( 4)=DV 4-DZ 4S 1*V( 1)-DZ 4S 2*V( 2)-DZ 4S 3*V( 3)-
* DZ 4S 4*V( 4)-DZ 4S 5*V( 5)-DZ 4S 6*V( 6)
DV( 5)=DV 5-DZ 5S 3*V( 3)-DZ 5S 4*V( 4)-DZ 5S 5*V( 5)
DV( 6)=DV 6-DZ 6S 3*V( 3)-DZ 6S 4*V( 4)-DZ 6S 6*V( 6)
CALL SOL( 6,30,Z,DV,1PS)
VX 1=V( 1)
DVX 1=DV( 1)
VX 2=V( 2)
DVX 2=DV( 2)
V( 1)=0.0
DV 1=0.0
V( 2)=0.0
DV 2=0.0
V( 3)=X 1
DV 3=DX 1
V( 4)=X 2
DV 4=DX 2
V( 5)=X 1
DV 5=DX 1
V( 6)=X 2
DV 6=DX 2
CALL SOL( 6,30,Z,V,1PS)
DV( 1)=DV 1-DZ 1S 2*V( 2)-DZ 1S 3*V( 3)-DZ 1S 4*V( 4)
DV( 2)=DV 2-DZ 2S 1*V( 1)-DZ 2S 3*V( 3)-DZ 2S 3*V( 3)-
* DZ 2S 4*V( 4)
DV( 2)=DV 2-DZ 2S 1*V( 1)-DZ 2S 3*V( 3)-DZ 2S 4*V( 4)
DV( 3)=DV 3-DZ 3S 1*V( 1)-DZ 3S 2*V( 2)-DZ 3S 3*V( 3)-
* DZ 3S 4*V( 4)-DZ 3S 5*V( 5)-DZ 3S 6*V( 6)
DV( 4)=DV 4-DZ 4S 1*V( 1)-DZ 4S 2*V( 2)-DZ 4S 3*V( 3)-
* DZ 4S 4*V( 4)-DZ 4S 5*V( 5)-DZ 4S 6*V( 6)
DV( 5)=DV 5-DZ 5S 3*V( 3)-DZ 5S 4*V( 4)-DZ 5S 5*V( 5)
DV( 6)=DV 6-DZ 6S 3*V( 3)-DZ 6S 4*V( 4)-DZ 6S 6*V( 6)

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FIN 4.8*498

76/76 OPT=1 ROUNDO=+-*/ TRACE

SUBROUTINE F

```

345 CALL SCL( 6,30,Z,DV,1PS)
      VT 1=-2.5*RH*DT*V( 1)/(T* 5.000000E-05)
      VT 2=-2.5*RH*DT*V( 2)/(T* 5.000000E-05)
      DDT=UPH2(NPDE)* 1.000000E+03
      DVT 1=-2.5*(DRH*DT*V( 1)+RH*DDT*V( 1)-RH*DT*V( 1))*
      * DT/T)/(T* 5.000000E-05)
      DVT 2=-2.5*(DRH*DT*V( 2)+RH*DDT*V( 2)-RH*DT*V( 2))*
      * DT/T)/(T* 5.000000E-05)
      UV 1=U 1*(VX 1+VT 1)
      UV 2=U 2*(VX 2+VT 2)
      DUV 1=DU 1*(VX 1+VT 1)+U 1*(DVX 1+DVT 1)
      DUV 2=DU 2*(VX 2+VT 2)+U 2*(DVX 2+DVT 2)
      RHUV(1ST+ 1)=RH*UV 1
      RHUV(1ST+ 2)=RH*UV 2
      DRHUV(1ST+ 1)=DRH*UV 1+RH*DUV 1
      DRHUV(1ST+ 2)=DRH*UV 2+RH*DUV 2
      SUM=+X 1*V( 3)+X 2*V( 4)
      USUM=+DX 1*V( 3)+X 1*DV( 3)+DX 2*V( 4)+X 2*DV( 4)
      RLTRS= -1.513711E-01*SUM/T
      URLTRS= -1.513711E-01*(DSUM-SUM*DT/T)/T
      SUM=+X 1*V( 5)+X 1*DV( 5)+X 2*V( 6)
      USUM=+DX 1*V( 5)+X 1*DV( 5)+DX 2*V( 6)+X 2*DV( 6)
      RLINT= -1.513711E-01*SUM/T
      DRLINT= -1.513711E-01*(DSUM-SUM*DT/T)/T
      RLM=RLTRS+RLINT
      DRLM=DRLTRS+DRLINT
      RHLM(1C)=RH*RLM
      DRHLM(1C)=DRH*RLM+RH*DRLM
      SUM=+DX 1*V( 1)+DX 2*V( 2)
      DSUM=+DDX 1*V( 1)+DX 1*DV( 1)+DX 2*V( 2)+DX 2*DV( 2)
      OX= -1.210968921389E+03*RH*SUM
      DUX(1C)= -1.210968921389E+03*(D-H*SUM+RH*DSUM)
      C FIND THE TIME DERIVATIVES.
      SP=ASP+RSP*TIME
100 CONTINUE
      IF (KPDE.EQ.NPDE)GO TO 150
      RY= 1.0000000000E-03*R(KPDE)
      DY=- 2.0000000000E+01*DRHUV(1ST+KPDE)
      FVAL=SP*UPH(KPDE)+DY+RY
      RETURN
150 CONTINUE
      TL= 4.0000000000E+05*
      * (DRHLM(1C)*UPH(NPDE)+RHLM(1C)*UPH2(NPDE))
      TU=- 2.0000000000E+01*UPH(NPDE)*( +C(1ST+ 1)*RHUV(1ST+ 1) +
      * C(1ST+ 2)*RHUV(1ST+ 2))
      TH=- 1.0000000000E-06*( +R( 1)*H(1ST+ 1) +R( 2)*H(1ST+ 2))
      TX= -2.000000000000E-02*DX(1C)
      FVAL=SP*UPH(NPDE)+(TL+TH+TD+TX)/UM(1C)
      RETURN
      END

```

```

1  PROGRAM LOADF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
    * TAPE3,TAPE9,TAPE15)
2  MAIN
3  MAIN
4  MAIN
5  C LOADF CREATES THE SUBROUTINE F IN FLSC.
6  MAIN
7  DIMENSION II(72)
8  MAIN
9  DIMENSION LB(25),W(25),AU(7,25),AL(7,25)
10  DIMENSION ALO(25),BLU(25),ABD(25,25),BBU(25,25)
11  DIMENSION LBPR(25)
12  DIMENSION III(44)
13  DIMENSION LBROT(25),SGA(25),ESK(25),UM(25),ALP(25),ZROT(25),OF(25)
14  DIMENSION AV(25),BV(25)
15  WRITE(3,1000)
16  FORMAT(1HC,2X,34HWE WANT TO AVOID DIVISION BY ZERO. )
17  WRITE(3,1012)
18  FORMAT(6X,14H00 5 K=1,NPOEM)
19  WRITE(3,1014)
20  FORMAT(6X,32HIF (ABS(U(K)).LT.SMALL)U(K)=SMALL )
21  WRITE(3,1016)
22  FORMAT(1X,1H5,4X,36HIF (ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL )
23  READ(5,12)NLINE
24  C NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
25  DO 20 K=1,NLINE
26  READ(5,22)II
27  WRITE(3,22)II
28  CONTINUE
29  FORMAT(72A1)
30  FORMAT(1X,72A1/)
31  READ(5,12)NSPC
32  NM=NSPC-1
33  LHM=1H-
34  LBU=2HU(
35  LBP=1H)
36  WRITE(3,1020)((LHM,LBU,K,LBP),K=1,NM)
37  FORMAT(6X,6HYN=1,0,8(A1,A2,12,A1),A1,2/(5X,1H*,1X,
38  * 8(A2,12,A1,A1)) )
39  WRITE(3,1025)
40  FORMAT(6X,33HCALL RT(U,YN,R,NPOE,KPDE,IC,KSKR) )
41  WRITE(3,18)NSPC
42  FORMAT(6X,4HIST=,12,7H*(IC-1) )
43  C ASSUME AT MOST ONE POLAR SPECIES. (OIPOLE MUMENT NON-ZERO).
44  C THEN A* AND B* CAN BE APPROXIMATED BY LENNARD-JONES COLLISION
45  C INTEGRALS, EVEN IF THE INPUT PARAMETERS ARE STOCKMAYER.
46  DO 30 K=1,NSPC
47  READ(5,32) LB(K),W(K),OF(K),SGA(K),ESK(K),UM(K),ALP(K),ZROT(K),
48  * LBROT(K)
49  WRITE(6,34)K,LB(K),W(K),OF(K),SGA(K),ESK(K),UM(K),ALP(K),ZROT(K),
50  * LBROT(K)
51  READ(15,36)(AU(L,K),L=1,5),(III(L),L=1,5)
52  WRITE(6,36)(AU(L,K),L=1,5),(III(L),L=1,5)
53  READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
54  WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
55  READ(15,37)(AL(L,K),L=4,7),(III(L),L=1,2U)
56  WRITE(6,37)(AL(L,K),L=4,7),(III(L),L=1,2U)
57  CONTINUE
58  FORMAT(A5,7F7.0,A5)
59  FORMAT(2X,14,4X,A5,4X,7F8.2,4X,A5/)
60  FORMAT(5E15.8,5A1)

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FTN 4.8+498

PROGRAM LOADF 76/76 OPT=1 ROUND=**/ TRACE

```

37  FORMAT(4E15.8,20A1)
    READ(5,232)IPN,PHN,TMN
232  FORMAT(1P3E12.4)
    WRITE(3,27)
27   FORMAT(6X,22HIF(KSKI,GT,1)GO TO 100)
    WRITE(3,28)
28   FORMAT(6X,22HIF(KSKR,GT,1)GO TO 125 )
    READ(5,12)NLINE
    DO 40 K=1,NLINE
    READ(5,22)II
    WRITE(3,22)II
40   CONTINUE
C *****
C   ENTHALPIES AND HEAT CAPACITIES.
C *****
    WRITE(3,42)
42   FORMAT(6X,24HIF(T,GT,1000.)GO TO 2000)
    DO 50 K=1,NSPC
    WRITE(3,52)K,AL(1,K),AL(2,K)
    WRITE(3,54)AL(L,K),L=3,5)
    WRITE(3,62)K,AL(6,K),AL(1,K)
    WRITE(3,64)AL(2,K),AL(3,K)
    WRITE(3,66)AL(4,K),AL(5,K)
50   CONTINUE
52   FORMAT(6X,1HC,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
54   FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8),5H))))))
    WRITE(3,56)
56   FORMAT(6X,10HGO TO 3000)
    WRITE(3,58)
58   FORMAT(4H2000,2X,8HCONTINUE)
    DO 60 K=1,NSPC
    WRITE(3,52)K,AL(1,K),AU(2,K)
    WRITE(3,54)AU(L,K),L=3,5)
    WRITE(3,62)K,AU(6,K),AU(1,K)
    WRITE(3,64)AU(2,K),AU(3,K)
    WRITE(3,66)AU(4,K),AU(5,K)
60   CONTINUE
62   FORMAT(6X,1H*,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
64   FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/2.0,4H+T*(,1PE16.8,4H/3.0)
66   * 4H/5.0,6H))))))
    WRITE(3,68)
68   FORMAT(4H3000,2X,8HCONTINUE)
    WRITE(3,134)
134  FORMAT(1HC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES. )
    DO 140 K=1,NSPC
    WRITE(3,142)K,K,W(K)
    WRITE(3,144)K,K,W(K)
140  CONTINUE
142  FORMAT(6X,6HC(1ST+,12,3H)=C,12,1H/,F6.2)
144  FORMAT(6X,6HH(1ST+,12,3H)=H,12,1H/,F6.2)
    WRITE(3,146)
146  FORMAT(1X,3H125,2X,8HCONTINUE)
C *****
C   THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
C   READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
C   COEFFICIENTS FROM A FILE CREATED BY VALUES. CY=5.

```

```
115 C *****
      READ(5,12)NLINE
      DO 72 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
      CONTINUE
120 72 FORMAT(1HC,5X,IHV,12,1H=,1PE14.6,5H*(T**,1PE14.6,1H) )
      READ(5,12)NLINE
      DO 70 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
      CONTINUE
125 70 DO 80 K=1,NSPC
      READ(9,82)AV(K),BV(K),III
      WRITE(6,84)K,L8(K),AV(K),BV(K),III
      READ(9,82)ALD(K),BLD(K),III
      WRITE(6,84)K,L8(K),ALD(K),BLD(K),III
      CONTINUE
130 80 FORMAT(1P2E14.6,44A1)
      82 FORMAT(2X,I4,4X,A4,4X,1P2E14.6,44A1/)
      84 DO 76 K=1,NSPC
      WRITE(3,78)K,AV(K),BV(K)
      DO 90 K=1,NSPC
      WRITE(3,92)K,ALD(K),BLD(K)
      CONTINUE
135 90 CONTINUE
      92 FORMAT(6X,2HRL,12,1H=,1PE14.6,5H*(T**,1PE14.6,1H) )
      READ(5,12)NLINE
      DO 100 K=1,NLINE
      READ(5,22)II
      WRITE(3,22)II
      CONTINUE
140 100 NM=NSPC-1
      DO 110 I=1,NSPC
      DO 110 J=1,NSPC
      READ(9,82)ABD(I,J),HBD(1,J),III
      WRITE(6,112)I,J,LH(1),LB(J),ABD(I,J),HBD(1,J),III
      CONTINUE
145 110 CONTINUE
      112 FORMAT(2X,I4,4X,I4,4X,A4,4X,1P2E14.6,44A1/)
      114 HEAD(5,114)PRESS
      FORMAT(6,0)
      WRITE(3,116)PRESS
      WRITE(6,116)PRESS
      116 FORMAT(1HC,2X,7HPRESS =,F6.2)
      DO 120 I=1,NSPC
      DO 120 J=1,NSPC
      ABD(I,J)=ABD(I,J)/PRESS
      WRITE(3,122)I,J,ABD(I,J),HBD(1,J)
      CONTINUE
160 120 CONTINUE
      122 FORMAT(6X,IHD,2I2,1H=,1PE14.6,5H*(T**,1PE14.6,1H) )
      C *****
      C SPACE DERIVATIVES.
      C *****
      LHP=LH*
      WRITE(3,148)
      148 FORMAT(1HC,2X,1HHSPEACE DERIVATIVE+S.)
      NS=NSPC+1
      WRITE(3,149)NS
170 172
```

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PROGRAM LOAOF 76/76 OPT=1 ROUNO=+*/ THACE FTN 4.8+98

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149  FORMAT(6X,4HYS=Y,I2)
150  DO 150 K=1,NSPC
151  WRITE(3,152)K,K
152  CONTINUE
153  FORMAT(6X,1HX,I2,2H=Y,I2,3H/YS)
154  DO 160 K=1,NM
155  WRITE(3,162)K,K
156  WRITE(3,164)K,K
157  WRITE(3,166)K,K
158  CONTINUE
159  FORMAT(6X,1HU,I2,3H=U(,I2,1H))
160  FORMAT(6X,2H DU,I2,5H=UPH(,I2,1H))
161  FORMAT(6X,3HDDU,I2,6H=UPH2(,I2,1H))
162  LBU=1HU
163  WRITE(3,172)NSPC,((LBM,LBU,K),K=1,NM)
164  FORMAT(6X,1HU,I2,4H=1.0,8(A1,I2),A1,2(/5X,1H*,1X,
165  * 8(A1,I2,A1)) )
166  LBDU=2H DU
167  WRITE(3,174)NSPC,((LBM,LBDU,K),K=1,NM)
168  FORMAT(6X,2H DU,I2,1H=8(A1,A2,I2),A1,2(/5X,1H*,1X,
169  * 8(A2,I2,A1)) )
170  LBDU=3HDDU
171  WRITE(3,176)NSPC,((LBM,LBDU,K),K=1,NM)
172  FORMAT(6X,3HDDU,I2,1H=8(A1,A3,I2),A1,2(/5X,1H*,1X,
173  * 8(A3,I2,A1)) )
174  DO 180 K=1,NSPC
175  WRITE(3,182)K,K,W(K)
176  CONTINUE
177  FORMAT(6X,2HDY,I2,3H=DU,I2,1H/,F6.2)
178  LBDY=2HDY
179  WRITE(3,186)((LBP,LBDY,K),K=1,NSPC)
180  FORMAT(6X,4HDYS=8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
181  PSR=PRESS/R2.05
182  WRITE(3,234)TPN,PHN,TMN
183  WRITE(6,234)TPN,PHN,TMN
184  FORMAT(1HC,2X,5HTPN =,1PE12.4,6X,5HPHN =,1PE12.4,6X,
185  * 5HTMN =,1PE12.4)
186  WRITE(3,226)TPN
187  FORMAT(6X,13HDT=UPH(,PDE)*,1PE12.4)
188  WRITE(3,242)PSR
189  FORMAT(6X,5HORH=-,1PE18.10,21H*(U/T+DYS/YS)/(T*YS))
190  WRITE(3,1202)
191  FORMAT(6X,16HDYS=DYS/(YS*YS) )
192  DO 1250 K=1,NSPC
193  WRITE(3,1204)K,K,K
194  FORMAT(6X,2HDX,I2,3H=DY,I2,5H=YS-Y,I2,5H*DYYS )
195  A=ALO(K)*BLO(K)
196  H=HLD(K)-1.0
197  WRITE(3,1208)K,A,H
198  FORMAT(6X,2HDL,I2,1H=,1PE20.12,4H*(T*(,1PE14.6,5H))*DT )
199  HG=1.9R72
200  A=15.0*RG*AV(K)/(4.0*W(K))
201  H=HV(K)
202  WRITE(3,1212)K,A,H
203  FORMAT(6X,3HRLZ,I2,1H=,1PE20.12,4H*(T*(,1PE14.6,5H))*DT )
204  A=Δ*H
205  H=H-1.0

```

```

230      WRITE(3,1216)K,A,B
      FORMAT(6X,3HDLZ,12,1H=,1PE20.12,6H*(T**,(,1PE14.6,2H)),3H*DT )
      A=ABD(K,K)*BBD(K,K)
      R=HBD(K,K)-1.0
235      WRITE(3,1220)K,K,A,B
      FORMAT(6X,2HDD,212,1H=,1PE20.12,6H*(T**,(,1PE14.6,5H))*DT )
      A=I.0/AV(K)
      B=-BV(K)
240      WRITE(3,1224)K,A,B
      FORMAT(6X,2HVV,12,1H=,1PE20.12,6H*(T**,(,1PE14.6,2H)) )
      A=A*B
      B=B-1.0
245      WRITE(3,1228)K,A,B
      FORMAT(6X,3HVV,12,1H=,1PE20.12,6H*(T**,(,1PE14.6,5H))*DT )
      WRITE(3,1232)K,K,K,K
250      FORMAT(6X,4HXXSV,12,2H=X,12,2H*X,12,3H*VV,12)
      WRITE(3,1236)K,K,K,K,K,K
255      FORMAT(6X,5HDXSV,12,6H=2.0*X,12,3H*DX,12,3H*VV,12,2H*X,12,2H*X,
      * 12,4H*DVV,12)
260      CONTINUE
      DO 1300 I=1,NM
      IP=1+I
      DO 1300 J=IP,NSPC
      A=I.0/ABD(I,J)
      B=-BBD(I,J)
      WRITE(3,1258)I,J,A,B
265      FORMAT(6X,2HVD,212,1H=,1PE20.12,6H*(T**,(,1PE14.6,2H)) )
      A=A*B
      B=B-1.0
      WRITE(3,1262)I,J,A,B
270      FORMAT(6X,3HVD,212,1H=,1PE20.12,6H*(T**,(,1PE14.6,5H))*DT )
      WRITE(3,1268)((I,J),L=1,3)
      FORMAT(6X,4HXXSD,212,2H=X,12,2H*X,12,3H*VD,212)
      WRITE(3,1274)((I,J),L=1,7)
275      FORMAT(6X,5HDXSD,212,3H=DX,12,2H*X,12,2H*X,12,2H*X,12,
      * 3H*DX,12,3H*VD,212,2H*X,12,2H*X,12,4H*VD,212)
      WRITE(3,1278)I,J,1,J
280      FORMAT(6X,5HXTSD,212,5H=XXSD,212,2H*1)
      WRITE(3,1282)((I,J),L=1,3)
      FORMAT(6X,5HXTSD,212,6H=DXSD,212,7H*1+XXSD,212,3H*DT)
285      CONTINUE
      C *****
      C SPECIFIC HEAT OF THE MIXTURE.
      C *****
290      WRITE(3,124)
      FORMAT(1HC,2X,44HSPECIFIC HEAT OF THE MIXTURE. NTIS FORMULA. )
      LHC=6HC(IST+
      LHO=3H)*U
295      WRITE(3,132)((LHPL,LHC,K,LBU,K),K=1,NSPC)
      FORMAT(6X,7HCM(IC)=,4(A1,A6,12,A3,12),A1,
      * 4(/5X,1H,1X,4(A6,12,A3,12,A1)) )
300      C *****
305      C THERMAL CONDUCTIVITY OF THE MIXTURE.
310      C *****
      C BOLTZMAN CONSTANT.
      HK=1.38054E-16
      WRITE(3,272)

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FTN 4.8+498

PROGRAM LOADF 76/76 OPT=I ROUND=+*/ TRACE

```

272 WRITE(3,274)
274 FORMAT(1HC,2X,36HTHERMAL CONDUCTIVITY OF THE MIXTURE.)
276 WRITE(3,276)
276 FORMAT(1HC,2X,35HHIRSHFELDER METHOD FOR MONATOMICS. )
277 WRITE(3,277)
277 FORMAT(1HC,2X,39HP. 37A. TOULOUKIEN, LILEY, AND SAXENA. )
278 *NITS AS D*P/T.
278 WRITE(3,278)
278 FORMAT(1HC,2X,63HLMHDA=15*R*VISC/(4*M), WHERE R=82.05 CM**3-ATM/M
*OLE-K.
279 WRITE(3,279)
279 FORMAT(1HC,2X,69HTO CONVERT LAMHDA BACK TO CAL/CM-SEC-K, MULTIPLY
*BY 1.9872/82.05.
280 READ(5,82)AAS1,8AS1,I11
280 WRITE(6,123)AAS1,8AS1,I11
280 FORMAT(/2X,1P2E14.6,44A1)
280 READ(5,82) ABST,8BS1,I11
280 WRITE(6,123)ABST,8BS1,I11
280 WRITE(3,282)8AS1
282 FORMAT(6X,11HTAS1LJ=1**(.1PE14.6,1H) )
284 WRITE(3,284)8BS1
284 FORMAT(6X,11HTBS1LJ=1**(.1PE14.6,1H) )
284 BM=8AS1-1.0
284 WRITE(3,1382)8AS1,8M
284 FORMAT(6X,6HDTAST=,1PE14.6,8H*DT*1**(.1PE14.6,1H) )
284 BM=8BS1-1.0
284 WRITE(3,1384)8BS1,8M
284 FORMAT(6X,6HDT8ST=,1PE14.6,8H*DT*1**(.1PE14.6,1H) )
284 OO 280 I=1,NM
284 IP=1+1
284 DO 280 J=1P,NSPC
284 A=16.0*M*(1)*W(J)/(25.0*(W(1)+W(J))*(W(1)+W(J))*PRESS)
284 B=13.75
284 ESK1J=SORT(ESK(1)*ESK(J))
284 IF(UM(1).EQ.0.0.AND.UM(J).EQ.0.0)GO TO 287
284 C COMBINING RULE. P. 528, REID AND SHERWOOD.
284 IF(UM(1).NE.0.0)LP=1
284 IF(UM(J).NE.0.0)LP=J
284 IF(LP.EQ.1)LNP=J
284 IF(LP.EQ.J)LNP=I
284 UMP=UM(LP)*1.0E-18
284 SGC=SGA(LP)*1.0E-8
284 TPSTAH=UMP*UMP/(ESK(LP)*RK*SGC*SGC*SORT(8.0))
284 FC=1.0+(1.0/SORT(2.0))* (ALP(LNP)*TPSTAH/(SGA(LNP)**3))*
* SORT(ESK(LP)/ESK(LNP))
284 WRITE(6,1234)1J,LP,LNP,FC
284 FORMAT(4I4,1PE12.4)
284 ESK1J=ESK1J*FC*FC
287 CONTINUE
287 C=3.0*AHST/(ESK1J**8BS1)
287 D=4.0*AAS1/(ESK1J**8BS1)
287 AH=A*R
287 AC=A*C
287 AU=A*U
287 WHITE(3,286)AH,AC,AU
286 FORMAT(6X,5HCNST=,1PE20.12,1H-,1PE20.12,1H*,/5X,1H*,1X,

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```

345      * 7HTBSTLJ-,IPE20.12,7H*TASTLJ)
      WRITE(3,1386)AC,AD
1386    FORMAT(6X,6HDCNST=,IH-,IPE20.12,IH*,6HDTBST-,IPE20.12,6H*DTAST)
      WRITE(3,288)I,J,I,J
288    FORMAT(6X,2HZ(,I2,IH,12,IH,12,12H)=CONST*XXTSU,2I2)
      WRITE(3,290)I,J,I,J,I,J,I,J
290    FORMAT(6X,2HDZ,12,IHS,12,IH=CNST*DXTSU,2I2,
      * 12H*DCNST*XXTSU,2I2 )
      WRITE(3,292)J,I,I,J
292    FORMAT(6X,2HZ(,I2,IH,12,4H)=Z(,I2,IH,12,IH) )
      WRITE(3,294)J,I,I,J
294    FORMAT(6X,2HDZ,12,IHS,12,3H=OZ,I2,IHS,I2)
280    CONTINUE
      DO 300 I=I,NSPC
      DO 295 K=I,NSPC
      IF(I.EQ.K)GO TO 295
      IMIN=MIN0(I,K)
      IMAX=MAX0(I,K)
      C=16.0/(25.0*(W(I)+W(K))*(W(I)+W(K))*PRESS)
      D=7.5*W(I)*W(I)+6.25*W(K)*W(K)
      ESKIK=SQRT(ESK(I)*ESK(K))
      IF(UM(I).EQ.0.0.AND.UM(K).EQ.0.0)GO TO 299
      IF(UM(I).NE.0.0)LP=I
      IF(UM(K).NE.0.0)LP=K
      IF(LP.EQ.I)LNP=K
      IF(LP.EQ.K)LNP=I
      UMP=UM(LP)*I.0E-18
      SGC=SGA(LP)*I.0E-8
      TPSTAR=UMP*UMP/(ESK(LP)*RK*SGC*SGC*SGC*SQRT(8.0))
      FC=1.0*(1.0/SQRT(2.0))*(ALP(LNP)*TPSTAR/(SGA(LNP)**3))*
      * SQRT(ESK(LP)/ESK(LNP))
      WRITE(6,1234)I,J,LP,LNP,FC
      ESKIK=ESKIK*FC*FC
299    CONTINUE
      E=3.0*W(K)*W(K)*AHST/(ESKIK**BBST)
      F=4.0*W(I)*W(K)*AAST/(ESKIK**BAST)
      CD=C*D
      CE=C*E
      CF=C*F
      WRITE(3,296)CD,CE,CF
296    FORMAT(6X,6HDCNST=,IPE20.12,IH*,IPE20.12,IH*,5X,IH*,IX,
      * 7HTBSTLJ-,IPE20.12,7H*TASTLJ )
      WRITE(3,1396)CE,CF
1396    FORMAT(6X,6HDCNST=,IPE20.12,IH*,6HDTBST-,IPE20.12,6H*DTAST)
      WRITE(3,297)K,IMIN,IMAX
297    FORMAT(6X,IHT,I2,7H=-XXTSU,2I2,5H*CNST)
      WRITE(3,298)K,IMIN,IMAX,IMIN,IMAX
298    FORMAT(6X,2HDT,I2,7H=-DXTSU,2I2,5H*CNST,6H-XXTSU,2I2,6H*DCNST )
295    CONTINUE
      LBL=IH
      LBT=IHT
395    C GAS CONSTANT IN CM**3-ATM/MOLE-K.
      RGA=82.05
      A=-16.0*W(I)/(15.0*RGA)
      WRITE(3,302)I,I,A,I
302    FORMAT(6X,2HZ(,I2,IH,12,2H)=,I,20.12,5H*XXSV,I2,1H--)

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FTN 4.8+498

PROGRAM LOAUF 76/76 OPT=1 KOUNO=***/ TRACE

```

400      LBLP=1H(
304      IF(1.EQ.1)WRITE(3,304)LBLP,((LBHL,LBPL,LBT,K),K=2,NSPC),LBP
      FORMAT(5X,1H*,IX,2A1,10(2A1,12,A1),A1,/5X,1H*,IX,10(2A1,12,A1) )
      IF(1.EQ.NSPC)WRITE(3,304)LBLP,((LBHL,LBPL,LBT,K),K=1,NM),LBP
      IF(1.EQ.1.OR.1.EQ.NSPC)GO TO 307
405      IM=1-1
      IP=1+1
      WRITE(3,304)LBLP,((LBHL,LBPL,LBT,K),K=1,1M),((LBHL,LBPL,LBT,K),
      * K=IP,NSPC),LBP
307      CONTINUE
      WRITE(3,305)1,1,A,1
305      FORMAT(6X,2H0Z,12,1H5,12,1H=,1PE20,12,6H*UXXSV,12,1H- )
      LBDT=2H0T
306      IF(1.EQ.1)WRITE(3,306)LBLP,((LBHL,LBPL,LBT,K),K=2,NSPC),LBP
      FORMAT(5X,1H*,IX,2A1,10(A1,A2,12,A1),A1,/5X,1H*,1X,
      * 10(A1,A2,12,A1) )
415      IF(1.EQ.NSPC)WRITE(3,306)LBLP,((LBHL,LBPL,LBT,K),K=1,NM),LBP
      IF(1.EQ.1.OR.1.EQ.NSPC)GO TO 309
      IM=1-1
      IP=1+1
      WRITE(3,306)LBLP,((LBHL,LBPL,LBT,K),K=1,1M),((LBHL,LBPL,LBT,K),
      * K=IP,NSPC),LBP
309      CONTINUE
300      CONTINUE
      OO 310 K=1,NSPC
425      WRITE(3,312)K,K
310      CONTINUE
312      FORMAT(6X,2HV,(,12,3H)=X,12)
      NDIM=20
      WRITE(3,428)NSPC,NDIM
430      WRITE(3,432)NSPC,NDIM
      LBX=1HX
      LBV=3H*V(
      C CONVERT RLM FROM CM**3-ATM/CM-SEC-K TO CAL/CM-SEC-K.
      A=-4.0*RG/RGA
435      WRITE(3,316)A,((LBHL,LBPL,LBX,K,LBV,K,LBP),K=1,NSPC),LBP
      FORMAT(6X,4HRLM=,1PE14.6,2H*(,4(3A1,12,A3,12,A1),2A1,2(/5X,1H*,1X,
      * 5(A1,12,A3,12,3A1)) )
      LBDZ=2H0Z
      LBV=3H*V(
440      LBP=1H
      LHS=1HS
      LBSP=1HS
      DO 320 I=1,NSPC
445      WRITE(3,322)1,1,((LBH,LBDZ,1,LB'S,J,LBV,J,LBP),J=1,NSPC)
320      CONTINUE
322      FORMAT(6X,3H0V,(,12,4H)=OX,12,3(A1,A2,12,A1,12,A3,12,A1),A1,
      * 5(/5X,1H*,1X,4(A2,12,A1,12,A3,12,2A1)) )
      WRITE(3,546)NSPC,NDIM
      LBHL=1H
      LBX=1HX
      LBV=4H*DV(
450      LBDX=2H0X
      LBV=3H*V(
      * K=1,NSPC),LBP
      FORMAT(6X,5H0RLM=,1PE14.6,2H*(,4(3A1,12,A4,12,2A1,A2,12,A3,12,A1,
      * 5(A1,12,A3,12,3A1)) )
455      WRITE(3,326)A,((LBHL,LBPL,LBX,K,LBDV,K,LBP,LBDX,K,LBV,K,LBP),
      * K=1,NSPC),LBP
      FORMAT(6X,5H0RLM=,1PE14.6,2H*(,4(3A1,12,A4,12,2A1,A2,12,A3,12,A1,
      * 5(A1,12,A3,12,3A1)) )

```

```

460      * 2A1,10(/5X,1H*,1X,2(A1,12,A4,12,A4,12,2A1,A2,12,A3,12,3A1)) )
C THE ABOVE IS THE THERMAL CONDUCTIVITY FOR A MIXTURE OF MONATOMIC
C GASES. COMPUTE THE CORRECTION FACTOR FOR POLYATOMIC GASES.
      I=1
      LBX=IHX
      LBDV=3H*VD
      LHDV=2HDX
      LHDVD=4H*DVD
      IF (DF(1),EQ.0.0160 TO 725)
        WRITE(3,702)((LBPL,LBX,J,LBVD,I,J),J=2,NSPC)
        FORMAT(6X,4HSUM=,5(2A1,12,A3,2I2),A1,3(/5X,1H*,1X,
702      * 5(A1,12,A3,2I2,A1)) )
        WRITE(3,706)((LBPL,LHDV,J,LBVD,I,J,LBPL,LBX,J,LBDVD,I,J),J=2,NSPC)
        FORMAT(6X,5HDSUM=,2(A1,A2,12,A3,2I2,A1,12,A4,2I2),A1,
470      * 9(/5X,1H*,1X,2(A2,12,A3,2I2,2A1,12,A4,2I2,A1)) )
        WRITE(3,710)1,1,1
        FORMAT(6X,6H8=1.0,1H0,2I2,6H*SUM/X,12)
710      WRITE(3,714)((1),L=1,1)
        FORMAT(6X,5H8=DU,2I2,6H*SUM/X,12,2H+D,2I2,7H*DSUM/X,12,
475      * 2H-D,2I2,7H*SUM*DX,12,3H/(X,12,2H*X,12,1H) )
        WRITE(3,718)1,1
        FORMAT(6X,11HRLM=RLM*(RL,12,4H*RLZ,12,3H)/B )
718      WRITE(3,722)1,1,1
        FORMAT(6X,13HDLRM=DRLM*(DL,12,4H-DLZ,12,5H)/B-,(2HRL,12,4H-RLZ,
480      * 12,10H)*DB/(B*B) )
722      CONTINUE
725      DO 730 I=2,NM
        IF (DF(1),EQ.0.0160 TO 730)
          IM=I-1
          IP=I+1
          WRITE(3,702)((LBPL,LBX,J,LBVD,I,J),J=I,IM),
          * ((LBPL,LBX,J,LBVD,I,J),J=IP,NSPC)
          WRITE(3,706)((LBPL,LHDV,J,LBVD,I,J,LBPL,LBX,J,LBDVD,I,J),J=I,IM),
          * ((LBPL,LHDV,J,LBVD,I,J,LBPL,LBX,J,LBDVD,I,J),J=IP,NSPC)
          WRITE(3,710)I,1,1
          WRITE(3,714)((1),L=I,1,1)
          WRITE(3,718)I,1
          WRITE(3,722)I,1,1,1
          CONTINUE
730      I=NSPC
        IF (DF(1),EQ.0.0160 TO 735)
          WRITE(3,702)((LBPL,LBX,J,LBVD,I,J),J=I,NM)
          WRITE(3,706)((LBPL,LHDV,J,LBVD,I,J,LBPL,LBX,J,LBDVD,I,J),J=I,NM)
          WRITE(3,710)I,1,1
          WRITE(3,714)((1),L=I,1,1)
          WRITE(3,718)I,1
          WRITE(3,722)I,1,1,1
          CONTINUE
735      WRITE(3,738)
738      FORMAT(6X,15HRLM(IC)=RH*RLM)
742      WRITE(3,742)
742      FORMAT(6X,25HDLRM(IC)=RH*DRLM*(1+H*RLM) )
C *****
C SOLVE FOR UV.
C *****
400      WRITE(3,400)
        FORMAT(1HC,2X,13HSOLVE FOR UV.)

```

```
515      WRITE(3,402)NSPC
516      FORMAT(6X,2HV(,I2,5H)=0.0 )
517      DO 405 K=1,NM
518      WRITE(3,408)K,K,PHW
519      CONTINUE
520      FORMAT(6X,2HV(,I2,4H)=DX,I2,4H*KKH/,IPEI2.4 )
521      DO 410 K=1,NSPC
522      WRITE(3,412)NSPC,K,K
523      CONTINUE
524      FORMAT(6X,2HZ(,I2,IH,,I2,3H)=U,I2)
525      FORMAT(6X,2HDZ,I2,IHS,I2,3H=DU,I2)
526      DO 415 I=1,NM
527      IP=I+1
528      DO 415 J=IP,NSPC
529      WRITE(3,416)I,J,I,J
530      FORMAT(6X,2HZ(,I2,IH,,I2,6H)=XXSD,2I2)
531      IF(J.NE.NSPC)WRITE(3,416)J,I,I,J
532      WRITE(3,418)I,J,I,J
533      FORMAT(6X,2HDZ,I2,IHS,I2,6H=DXSD,2I2)
534      IF(J.NE.NSPC)WRITE(3,418)J,I,I,J
535      CONTINUE
536      I=1
537      LBXXSD=4HXXSD
538      WRITE(3,422)I,I,((LBH,LBXXSD,I,J),J=2,NSPC)
539      FORMAT(6X,2HZ(,I2,IH,,I2,2H)=,4(A1,A4,2I2),A1,
540      * 3(/5X,IH*,IX,5(A4,2I2,A1)) )
541      LBDS=5HDXSD
542      WRITE(3,424)I,I,((LBH,LBD,I,J),J=2,NSPC)
543      FORMAT(6X,2HDZ,I2,IHS,I2,IH=,4(A1,A5,2I2),A1,
544      * 3(/5X,IH*,IX,5(A5,2I2,A1)) )
545      DO 420 I=2,NM
546      IM=I-1
547      IP=I+1
548      WRITE(3,422)I,I,((LBH,LBXXSD,J,I),J=1,IM),
549      * ((LBH,LBXXSD,I,J),J=IP,NSPC)
550      WRITE(3,424)I,I,((LBH,LBD,J,I),J=1,IM),((LBH,LBD,I,J),J=IP,NSPC)
551      CONTINUE
552      WRITE(3,428)NSPC,NDIM
553      FORMAT(6X,9HCALL DEC(,I2,IH,,I2,1IH,Z,IPS,IER) )
554      WRITE(3,432)NSPC,NDIM
555      FORMAT(6X,9HCALL SOL(,I2,IH,,I2,9H,Z,V,IPS) )
556      DO 435 K=1,NSPC
557      WRITE(3,438)K,K,K
558      CONTINUE
559      FORMAT(6X,2HUV,I2,2H=U,I2,3H*V(,I2,IH) )
560      DO 440 K=1,NSPC
561      WRITE(3,442)K,K
562      CONTINUE
563      FORMAT(6X,9HRHUV(IST,.,I2,7H)=RH*UV,I2)
564      C *****
565      C SOLVE FOR THE SPACE DERIVATIVE OF UV.
566      C *****
567      WRITE(3,522)
568      FORMAT(1HC,2X,30HSPACE DER OF UTILITY TIMES UV.)
569      DO 500 K=1,NSPC
570      WRITE(3,502)K,K,K(K)
```

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PROGRAM LOADF 76/76 OPT=I ROUNO=+*+* TRACE FTN 4.8+498

```

500 CONTINUE
502 FORMAT(6X,3HDDY,I2,4H=DDU,I2,IH/,F6.2)
LDDY=3HDDY
506 WRITE(3,506)((LHPL,LHDDY,K),K=1,NSPC)
575 FORMAT(6X,5HDDYS=,8(A1,A3,I2),A1,2(/5X,1H*,1X,8(A3,I2,A1)) )
577 WRITE(3,510)
510 FORMAT(6X,18HDDYSU=(DYS/YS)**2 )
DO 515 K=1,NSPC
579 WRITE(3,518)K,K,K,K,K
580 CONTINUE
582 FORMAT(6X,3HDDX,I2,5H=(DDY,I2,7H-2.0*DY,I2,13H*DY/YS+2.0*Y,
583 * I2,9H*DDYSO-Y,I2,12H*DDYS/YS)/YS )
LHDZ=2HDZ
LHV=3H*V(
585 LBS=IHS
LBS=IHS
DO 525 I=1,NM
572 WRITE(3,528)I,I,I,PHN,((LBM,LBDZ,I,LBS,J,LBV,J,LBP),J=1,NSPC)
590 CONTINUE
592 FORMAT(6X,3HDV(I,I2,9H)=(RH*DDX,I2,7H*DRH*DX,I2,2H)/,
593 * 1PE12.4,A1,A2,I2,A1,I2,A3,I2,2A1,5(/5X,1H*,1X,
594 * 4(A2,I2,A1,I2,A3,I2,2A1)) )
I=NSPC
595 WRITE(3,532)I,((LBM,LBDZ,I,LBP,J,LBV,J,LBP),J=1,NSPC)
596 FORMAT(6X,3HDV(I,I2,2H)=,3(A1,A2,I2,A1,I2,A3,I2,A1),A1,
597 * 5(/5X,1H*,1X,4(A2,I2,A1,I2,A3,I2,2A1)) )
598 WRITE(3,546)NSPC,NDIM
599 FORMAT(6X,9HCALL SOL(,I2,IH,I2,10H,Z,DV,IPS) )
600 DO 550 K=1,NSPC
601 WRITE(3,552)K,K,K,K,K
602 CONTINUE
603 FORMAT(6X,3HDUV,I2,2H=U,I2,4H*UV(,I2,4H)+UU,I2,3H*V(,I2,IH) )
604 DO 810 K=1,NSPC
605 WRITE(3,812)K,K,K
610 CONTINUE
612 FORMAT(6X,10HDRVU(IST,*,I2,8H)=UHH*UV,I2,7H*RH*DUV,I2)
812 C *****
C FIND THE TIME DERIVATIVES.
C *****
612 WRITE(3,612)
612 FORMAT(1HC,2X,26H FIND THE TIME DERIVATIVES.)
622 WRITE(3,622)
622 FORMAT(6X,15HSP=ASP+RSP*TIME)
TMSPH2=TMN/(PHN*PHN)
615 WRITE(3,628)
615 FORMAT(1X,3H100,2X,6HCONTINUE)
632 WRITE(3,632)
632 FORMAT(6X,25HIF(KPDE.EQ.NPDE)GO TO 150)
636 WRITE(3,636)TMN
636 FORMAT(6X,3HRY=,1PE20.10,8H*(KPDE) )
TMSPH=TMN/PHN
638 WRITE(3,638)TMSPH
638 FORMAT(6X,4HDY=,1PE20.10,16H*UHH*UV(IST*KPDE) )
642 WRITE(3,642)
642 FORMAT(6X,23H FVAL=SP*UPH(KPDE)+UY+RY)
646 WRITE(3,646)
646 FORMAT(6X,6H KETURN)

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FIN 4.8+49H

PROGRAM LOADF 76/76 OPT=I ROUNO=-**/ TRACE

```

630      WRITE(3,648)
648      FORMAT(IX,3H150,2X,4HCONTINUE)
        WRITE(3,662)TMSPH2
662      FORMAT(6X,3HTL=,IPE20,I0,IH*)
        WRITE(3,664)
664      FORMAT(5X,IH*,IX,4IH(DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE)))
        LBL=IH
        LHC=6HC(IST+
        LBRHUV=10H)*RHUV(IST
        WRITE(3,668)TMSPH,((LBBL,LBPL,LHC,K,LBRHUV,LBPL,K,LBP),K=1,NSPC)
        * ,LBP
668      FORMAT(6X,4HTD=-,IPE20,I0,I2H*UPH(NPDE)*(.2AI,A6,I2,A10,AI,I2,3AI,
        * 10I/5X,IH*,IX,2(A6,I2,A10,AI,I2,3AI)) )
        TMSPT=TMN/TPN
        LBR=2HR(
        LBH=8H)*H(IST+
        WRITE(3,672)TMSPT,((LBBL,LBPL,LBR,K,LBH,K,LBP),K=1,NSPC),LBP
672      FORMAT(6X,4HTR=-,IPE20,I0,2H* (.2(2AI,A2,I2,A8,I2,A1),2AI,
        * 9I/5X,IH*,IX,2(A2,I2,A8,I2,3AI)) )
        WRITE(3,676)
676      FORMAT(6X,3SHFVAL=SP*UPH(NPDE)+ (TL+TR+TD)/CM(IC) )
        STOP
        END
650
629      MAIN
630      MAIN
631      MAIN
632      MAIN
633      MAIN
634      MAIN
635      MAIN
636      MAIN
637      MAIN
638      MAIN
639      MAIN
640      MAIN
641      MAIN
642      MAIN
643      MAIN
644      MAIN
645      MAIN
646      MAIN
647      MAIN
648      MAIN
649      MAIN
650      MAIN
651      MAIN

```

BLOCK	ADDRESS	LENGTH	FILE
LOADF	110	12777	LGO
/STP.END/	13107	1	SL-FINL18
/FCL.C./	13110	30	SL-FINL18
/QB.10./	13140	144	SL-FINL18
QENTRY=	13304	4	SL-FINL18
CUMIO=	13310	10	SL-FINL18
FECMSK=	13320	41	SL-FINL18
FEFST=	13361	3	SL-FINL18
FLTIN=	13364	156	SL-FINL18
FLTOUT=	13542	315	SL-FINL18
FMTAP=	14057	377	SL-FINL18
FORSYS=	14456	300	SL-FINL18
FORUTL=	14756	45	SL-FINL18
GETFIT=	15023	54	SL-FINL18
INCOM=	15077	144	SL-FINL18
INPC=	15243	173	SL-FINL18
KODER=	15436	476	SL-FINL18
KRAKER=	16134	454	SL-FINL18
OUTC=	16610	155	SL-FINL18
OUTCOM=	16765	204	SL-FINL18
ERRCAP=	17171	317	SL-FINL18
FERCAP=	17510	171	SL-FINL18
ALOG.	17701	63	SL-FINL18
EXP.	17764	73	SL-FINL18
EXP.MSG	20057	16	SL-FINL18
SQRT	20075	6	SL-FINL18
SQRT.	20103	32	SL-FINL18
SYS.AID=	20135	1	SL-FINL18
SYS=1ST	20136	65	SL-FINL18
SYS=AID	20223	7	SL-FINL18
XIOY*	20232	11	SL-FINL18
XIOY.	20243	32	SL-FINL18

1	H2	2.00	2.00	2.92	38.00	0.00	.79	280.00	CNST
.31001901E+01	.51119464E+03	.52644210E-07	-.34909973E-10	.36945345E-14	H2				
-.87738042E+03	-.19629421E+01	.30574451E+01	.26765200E-02	-.58099162E-05	H2				
.55210391E-08	-.18122739E-11	-.98890474E+03	-.22997056E+01		H2				
2	N2	28.00	2.00	3.62	97.50	0.00	0.00	15.70	VAR
.28963194E+01	.15154866E-02	-.57235277E-06	.99807393E-10	-.65223555E-14	N2				
-.90586184E+03	.61615148E+01	.36748261E+01	-.12081500E-02	.23240102E-05	N2				
-.63217559E-09	-.22577253E-12	-.10611588E+04	.23580424E+01		N2				
1	H2	2.188700E-06	6.502900E-01		H2				VISCOSITY.
1	H2	6.357900E-06	7.383300E-01		H2				HERMAL CONDUCTIVITY.
2	N2	4.266700E-06	6.613600E-01		N2				VISCOSITY.
2	N2	6.407700E-07	7.999600E-01		N2				HERMAL CONDUCTIVITY.

1	1	H2	H2	1.119300E-04	1.661400E+00	H2	H2	BINARY DIFFUSION.
1	2	H2	N2	5.951700E-05	1.663800E+00	H2	N2	BINARY DIFFUSION.
2	2	N2	N2	1.537400E-05	1.672900E+00	N2	N2	BINARY DIFFUSION.

PRESS = 1.00
 TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03
 1.088500E+00 9.055700E-03 A* P. 1128, HIRSHFELDER, ET. AL.
 1.129600E+00 -1.022500E-02 B* P. 1128, HIRSHFELDER, ET. AL.

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1 SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPDE,IC,KSKT,KSKR)
  DIMENSION Z(20,20),IPS(20)
  DIMENSION V(20),DV(20)
  DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
  COMMON/TABAR/ASP,ASP,TPN,PHN,IMN,TMSPH,TMSPH2,TMSTP,TPENT
  COMMON/TARP/PRESS,PSK,NPDEM
  COMMON/TARSM/SMALL
  COMMON/TARAM/YAB,WAB
  DIMENSION R(20)
  DIMENSION C(I000),H(I000),RHLM(I00),ORHLM(I00),CM(I00)
  COMMON/TABCT/RL,CPMK,H0(20),R2D(20),R2DM(20)
  COMMON/TARMF/RHUV(I000),ORHUV(I000)
  COMMON/TARRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
  C AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PUE IS RETURNED IN FVAL.
  C WE WANT TO AVOID DIVISION BY ZERO.
    00 5 K=I,NPDEM
    IF (ABS(U(K)).LT.SMALL)U(K)=SMALL
    IF (ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL
  5 C TEST CASE. BINARY MIX OF H2 AND N2. TRANSPORT WARNATZ PAR.
  C U = MASS FRACTIONS. Y = MASS FRACTIONS / MOLECULAR WEIGHTS.
    YN=1.0-U( 1)
    CALL RT(U,YN,R,NPDE,KPDE,IC,KSKK)
    IST= 2*(IC-I)
    IF (KSKT.GT.1)GO TO 100
    IF (KSKR.GT.1)GO TO 125
  25 C NTIS ENTHALPIES AND HEAT CAPACITIES.
    IF (T.GT.1000.)GO TO 2000
    C I=1.9872*( 3.05744510E+00+T*( 2.67652000E-03
      *+T*( -5.80991620E-06+T*( 5.52103910E-09+T*( -1.81227390E-12))))))
    H 1=1.9872*( -9.88904740E+02+T*( 3.05744510E+00
      *+T*( 2.67652000E-03/2.0+T*( -5.80991620E-06/3.0
      *+T*( 5.52103910E-09/4.0+T*( -1.81227390E-12/5.0))))))
    C 2=1.9872*( 3.67482610E+00+T*( -1.20815000E-03
      *+T*( 2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13))))))
    H 2=1.9872*( -1.06115880E+03+T*( 3.67482610E+00
      *+T*( -1.20815000E-03/2.0+T*( 2.32401020E-06/3.0
      *+T*( -6.32175590E-10/4.0+T*( -2.25772530E-13/5.0))))))
    GO TO 3000
  2000 CONTINUE
    C I=1.9872*( 3.10019010E+00+T*( 5.11194640E-04
      *+T*( 5.26442100E-08+T*( -3.49099730E-11+T*( 3.69453450E-15))))))
    H 1=1.9872*( -8.77380420E+02+T*( 3.10019010E+00
      *+T*( 5.11194640E-04/2.0+T*( 5.26442100E-08/3.0
      *+T*( -3.49099730E-11/4.0+T*( 3.69453450E-15/5.0))))))
    C 2=1.9872*( 2.89631940E+00+T*( 3.69453450E-15/5.0))))
    H 2=1.9872*( -9.05861840E+02+T*( 9.98073930E-11+T*( -6.52235550E-15))))
    *+T*( 1.51548660E-03/2.0+T*( -5.72352770E-07/3.0
      *+T*( 9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))
  3000 CONTINUE
  C SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
    C(IST+ 1)=C I/ 2.00
    H(IST+ 1)=H I/ 2.00
    C(IST+ 2)=C 2/ 28.00
    H(IST+ 2)=H 2/ 28.00
  125 CONTINUE
  C VISCOSITY FROM WARNATZ ST PAR.

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FTN 4.8+498

SUBROUTINE F 76/76 OPT=1 ROUNDO=+*/ TRACE

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60      C LEAST SQUARES FIT, T=300,2000.
        C THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
        C LEAST SQUARES FIT, T=300,2000.
        C V 1= 2.188700E-06*(T** 6.502900E-01)
        C V 2= 4.266700E-06*(T** 6.613600E-01)
        C RL 1= 6.357900E-06*(T** 7.383300E-01)
        C RL 2= 6.407700E-07*(T** 7.999400E-01)
65      C BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
        C LEAST SQUARES FIT, T=300,2000.
        C PRESS = 1.00
        D 1 1= 1.119300E-04*(T** 1.661400E+00)
        D 1 2= 5.951700E-05*(T** 1.663800E+00)
        D 2 2= 1.537400E-05*(T** 1.672900E+00)
70      C SPACE DERIVATIVES.
        YS=Y 3
        X 1=Y 1/Y5
        X 2=Y 2/Y5
        U 1=U( 1)
        DU 1=UPH( 1)
        DUU 1=UPH2( 1)
        U 2=1.0-U 1
        DU 2=-DU 1
        DUU 2=-DUU 1
        DY 1=DU 1/ 2.00
        DY 2=DU 2/ 28.00
        DYS=+DY 1+DY 2
80      C TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03
        DT=UPH(NPDE)* 1.0000E+03
        DRH=- 1.2187690433E-02*(DT/T+DYS/YS)/(T*YS)
        DYS=DYS/(YS*YS)
        DX 1=DY 1/YS-Y 1*DYSY
        DL 1= 4.694228307000E-06*(T**(-2.616700E-01))*DT
        RLZ 1= 8.155096200000E-06*(T**(-6.502900E-01))
        DLZ 1= 5.303177507898E-06*(T**(-3.497100E-01))*DT
        DD 1 1= 1.859605020000E-04*(T**(-6.614000E-01))*DT
        VV 1= 4.568922191255E+05*(T**(-6.502900E-01))
        DVV 1= -2.971124411751E+05*(T**(-1.650290E+00))*DT
        XXSV 1=X 1*X 1*VV 1
        DXXSV 1=2.0*X 1*DX 1*VV 1+X 1*X 1*DVV 1
        DX 2=DY 2/YS-Y 2*DYSY
        DL 2= 5.125903692000E-07*(T**(-2.000400E-01))*DT
        RLZ 2= 1.135551728571E-06*(T**(-6.613600E-01))
        DLZ 2= 7.510084912080E-07*(T**(-3.386400E-01))*DT
        DD 2 2= 2.571916460000E-05*(T**(-6.729000E-01))*DT
        VV 2= 2.343731689596E+05*(T**(-6.613600E-01))
        DVV 2= -1.550050390231E+05*(T**(-1.661360E+00))*DT
        XXSV 2=X 2*X 2*VV 2
        DXXSV 2=2.0*X 2*DX 2*VV 2+X 2*X 2*DVV 2
        VD 1 2= 1.680192213989E+04*(T**(-1.663800E+00))
        DVD 1 2= -2.795503805635E+04*(T**(-2.663800E+00))*DT
        XXSD 1 2=X 1*X 2*DVD 1 2
        DXXSD 1 2=DX 1*X 2*DVD 1 2+X 1*DX 2*DVD 1 2
        XXSD 1 2=XXSD 1 2*1
        DATSD 1 2=DXSD 1 2*(1+XXSD 1 2*1)
100      C SPECIFIC HEAT OF THE MIXTURE. NTIS FORMULA.
        CM(IC)=+C(IST+ 1)*U 1+C(IST+ 2)*U 2
105      C THERMAL CONDUCTIVITY OF THE MIXTURE.
110
111
112
113
114
115

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115 C HIRSHFELDER METHOD FOR MDNATDMICS.
C P. 37A, TOULDUKLEN, LILEY, AND SAXENA.
C NOTE IN THE FORMULA, LAMBDA MUST BE IN THE SAME UNITS AS D*P/T.
C LAMBDA=15*PI*VISC/(4*PI)*R, WHERE R=B2.05 CM**3-ATM/MOLE-K.
C TO CONVERT LAMBDA BACK TO CAL/CM-SEC-K, MULTIPLY BY 1.9872/82.05.
120 TASTLJ=T*( 9.055700E-03)
TASTLJ=T*( -1.022500E-02)
DIATSI= 9.055700E-03*DI*TI**(-9.909443E-01)
DTBST= -1.022500E-02*DT*TI**(-1.010225E+00)
CNST= 5.475555555555555E-01- 1.407397773742E-01*
* TASTLJ- 1.670532689818E-01*TASTLJ
DCNST=- 1.407397773742E-01*DTBST- 1.670532689818E-01*DIATSI
Z( 1, 2)=CNST*XTSD 1 2
DZ 1S 2=CNST*DXTSO 1 2+DCNST*XTSD 1 2
Z( 2, 1)=Z( 1, 2)
DZ 2S 1=DZ 1S 2
CNST=- 3.505777777777777E+00+ 1.970356883238E+00*
* TASTLJ- 1.670532689818E-01*TASTLJ
DCNST= 1.970356883238E+00*DTBST- 1.670532689818E-01*DIATSI
T 2=-XTSD 1 2*CNST
DT 2=-DXTSO 1 2*CNST-XTSD 1 2*DCNST
Z( 1, 1)= -2.600040625635E-02*XXSV 1-
* ( +T 2)
DZ 1S 1= -2.600040625635E-02*DXXSV 1-
* ( +DT 2)
CNST=- 4.199111111111111E+00+ 1.005284124101E-02*
* TASTLJ- 1.670532689818E-01*TASTLJ
DCNST= 1.005284124101E-02*DTBST- 1.670532689818E-01*DIATSI
T 1=-XTSD 1 2*CNST
DT 1=-DXTSO 1 2*CNST-XTSD 1 2*DCNST
Z( 2, 2)= -3.640056875889E-01*XXSV 2-
* ( +T 1)
DZ 2S 2= -3.640056875889E-01*DXXSV 2-
* ( +DT 1)
V( 1)=X 1
V( 2)=X 2
CALL DEC( 2*20,Z,IPS,IER)
CALL SCL( 2*20,Z,V,IPS)
RLM= -9.687751E-02*( +X 1*V( 1) +X 2*V( 2))
DV( 1)=DX 1-DZ 1S 1*V( 1)-DZ 1S 2*V( 2)
DV( 2)=DX 2-DZ 2S 1*V( 1)-DZ 2S 2*V( 2)
CALL SCL( 2*20,Z,DV,IPS)
DRLM= -9.687751E-02*( +X 1*DV( 1)+DX 1*V( 1) +
* X 2*DV( 2)+DX 2*V( 2))
SUM=+X 2*VD 1 2
DSUM=+DX 2*VD 1 2+X 2*DVD 1 2
B=1.0+D 1 1*SUM/X 1
DH=DD 1 1*SUM/X 1+D 1 1*DSUM/X 1-D 1 1*SUM*DX 1/(X 1*X 1)
RLM=RLM+(RL 1-RLZ 1)/H
DRLM=DRLM+(DL 1-DLZ 1)/H-(RL 1-RLZ 1)*DH/(B*B)
SUM=+X 1*VD 1 2+X 3*VD 2 3
DSUM=+DX 1*VD 1 2+X 1*DVD 1 2+X 3*VD 2 3
H=1.0+D 2 2*SUM/X 2
DH=DD 2 2*SUM/X 2+D 2 2*DSUM/X 2-D 2 2*SUM*DX 2/(X 2*X 2)
RLM=RLM+(RL 2-RLZ 2)/H
DRLM=DRLM+(DL 2-DLZ 2)/H-(RL 2-RLZ 2)*DH/(B*B)
SUM=+X 1*VD 1 2
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SUBROUTINE F 76/76 OPT=1 ROUNO=+--*/ TRACE

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175      USUM=DX 1*VD 1 2*X 1*DVD 1 2
      B=1.0+D 2 2*SUM/X 2
      DB=DD 2 2*SUM/X 2+D 2 2*DSUM/X 2-D 2 2*SUM*DX 2/(X 2*X 2)
      RLM=RLM+(RL 2-RLZ 2)/B
      DRLM=DRLM+(DL 2-DLZ 2)/B-(RL 2-RLZ 2)*DH/(B*B)
      RMLM(IC)=RH*RLM
      DRMLM(IC)=RH*DRLM+DRH*RLM
      C SOLVE FOR UV.
      V( 2)=0.0
      V( 1)=DX 1*RH/ 5.0000E-05
      Z( 2, 1)=U 1
      DZ 25 1=DU 1
      Z( 2, 2)=U 2
      DZ 25 2=DU 2
      Z( 1, 2)=XXSD 1 2
      DZ 15 2=DXSD 1 2
      Z( 1, 1)=-XXSD 1 2
      DZ 15 1=-DXSD 1 2
      Z( 2, 2)=-XXSD 1 2-XXSD 2 3
      DZ 25 2=-DXSD 1 2-DXSD 2 3
      CALL DEC( 2,20,Z,1PS,1ER)
      CALL SOL( 2,20,Z,V,1PS)
      UV 1=U 1*( 1)
      UV 2=U 2*( 2)
      RHUV(IST+ 1)=RH*UV 1
      RHUV(IST+ 2)=RH*UV 2
      C SPACE DER OF DENSITY TIMES UV.
      DDY 1=DDU 1/ 2.00
      DDY 2=DDU 2/ 28.00
      DDYS=DDY 1*DDY 2
      DYSYSQ=(DYS/YS)**2
      DDY 1=(DDY 1-2.0*DY 1*DYS/YS+2.0*Y 1*DYSYSQ-Y 1*DDYS/YS)/YS
      DDY 2=(DDY 2-2.0*DY 2*DYS/YS+2.0*Y 2*DYSYSQ-Y 2*DDYS/YS)/YS
      DV( 1)=(RH*DDX 1+DRH*DX 1)/ 5.0000E-05-DZ 15 1*(V( 1)-
      * DZ 15 2*(V( 2)
      DV( 2)=-DZ 25 1*(V( 1)-DZ 25 2*(V( 2)
      CALL SOL( 2,20,Z,DV,1PS)
      DUV 1=U 1*DV( 1)+DU 1*(V( 1)
      DUV 2=U 2*DV( 2)+DU 2*(V( 2)
      DRHUV(IST+ 1)=DRH*UV 1+RH*DUV 1
      DRHUV(IST+ 2)=DRH*UV 2+RH*DUV 2
      C FIND THE TIME DERIVATIVES.
      SP=ASP+BSP*TIME
      100 CONTINUE
      IF (KPDE.EQ.NPDE) GO TO 150
      RY= 1.000000000E-03*(KPDE)
      DY=- 2.000000000E+01*DRHUV(IST+KPDE)
      FVAL=SP*UPH(KPDE)+DY*RY
      RETURN
      150 CONTINUE
      TL= 4.000000000E+05*
      * (DRHLM(IC)*UPH(NPDE)+RMLM(IC)*UPH2(NPDE))
      TD=- 2.000000000E+01*UPH(NPDE)* ( *C(IST+ 1)*RHUV(IST+ 1) +
      * C(IST+ 2)*RHUV(IST+ 2))
      TR=- 1.000000000E-06*( *P( 1)*H(IST+ 1) +P( 2)*H(IST+ 2))
      FVAL=SP*UPH(NPDE)+ (TL+TR+TD)/CM(IC)
      RETURN

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SUBROUTINE F	76/76	OPT=1	ROUND=+-*/	IPACE	FTN 4.8+498	04/15/80	14.21.44	PAGE	5
•	END					F	230		

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PROGRAM LOADF 76/76 OPT=1 ROUND=**/ TRACE FTN 4.8+498

```

1      PROGRAM LOADF (INPUT,OUTPUT,TAPE4=INPUT,TAPE6=OUTPUT,
2      * TAPE3,TAPE9,TAPE15)
3      C  LOADF CREATES THE SUBROUTINE F IN FLSC.
4      DIMENSION II(72)
5      DIMENSION III(44)
6      DIMENSION LB(25),W(25),AU(7,25),AL(7,25)
7      DIMENSION ALD(25),HLD(25),ABD(25,25),BBD(25,25)
8      DIMENSION AV(25),BV(25)
9      DIMENSION LBPR(25)
10     WRITE(3,1000)
11     FORMAT(1HC,2X,63HFOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT T
12     *HE U VALUES OR)
13     WRITE(3,1005)
14     FORMAT(1HC,2X,62HTHEIR FIRST DERIVATIVES TO BE ZERO. THIS CAN LEA
15     *D TO DIVISION)
16     WRITE(3,1010)
17     FORMAT(1HC,2X,8HBY ZERO.)
18     WRITE(3,1012)
19     FORMAT(6X,14HDO 5 K=1,NPDEM)
20     WRITE(3,1014)
21     FORMAT(6X,32HF(ABS(U(K)).LT.SMALL)U(K)=SMALL)
22     WRITE(3,1016)
23     FORMAT(1X,1H5,4X,36HF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL)
24     READ(5,12)NLINE
25     C  NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
26     DO 20 K=1,NLINE
27     READ(5,22)II
28     WRITE(3,22)II
29     CONTINUE
30     FORMAT(72A1)
31     FORMAT(/1X,72A1/)
32     READ(5,12)NSPC
33     NM=NSPC-1
34     LBM=1H-
35     LBU=2HU(
36     LBP=1H)
37     WRITE(3,1020)((LHM,LHU,K,LBP),K=1,NM)
38     FORMAT(6X,6HYN=1.0,B(A1,A2,I2,A1),A1,2(/5X,IH*,1X,
39     * 8(A2,I2,A1,A1)) )
40     WRITE(3,1025)
41     FORMAT(6X,33HCALL RT(U,YN,R,NPUE,KPDE,IC,KSKR) )
42     WRITE(3,18)NSPC
43     FORMAT(6X,4HIST=,I2,7H*(IC-I) )
44     DO 30 K=1,NSPC
45     READ(5,32)LB(K),W(K)
46     WRITE(6,34)K,LB(K),W(K)
47     READ(15,36)(AU(L,K),L=1,5),(III(L),L=1,5)
48     WRITE(6,36)(AU(L,K),L=1,5),(III(L),L=1,5)
49     READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
50     WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(III(L),L=1,5)
51     READ(15,37)(AL(L,K),L=4,7),(III(L),L=1,20)
52     WRITE(6,37)(AL(L,K),L=4,7),(III(L),L=1,20)
53     CONTINUE
54     FORMAT(A5,7F7.0)
55     FORMAT(/2X,I4,4X,A15,4X,F8.2/)
56     FORMAT(5F15.8,5A1)
57
58

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37  FORMAT(4E15.8,20A1)
60  READ(5,232)TPN,PHN,1MN
232  FORMAT(1P3E12.4)
27  WRITE(3,27)
27  FORMAT(6X,22HIF(KSKT.GT.1)GO TO 100)
28  WRITE(3,28)
28  FORMAT(6X,22HIF(KSKK.GT.1)GO TO 125 )
65  READ(5,12)NLINE
    DO 40 K=1,NLINE
    READ(5,22)II
    WRITE(3,22)II
40  CONTINUE
70  C *****
    C ENTHALPIES AND HEAT CAPACITIES.
    C *****
42  WRITE(3,42)
75  FORMAT(6X,24HIF(T.GT.1000.)GO TO 2000)
    DO 50 K=1,NSPC
    WRITE(3,52)K,AL(1,K),AL(2,K)
    WRITE(3,54) (AL(L,K),L=3,5)
    WRITE(3,62)K,AL(6,K),AL(1,K)
    WRITE(3,64)AL(2,K),AL(3,K)
    WRITE(3,66)AL(4,K),AL(5,K)
80  CONTINUE
50  FORMAT(6X,1HC,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
52  FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8),5H))))
54  WRITE(3,56)
85  FORMAT(6X,10HG TO 3000)
    WRITE(3,58)
58  FORMAT(4H2000,2X,8HCONTINUE)
    DO 60 K=1,NSPC
    WRITE(3,52)K,AU(1,K),AU(2,K)
    WRITE(3,54) (AU(L,K),L=3,5)
    WRITE(3,62)K,AU(6,K),AU(1,K)
    WRITE(3,64)AU(2,K),AU(3,K)
    WRITE(3,66)AU(4,K),AU(5,K)
90  CONTINUE
60  FORMAT(6X,1HH,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
62  FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H+T*(,1PE16.8,4H+T*(,1PE16.8)
64  FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H+T*(,1PE16.8,4H+T*(,1PE16.8,
66  * 4H/5.0,6H))))))
    WRITE(3,68)
100  FORMAT(4H3000,2X,8HCONTINUE)
    WRITE(3,134)
134  FORMAT(1HC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES. )
    DO 140 K=1,NSPC
    WRITE(3,142)K,K,W(K)
    WRITE(3,144)K,K,W(K)
105  CONTINUE
140  FORMAT(6X,6HC(IST,12,3H)=C,12,1H/,F6.2)
142  FORMAT(6X,6HH(IST,12,3H)=H,12,1H/,F6.2)
144  WRITE(3,146)
110  FORMAT(1X,3HI25,2X,8HCONTINUE)
146  C *****
    C THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
    C READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
    C COEFFICIENTS FROM A FILE CREATED BY VALUES, CY=6.

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04/15/80 14.46.06

FTN 4.8+498

PROGRAM LOADF 76/76 OPT=1 ROUNO=**/ TRACE

```

115 C *****
116 READ(5,12)NLINE
117 DO 72 K=1,NLINE
118 READ(5,22)I1
119 WRITE(6,22)I1
120 72 WRITE(3,22)I1
121 FORMAT(1HC,5X,IHV,12,IH=,IPEI4.6,5H*(T**,IPEI4.6,IH) )
122 79 READ(5,12)NLINE
123 DO 70 K=1,NLINE
124 READ(5,22)I1
125 WRITE(3,22)I1
126 WRITE(6,22)I1
127 CONTINUE
128 DO 80 K=1,NSPC
129 READ(9,82)AV(K),HV(K),I11
130 WRITE(6,84)K,LR(K),AV(K),BV(K),I11
131 READ(9,82)ALD(K),BLD(K),I11
132 WRITE(6,84)K,LB(K),ALD(K),BLD(K),I11
133 CONTINUE
134 FORMAT(IP2EI4.6,44A1)
135 82 FORMAT(I2X,I4,4X,A4,4X,IP2EI4.6,44A1/)
136 84 DO 78 K=1,NSPC
137 WRITE(3,79)K,AV(K),BV(K)
138 CONTINUE
139 DO 90 K=1,NSPC
140 WRITE(3,92)K,ALD(K),BLD(K)
141 CONTINUE
142 90 FORMAT(6X,2HRL,I2,IH=,IPEI4.6,5H*(T**,IPEI4.6,IH) )
143 92 READ(5,12)NLINE
144 DO 100 K=1,NLINE
145 READ(5,22)I1
146 WRITE(3,22)I1
147 WRITE(6,22)I1
148 CONTINUE
149 NM=NSPC-1
150 DO 110 I=1,NSPC
151 DO 110 J=1,NSPC
152 READ(9,82)ABD(I,J),HBD(I,J),I11
153 WRITE(6,112)I,J,LB(I),LB(J),ABD(I,J),HBD(I,J),I11
154 CONTINUE
155 110 FORMAT(I2X,I4,4X,I4,4X,A4,4X,A4,4X,IP2EI4.6,44A1/)
156 112 READ(5,114)PRESS
157 FORMAT(F6.0)
158 114 WRITE(3,116)PRESS
159 116 FORMAT(1HC,2X,7HPRESS =,F6.2)
160 DO 120 I=1,NM
161 1P=I+1
162 DO 120 J=1P,NSPC
163 ABD(I,J)=ABD(I,J)/PRESS
164 WRITE(3,122)I,J,ABD(I,J),HBD(I,J)
165 CONTINUE
166 120 FORMAT(1HC,5X,IHV,212,IH=,IPEI4.6,5H*(T**,IPEI4.6,IH) )
167 122 C *****
168 C SPACE DERIVATIVES.
169 C *****
170 LbPL=1H+
171 WRITE(3,144)
172

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```

148  FORMAT(1HC,2X,18HSPACE DERIVATIVES.)
      NS=NSPC*1
      WRITE(3,149)NS
149  FORMAT(6X,4HYS=Y,I2)
      DO 150 K=1,NSPC
      WRITE(3,152)K,K
150  CONTINUE
152  FORMAT(6X,1HX,I2,2H=Y,I2,3H/YS)
      DO 160 K=1,NM
      WRITE(3,162)K,K
      WRITE(3,164)K,K
      WRITE(3,166)K,K
160  CONTINUE
162  FORMAT(6X,1HU,I2,3H=U(I,I2,1H))
164  FORMAT(6X,2HOU,I2,5H=UPH(I,I2,1H))
166  FORMAT(6X,3HODU,I2,6H=UPH2(I,I2,1H))
      LBU=1HU
172  WRITE(3,172)NSPC,((LBM,LBU,K)*K=1,NM)
      FORMAT(6X,1HU,I2,4H=1.0,8(A1,A1,I2),A1,2(/5X,1H*,1X,
      * 8(A1,I2,A1)) )
      LBDU=2HOU
174  WRITE(3,174)NSPC,((LBM,LBDU,K)*K=1,NM)
      FORMAT(6X,2HOU,I2,1H=8(A1,A2,I2),A1,2(/5X,1H*,1X,
      * 8(A2,I2,A1)) )
      LHOU=3HODU
176  WRITE(3,176)NSPC,((LBM,LHOU,K)*K=1,NM)
      FORMAT(6X,3HODU,I2,1H=8(A1,A3,I2),A1,2(/5X,1H*,1X,
      * 8(A3,I2,A1)) )
      DO 180 K=1,NSPC
      WRITE(3,182)K,K,W(K)
180  CONTINUE
182  FORMAT(6X,2HXY,I2,3H=DU,I2,1H/F6.2)
      LBDY=2HXY
186  WRITE(3,186)((LBP,LBDY,K)*K=1,NSPC)
      FORMAT(6X,4HYS=8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
      PSR=PRESS/82.05
      WRITE(3,234)TPN,PHN,TMN
      WRITE(6,234)TPN,PHN,TMN
234  FORMAT(1HC,2X,5HTPN =,1PE12.4,6X,5HPHN =,1PE12.4,6X,
      * 5HTMN =,1PE12.4)
      WRITE(3,226)TPN
226  FORMAT(6X,13HDT=UPH(NPDE)*,1PE12.4)
      WRITE(3,242)PSR
242  FORMAT(6X,5HDRH=,1PE18.10,21H*(DT/1+OYS/YS)/(T*YS))
      DO 815 I=1,NSPC
      DO 815 J=1,NSPC
      IF(1.E0.J)GO TO 815
      A=1.0/ABD(I,J)
      B=-880(I,J)
      WRITE(3,818)I,J,A,B
815  CONTINUE
818  FORMAT(6X,2HVD,I2,1H=,1PE16.8,6X,(T**(.1PE16.8,2H)) )
      DO 820 I=1,NSPC
      DO 820 J=1,NSPC
      IF(1.E0.J)GO TO 820
      A=1.0/ABD(I,J)
      H=-880(I,J)

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FTN 4.8+498

PROGRAM LOADF 76/76 OPT=I ROUND=+*/ TRACE

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230      A=A*B
      H=B-I.0
      WRITE(3,822)I,J,A,H
      CONTINUE
820      FORMAT(6X,3H0V0,2I2,1H=,1PEI6.8,6H*(T**(.1PEI6.8,5H))=DT)
822      C *****
      C SPECIFIC HEAT OF THE MIXTURE.
      C *****
235      WRITE(3,124)
124      FORMAT(1HC,2X,44HSPECIFIC HEAT OF THE MIXTURE. NTIS FORMULA. )
      LHC=6HC(1ST+
      LBU=3H)*U
      WRITE(3,132)((LBP, LHC,K,LHU,K),K=I,NSPC)
132      FORMAT(6X,7HCM(1C)=,4(AI,A6,I2,AJ,I2),AI,
      * 4(/5X,1H=,IX,4(A6,I2,A3,I2,AI)) )
      C *****
      C THERMAL CONDUCTIVITY OF THE MIXTURE.
      C *****
245      WRITE(3,272)
      WRITE(3,274)
272      FORMAT(1HC,2X,36HTHERMAL CONDUCTIVITY OF THE MIXTURE.)
274      FORMAT(1HC,2X,24HMASON AND SAXENA METHOD. )
      WRITE(3,252)
252      FORMAT(1HC,2X,55HLMIX=SUM(I) (L 1/(1.0+(SUM(J)P I J*X J)/X I))
      *I,NE,J )
      WRITE(3,254)
254      FORMAT(1HC,2X,69HP I J=(1.065/SUMT(8.0*(1.0+M I/M J)))*(1.0+SQRT((
      *M J*V I)/(M I*V J))* )
      WRITE(3,255)
255      FORMAT(1HC,2X,23HSQRT(SQRT(M I/M J))**2 )
      WRITE(3,256)
256      FORMAT(1HC,2X,45HP 1 J IS A FUNCTION OF T AND CONSTANTS. )
      WRITE(3,258)
258      FORMAT(1HC,2X,45HFOR CONVENIENCE, P I J = A*(1.0+B*T**C)**2 )
      DO 275 I=1,NSPC
      DO 275 J=1,NSPC
      IF(1.EQ.J)GO TO 275
      A=1.065/(2.0*SQRT(2.0*(1.0+W(I)/W(J))))
      B=SQRT(AV(I)/AV(J))*SQRT(SQRT(W(J)/W(I)))
      C=(BV(I)-BV(J))/2.0
      WRITE(3,271)B,C
271      FORMAT(6X,8HBTIC=1.0,1PE20.10,5H*T**(.1PE20.10,1H) )
      WRITE(3,278)I,J,A
      D=2.0*A*B*C
      E=C-I.0
      WRITE(3,279)I,J,D,E
275      CONTINUE
278      FORMAT(6X,1HP,12,1HS,I2,1H=,1PE20.10,7H*BTIC**2)
279      FORMAT(6X,2HDP,12,1HS,I2,1H=,1PE20.10,5H*T**(.1PE20.10,8H)*BTIC*U)
      LBP=1HP
      LHX=2H*X
      LHP=1HS
      K=1
      WRITE(3,282)K,((LHP,LHPS,K,LBSP,J,LHX,J),J=2,NSPC)
282      FORMAT(6X,4HSUMP,I2,1H=,5(2A1,I,A1,I2,A2,I2),A1,
      * 3(/5X,1H=,IX,5(A1,I2,A1,I2,A2,I2,A1)) )
      IF((NM.EQ.1)GO TO 284
      LOAD5

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290      DO 280 K=2,NM
          KM=K-1
          KP=K+1
          WRITE(3,282)K,((LBPL,LBPS,K,LBSP,J,LBX,J),J=1,KM),
          * ((LBPL,LBPS,K,LBSP,J,LBX,J),J=KP,NSPC)
          CONTINUE
280      CONTINUE
284      K=NSPC
          WRITE(3,282)K,((LBPL,LBPS,K,LBSP,J,LBX,J),J=1,NM)
          DO 285 K=1,NSPC
          WRITE(3,288)K,K,K
          CONTINUE
285      CONTINUE
288      FORMAT(6X,1H8,I2,9H=1.0+SUMP,I2,2H/X,I2)
          LBRL=2HRL
          LBSB=2H/B
          WRITE(3,292) ((LBPL,LBRL,K,LBSB,K),K=1,NSPC)
          FORMAT(6X,4HRLM=,6(A1,A2,I2,A2,I2),A1,3(/5X,1H*,1X,
292      * 6(A2,I2,A2,I2,A1)) )
          WRITE(3,306)
          FORMAT(6X,15HRLM(IC)=RH*RLM)
          C *****
          C DERIVATIVE OF THE THERMAL CONDUCTIVITY OF THE MIXTURE.
          C *****
          WRITE(3,312)
          FORMAT(1HC,2X,40HSPACE DER OF DENSITY TIMES THERMAL COND.,)
          DO 740 K=1,NSPC
          A=ALD(K)*BLD(K)
          B=BLD(K)-1.0
          WRITE(3,742)K,A,B
          CONTINUE
          FORMAT(6X,3HDL,I2,1H=,1PE14.6,6H*(T**(:,1PE14.6,5H))*DT )
          WRITE(3,745)
          FORMAT(6X,16HDYSY=DYS/(YS*YS) )
          DO 750 K=1,NSPC
          WRITE(3,752)K,K,K
          CONTINUE
          FORMAT(6X,2HDY,I2,3H=DY,I2,5H/YS-Y,I2,5H*DY SY )
          LBX=2H*X
          LBDX=3H*DX
          LBPS=1HP
          LDUP=2HDP
          K=1
          WRITE(3,762)K,((LBPL,LBDP,K,LBSP,J,LBX,J,LBPL,LBPS,K,LBSP,J,
          * LBDX,J),J=2,NSPC)
          IF (NM.EQ.1)GO TO 761
          DO 760 K=2,NM
          KM=K-1
          KP=K+1
          WRITE(3,762)K,((LBPL,LBDP,K,LBSP,J,LBX,J,LBPL,LBPS,K,LBSP,J,LBDX,
          * J),J=1,KM),((LBPL,LBDP,K,LBSP,J,LBX,J,LBPL,LBPS,K,LBSP,J,LBDX,J),
          * J=KP,NM)
          CONTINUE
          CONTINUE
          K=NSPC
          WRITE(3,762)K,((LBPL,LBDP,K,LBSP,J,LBX,J,LBPL,LBPS,K,LBSP,
          * J,LBDX,J),J=1,NM)
          FORMAT(6X,5HDSUMP,I2,1H=,2(A1,I2,A1,I2,A2,I2,2A1,I2,A1,I2,A3,
762

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FTN 4.8+498

THACE

76/76 OPT=I HOUND=+*/

PROGRAM LOADF

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345      * I2,A1,9(/5X,IH*,IX*2(A2,I2,A1,I2,A2,I2,2A1,I2,A1,I2,A3,I2,A1)) ) MAIN
      DO 765 K=1,NSPC
      WRITE(3,76R)K,K,K,K,K,K,K
      CONTINUE
      FORMAT(6X,2HDR,I2,IH=,6H(OSUMP,I2,5H-SUMP,I2,3H*OX,I2,2H/X,I2,
      * 3H)/X,I2)
      DO 770 K=1,NSPC
      WRITE(3,772)K,K,K,K,K,K,K
      CONTINUE
      FORMAT(6X,IHT,I2,5H=(ORL,I2,3H-RL,I2,3H*OB,I2,2H/B,I2,3H)/B,I2)
      LBT=IHT
      WRITE(3,776)((LBPL,LHT,K),K=1,NSPC)
      FORMAT(6X,5HORLM=,10(2A1,I2),A1,/5X,IH*,IX,10(A1,I2,A1) )
      WRITE(3,778)
      FORMAT(6X,25HORLM(IC)=ORH*RLM+K*H*DRLM)
      C *****
      C SOLVE FOR UV.
      C ZERO ORDER BORIS AND OHAN APPROXIMATION.
      C *****
      WRITE(3,400)
      FORMAT(1HC,2X,I3HSOLVE FOR UV.)
      LBX=IHX
      LBVD=3H*VD
      K=1
      WRITE(3,402)K,((LBPL,LBX,J,LBVD,K,J),J=2,NSPC)
      FORMAT(6X,3HSUM,I2,IH=,5(2A1,I2,3,2I2),A1,3(/5X,IH*,IX,
      * 5(A1,I2,A3,2I2,A1)) )
      IF(NM.EQ.1)GO TO 412
      DO 410 K=2,NM
      KM=K-1
      KP=K+1
      WRITE(3,402)K,((LBPL,LBX,J,LBVD,J,K),J=1,KM),((LBPL,LBX,J,
      * LBVD,K,J),J=KP,NSPC)
      CONTINUE
      CONTINUE
      K=NSPC
      WRITE(3,402)K,((LBPL,LBX,J,LBVD,J,K),J=1,NM)
      DO 415 K=1,NSPC
      WRITE(3,418)K,K,K,PHN
      CONTINUE
      FORMAT(6X,IHB,I2,2H=X,I2,4H*SUM,I2,IH*,1PLEI2.4)
      DO 420 K=1,NSPC
      WRITE(3,422)K,K
      CONTINUE
      FORMAT(6X,IHT,I2,IH=-RH*(1.0-U,I2,IH) )
      DO 425 K=1,NSPC
      WRITE(3,428)K,K,K
      CONTINUE
      FORMAT(6X,3HFAC,I2,2H=T,I2,2H/B,I2)
      DO 465 K=1,NSPC
      WRITE(3,468)K,K,K
      CONTINUE
      FORMAT(6X,IHV,I2,4H=FAC,I2,3H*UX,I2)
      DO 470 K=1,NSPC
      WRITE(3,472)K,K,K
      CONTINUE
      FORMAT(6X,2HUV,I2,2H=U,I2,2H*V,I2)

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400      LBUV=2HUV
      WRITE(3,476)((LBML,LBUD,K),K=1,NSPC)
476      FORMAT(6X,3HUV=,8(A1,A2,12),A1,2(/5X,1H*,1X,8(A2,12,A1)))
      DO 480 K=1,NSPC
      WRITE(3,482)K,K,K
480      CONTINUE
482      FORMAT(6X,2HUV,12,3H=UV,12,5H+UV*U,12)
      DO 485 K=1,NSPC
      WRITE(3,488)K,K
485      CONTINUE
488      FORMAT(6X,9HURUV(1ST,12,7H)=RH*UV,12)
C *****
C SOLVE FOR THE SPACE DERIVATIVE OF UV.
C *****
      WRITE(3,522)
522      FORMAT(1HC,2X,30HSPACE DER OF DENSITY TIMES UV.)
      DO 500 K=1,NSPC
      WRITE(3,502)K,K,K
500      CONTINUE
502      FORMAT(6X,3HDDY,12,4H=DDU,12,1H/,F6.2)
      LBDDY=3HDDY
      WRITE(3,506)((LBPL,LBDDY,K),K=1,NSPC)
506      FORMAT(6X,5HDDYS=,8(A1,A3,12),A1,2(/5X,1H*,1X,8(A3,12,A1)))
      WRITE(3,510)
510      FORMAT(6X,18HDDYSYSO=(DYS/YIS)**2)
      DO 515 K=1,NSPC
      WRITE(3,518)K,K,K,K
515      CONTINUE
518      FORMAT(6X,3HDDX,12,5H=(DDY,12,7H-2.0*DY,12,13H*DYIS/YIS+2.0*Y,
      * 12,9H*DYISYSO-Y,12,12H*DDYS/YIS)/YIS)
      LBDDX=2HDX
      LBVD=3H*VD
      LBX=1HX
      LBVDV=4H*DVD
      K=1
      WRITE(3,532)K,((LBPL,LBDDX,J,LBUD,K,J),LBPL,LBX,J,LBDDVD,K,J),
      * J=2,NSPC)
532      FORMAT(6X,4HDSUM,12,1H=,2(A1,A2,12,A3,212,2A1,12,A4,212),A1,
      * 9(/5X,1H*,1X,2(A2,12,A3,212,2A1,12,A4,212,A1)))
      IF(NM.EQ.1)GO TO 541
      DO 535 K=2,NM
      KN=K-1
      KP=K+1
      WRITE(3,532)K,((LBPL,LBDDX,J,LBUD,K,J),LBPL,LBX,J,LBDDVD,K,J),
      * J=1,KM),((LBPL,LBDDX,J,LBUD,K,J),LBPL,LBX,J,LBDDVD,K,J),J=KP,NSPC)
535      CONTINUE
      K=NSPC
      WRITE(3,532)K,((LBPL,LBDDX,J,LBUD,K,J),LBPL,LBX,J,LBDDVD,K,J),J=1,NM)
      DO 540 K=1,NSPC
      WRITE(3,542)K,K,K,K
540      CONTINUE
541      CONTINUE
542      FORMAT(6X,2HDS,12,1H=,1PE12.4,4H*(DX,12,4H*SUM,12,2H+X,12,
      * 5H*DSUM,12,1H))
      DO 545 K=1,NSPC
      WRITE(3,548)K,K,K
545      CONTINUE

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548      FORMAT(6X,2HDT,I2,I2H=-DRH*(1.0-U,I2,7H)+RH*DU,I2)
      DO 550 K=1,NSPC
      WRITE(3,552)(K,L=1,7)
      CONTINUE
550      FORMAT(6X,4HDFAC,I2,I2H=,2HDT,I2,2H/B,I2,2H-T,I2,3H*DR,I2,
552      * 3H/(B,I2,2H*B,I2,1H) )
      DO 590 K=1,NSPC
      WRITE(3,592)K,K,K,K,K
      CONTINUE
590      CONTINUE
592      FORMAT(6X,2HUV,I2,5H=DFAC,I2,3H*UX,I2,4H+FAC,I2,4H*OXX,I2)
      DO 595 K=1,NSPC
      WRITE(3,598)K,K,K,K,K
      CONTINUE
595      CONTINUE
598      FORMAT(6X,3HUV,I2,3H=DU,I2,2H*V,I2,2H+U,I2,3H*DV,I2)
      LDUV=3HUV
      WRITE(3,802)((LHM,LBDUV,K),K=1,NSPC)
      FORMAT(6X,4HDDV=,8(A1,A3,I2),A1,2(/5X,IH*,IX,8(A3,I2,A1))) )
      DO 805 K=1,NSPC
      WRITE(3,808)K,K,K,K,K
      CONTINUE
805      CONTINUE
808      FORMAT(6X,3HUV,I2,4H=DUV,I2,6H+UV*DU,I2,6H+DDV*U,I2)
      DO 810 K=1,NSPC
      WRITE(3,812)K,K,K
      CONTINUE
810      CONTINUE
812      FORMAT(6X,10HURUV(IST*,I2,8H)=URH*UV,I2,7H+RH*DUV,I2)
      C *****
      C FIND THE TIME DERIVATIVES.
      C *****
      WRITE(3,612)
      FORMAT(1HC,2X,26HFINO THE TIME DERIVATIVES.)
      WRITE(3,622)
      FORMAT(6X,15HSP=ASP*8SP*TIME)
      TMSPH2=TMN/(PHN*PHN)
      WRITE(3,628)
      FORMAT(1X,3H100,2X,8HCONTINUE)
      WRITE(3,632)
      FORMAT(6X,25HIF(KPDE.EQ.NPDE)GO TO 150)
      WRITE(3,636)TMN
      TMSPH=TMN/PHN
      WRITE(3,638)TMSPH
      FORMAT(6X,4HUY=,IPE<0.10,16H*URHUV(IST+KPDE) )
      WRITE(3,642)
      FORMAT(6X,23HFVAL=SP*UPH(KPDE)+UY*RY)
      WRITE(3,646)
      FORMAT(6X,6HRETURN)
      WRITE(3,648)
      FORMAT(1X,3H150,2X,8HCONTINUE)
      DO 650 K=1,NM
      WRITE(3,652)K,K
      CONTINUE
650      CONTINUE
652      FORMAT(6X,2HUU,I2,5H=UPH(,I2,1H) )
      K=NSPC
      LDUU=2HUU
      WRITE(3,656)K,((LBM,LDDU,J),J=1,NM)
      FORMAT(6X,2HUU,I2,IH=,8(A1,A2,1/),A1,2(/5X,1H*,IX,8(A2,I2,A1)) )
      WRITE(3,662)TMSPH2

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PROGRAM	LOADF	76/76	OPT=1	ROUND=+--*/	TRACE	FTN	4.8+498	04/15/80	14.46.06	PAGE	10	
515	662	FORMAT(6X,3HTL=,1PE20.10,1H*)										507
		WRITE(3,664)										508
	664	FORMAT(5X,1H*,1X,41H(ORHLM(1C)*UPH(NPDE)+RHLM(1C)*UPH2(NPDE)))										509
		LBBL=1H										510
		LBC=6HC(1ST+										511
		LBRHUV=10H)*RHUV(1ST										512
520		WRITE(3,668)TMSPH,((LBBL,LBPL,LHC,K,LBRHUV,LBPL,K,LBP),K=1,										513
		* NSPC),LBP										514
	668	FORMAT(6X,4HID=-,1PE20.10,12H*UPH(NPDE))*((2A1,A6,12,A10,A1,12,										515
		* 3A1,10(/5X,1H*,1X,2(A6,12,A10,A1,12,3A1)))										516
		TMSPT=TMN/TPN										517
525		LBR=2HR(										518
		LRH=8H)*H(1ST+										519
		WRITE(3,672)TMSPT,((LBBL,LBPL,LHC,K,LBP),K=1,NSPC),LBP										520
	672	FORMAT(6X,4HTR=-,1PE20.10,2H*((2A1,A2,12,A8,12,A1),2A1,										521
		* 9(/5X,1H*,1X,2(A2,12,A8,12,3A1)))										522
		WRITE(3,676)										523
530	676	FORMAT(6X,3SHFVAL=SP*UPH(NPDE))*((TL+TR*TD)/CM(1C))										524
		STOP										525
		END										526

SCOPE 2 LOAD MAP
PROGRAM WILL BE ENTERED AT LOADF

BLOCK	ADDRESS	LENGTH	FILE
LOADF	1110	11104	LGO
/STP.END/	11214	1	SL-F TNL1
/FCL.C./	11215	30	SL-F TNL1
/Q8.10./	11245	144	SL-F TNL1
Q2NTRY=	11411	4	SL-F TNL1
COM10=	11415	10	SL-F TNL1
FECMSK=	11425	41	SL-F TNL1
FEIFST=	11466	3	SL-F TNL1
FLFLIN=	11471	156	SL-F TNL1
FLFIOUT=	11647	315	SL-F TNL1
FMTAP=	12164	377	SL-F TNL1
FORSYS=	12563	300	SL-F TNL1
FORUTL=	13063	45	SL-F TNL1
GETFLIT=	13130	54	SL-F TNL1
IINCOM=	13204	144	SL-F TNL1
INPC=	13350	173	SL-F TNL1
KODER=	13543	476	SL-F TNL1
KRAKER=	14241	454	SL-F TNL1
UUTC=	14715	155	SL-F TNL1
UUTCOM=	15072	204	SL-F TNL1
ERRCAP=	15276	317	SL-F TNL1
FERCAP=	15615	171	SL-F TNL1
EXP.MSG	16006	16	SL-F TNL1
ISORT	16024	6	SL-F TNL1
ISORT.	16032	32	SL-F TNL1
SYS:=	16064	1	SL-F TNL1
SYS:=1ST	16065	65	SL-F TNL1

1	H2	2.00
---	----	------

H2	-.31001901E+01	.51119464E-03	.52644210E-07	-.34909973E-10	.36945345E-14
H2	-.87738042E+03	-.19629421E+01	.30574451E+01	.26765200E-02	-.58099162E-05
H2	.55210391E-08	-.18122739E-11	-.98890474E+03	-.22997056E+01	

?	N2	28.00
28963194E+01	.15154866E-02	-.5
-90586184E+03	.61615148E+01	.3
-.63217559E-09	-.22577253E-12	.1
VISCOSITY FROM WAINALZ ST PAR.		
LEAST SQUARES FIT,	T=300+2000.	
LEAST SQUARES FIT,	T=300+2000.	
LEAST SQUARES FIT,	T=300+2000.	

Run	Temperature, °C	Time, min	Viscosity, cP	Thermal Conductivity, W/mK
1	110	10	2.188700E-06	6.502900E-01
2	110	10	6.357900E-06	7.383300E-01
3	110	10	4.266700E-06	6.613600E-01
4	110	10	6.407700E-07	7.999600E-01

BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
 LEAST SQUARES FIT, $T=300.2000$.

1	1	H2	H2	1.119300E-04	1.661400E+00	H2	H2	BINARY DIFFUSION.
1	2	H2	N2	5.951700E-05	1.663800E+00	H2	N2	BINARY DIFFUSION.
2	2	N2	N2	1.537400E-05	1.672900E+00	N2	N2	BINARY DIFFUSION.

TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03

04/15/80 14.46.29

FTN 4.8+498

76/76 OPT=1 ROUNO=-*/ THACE

SUBROUTINE F

```

1  SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPDE,IC,KSKT,KSKR)
2  DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
3  COMMON/TABAB/ASP,RSP,TPN,PHN,TMN,TMSPH,TMSPH2,TMSTP,TPENT
4  COMMON/TARP/PRESS,PSK,NPDEM
5  COMMON/TARSM/SMALL
6  COMMON/TARAM/YAB,WAH
7  DIMENSION R(20)
8  DIMENSION C(1000),H(1000),RHLM(100),DRHLM(100),CM(100)
9  COMMON/TABCT/RL,CPMA,H0(20),R2D(20),R2DM(20)
10 COMMON/TABMF/RHUV(1000),DRHUV(1000)
11 COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
12 C AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.
13 C FOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT THE U VALUES OR
14 C THEIR FIRST DERIVATIVES TO BE ZERO. THIS CAN LEAD TO DIVISION
15 C BY ZERO.
16 DO 5 K=1,NPDEM
17 IF (ABS(U(K)).LT.SMALL)U(K)=SMALL
18 IF (ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL
19 S TEST CASE. BINARY MIX OF H2 AND N2. TRANSPORT WARNATZ PAR.
20 C U = MASS FRACTIONS. Y = MASS FRACTIONS / MOLECULAR WEIGHTS.
21 YN=1.0-U(1)
22 CALL RT(U,YN,R,NPDE,KPDE,IC,KSKR)
23 IST= 2*(IC-1)
24 IF(KSKT.GT.1)GO TO 100
25 IF(KSKR.GT.1)GO TO 125
26 C NTIS ENTHALPIES AND HEAT CAPACITIES.
27 IF(T.GT.1000.)GO TO 2000
28 C 1=1.9872*( 3.05744510E+00+T*( 2.67652000E-03
29 * +T*( -5.80991620E-06+T*( 5.52103910E-09+T*( -1.81227390E-12))))
30 H 1=1.9872*( -9.88904740E+02+T*( 3.05744510E+00
31 * +T*( 2.67652000E-03/2.0+T*( -5.80991620E-06/3.0
32 * +T*( 5.52103910E-09/4.0+T*( -1.81227390E-12/5.0))))))
33 C 2=1.9872*( 3.67482610E+00+T*( -1.20815000E-03
34 * +T*( 2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13))))
35 H 2=1.9872*( -1.06115880E+03+T*( 3.67482610E+00
36 * +T*( -1.20815000E-03/2.0+T*( 2.32401020E-06/3.0
37 * +T*( -6.32175590E-10/4.0+T*( -2.25772530E-13/5.0))))))
38 GO TO 3000
39 2000 CONTINUE
40 C 1=1.9872*( 3.10019010E+00+T*( 5.11194640E-04
41 * +T*( 5.26442100E-08+T*( -3.49099730E-11+T*( 3.69453450E-15))))))
42 H 1=1.9872*( -8.77380420E+02+T*( 3.10019010E+00
43 * +T*( 5.11194640E-04/2.0+T*( 5.26442100E-08/3.0
44 * +T*( -3.49099730E-11/4.0+T*( 3.69453450E-15/5.0))))))
45 C 2=1.9872*( 2.89631940E+00+T*( 1.51548660E-03
46 * +T*( -5.72352770E-07+T*( 9.98073930E-11+T*( -6.52235550E-15))))))
47 H 2=1.9872*( -9.05861840E+02+T*( 2.89631940E+00
48 * +T*( 1.51548660E-03/2.0+T*( -5.72352770E-07/3.0
49 * +T*( 9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))
50 3000 CONTINUE
51 C SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
52 C(1ST+ 1)=C 1/ 2.00
53 H(1ST+ 1)=H 1/ 2.00
54 C(1ST+ 2)=C 2/ 24.00
55 H(1ST+ 2)=H 2/ 24.00
56 125 CONTINUE
57 C VISCOSITY FROM WARNATZ ST PAR.
58

```

```
60 C LEAST SQUARES FIT, T=300,2000.
C THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
C LEAST SQUARES FIT, T=300,2000.
C V 1= 2.188700E-06*(T** 6.502900E-01)
C V 2= 4.266700E-06*(T** 6.613600E-01)
C RL 1= 6.357900E-06*(T** 7.383300E-01)
C RL 2= 6.407700E-07*(T** 7.999600E-01)
65 C BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
C LEAST SQUARES FIT, T=300,2000.
C PRESS = 1.00
C D 1 2= 5.951700E-05*(T** 1.663800E+00)
C SPACE DERIVATIVES.
70 YS=Y 3
X 1=Y 1/YS
X 2=Y 2/YS
U 1=U( 1)
DU 1=UPH( 1)
DUU 1=UPH2( 1)
U 2=1.0-U 1
DU 2=-DU 1
DUU 2=-DUU 1
DY 1=DU 1/ 2.00
DY 2=DU 2/ 28.00
80 DYS=+DY 1+DY 2
C TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03
DT=UPH(NPDE)* 1.0000E+03
DRH=- 1.2187690433E-02*(DT/T+DYS/YS)/(T*YS)
85 VD 1 2= 1.68019221E+04*(T**(-1.66380000E+00))
DUU 1 2= -2.79550381E+04*(T**(-2.66380000E+00))*DT
C SPECIFIC HEAT OF THE MIXTURE. NTIS FORMULA.
CM(IC)=C(IST+ 1)*U 1+C(1ST+ 2)*U 2
C THERMAL CONDUCTIVITY OF THE MIXTURE.
C MASON AND SAXENA METHOD.
90 LMIX=SUM(I)/(L 1/(1.0+(SUM(J)P 1 J*X J)/X 1)) 1.NE.J
C P 1 J=(1.065/SQRT(8.0*(1.0+M 1/M J)))*(1.0+SQRT((M J*V 1)/(M 1*V J)))*
C SQR(SQRT(M 1/M J))**2
C P 1 J IS A FUNCTION OF T AND CONSTANTS.
C FOR CONVENIENCE, P 1 J = A*(1.0+B*T**C)**2
95 HTC=1.0+ 1.3854124113E+00*T**(-5.5350000000E-03)
P 1S 2= 3.6376675219E-01*HTC**2
UP 1S 2= -5.5789143943E-03*T**(-1.0055350000E+00)*HTC*DT
100 HTC=1.0+ 7.2180672836E-01*T**(-5.5350000000E-03)
P 2S 1= 9.7220753957E-02*HTC**2
UP 2S 1= 7.7683275937E-04*T**(-9.9446500000E-01)*HTC*DT
SUMP 1=+P 1S 2*X 2
SUMP 2=+P 2S 1*X 1
B 1=1.0+SUMP 1/X 1
H 2=1.0+SUMP 2/X 2
RLM=+RL 1/B 1+KL 2/B 2
RHLM(IC)=RH*RLM
C SPACE DER OF DENSITY TIMES THERMAL COND.
110 DRL 1= 4.694228E-06*(T**(-2.616700E-01))*DT
DRL 2= 5.125904E-07*(T**(-2.000400E-01))*DT
DYS=DYS/(YS*YS)
DX 1=DY 1/YS-Y 1*DYYS
DX 2=DY 2/YS-Y 2*DYYS
USUMP 1=+OP 1S 2*X 2+P 1S 2*DX 2
```

```

115 USUMP 2=+DP 2S 1*X 1+P 2S 1*DX 1
    DH 1=(DSUMP 1-SUMP 1*DX 1/X 1)/X 1
    DH 2=(DSUMP 2-SUMP 2*DX 2/X 2)/X 2
    T 1=(DURL 1-RL 1*DH 1/B 1)/H 1
    T 2=(DURL 2-RL 2*DH 2/B 2)/H 2
    DRLM=+T 1+T 2
    DHLM(1C)=DRH*KLM+H*DRLM
120 C SOLVE FOR UV.
    SUM 1=+X 2*VD 1 2
    SUM 2=+X 1*VD 1 2
    H 1=X 1*SUM 1* 5.0000E-05
    H 2=X 2*SUM 2* 5.0000E-05
    T 1=-RH*(1.0-U 1)
    T 2=-RH*(1.0-U 2)
    FAC 1=T 1/B 1
    FAC 2=T 2/B 2
    V 1=FAC 1*DX 1
    V 2=FAC 2*DX 2
    UV 1=U 1*V 1
    UV 2=U 2*V 2
    UV=-UV 1-UV 2
    UV 1=UV 1+DV*U 1
    UV 2=UV 2+DV*U 2
    RHUV(1ST+ 1)=RH*UV 1
    RHUV(1ST+ 2)=RH*UV 2
    DUY 1=DDU 1/ 2.00
    DUY 2=DDU 2/ 28.00
    DDYS=DDY 1+DDY 2
    DYSQS=(DYS/Y S)**2
    DUX 1=(DDY 1-2.0*DY 1*UYS/Y S+2.0*Y 1*UYSYSU-Y 1*DDYS/Y S)/Y S
    DUX 2=(DDY 2-2.0*DY 2*UYS/Y S+2.0*Y 2*UYSYSU-Y 2*DDYS/Y S)/Y S
    DSUM 1=+DX 2*VD 1 2+X 2*DDVD 1 2
    DT 1=-DRH*(1.0-U 1)+RH*DU 1
    DT 2=-DRH*(1.0-U 2)+RH*DU 2
    DFAC 1=DT 1/B 1-1*T 1*UH 1/(B 1*H 1)
    DFAC 2=DT 2/B 2-1*T 2*UH 2/(B 2*H 2)
    UV 1=DFAC 1*DX 1+FAC 1*DDX 1
    UV 2=DFAC 2*DX 2+FAC 2*DDX 2
    UVV 1=DU 1*V 1+U 1*UVV 1
    UVV 2=DU 2*V 2+U 2*UVV 2
    UVV=-DUV 1-DUV 2
    DUV 1=DUV 1+DV*DU 1+UDV*U 1
    DUV 2=DUV 2+DV*DU 2+UDV*U 2
    URHUV(1ST+ 1)=DRH*UV 1+RH*DUV 1
    URHUV(1ST+ 2)=DRH*UV 2+RH*DUV 2
160 C FIND THE TIME DERIVATIVES.
    SP=ASP+RSP*TIME
100 CONTINUE
    IF(KPDE.EQ.NPDE)GO TO 150
    HY= 1.000000000E-03*R(KPDE)
    DY=- 2.000000000E+01*PHUV(1-T*KPDE)
    FVAL=SP*UPH(KPDE)+DY*HY
    RETURN
150 CONTINUE
    DU 1=UPH( 1)
    DU 2=UPH( 1)
170

```

```

      TL= 4.0000000000E+05*
      * (URHLM(IC)*UPH(NPDE)+RHLM(IC)*UFH2(NPDE))
      TD=- 2.0000000000E+01*UPH(NPDE)*( +C(IST+ 1)*RHUV(IST+ 1) +
      * C(IST+ 2)*RHUV(IST+ 2))
      TH=- 1.0000000000E-06*( +R( 1)*H(IST+ 1) +R( 2)*H(IST+ 2))
      FVAL=SP*UPH(NPDE)+(TL+TR*TD)/CM(IC)
      RETURN
      END

```

175

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      F 173
      F 174
      F 175
      F 176
      F 177
      F 178
      F 179
      F 180

```

04/15/80 14.10.20

FTN 4.8+498

IRACE

76/76

PROGRAM LOAD

1

```

1      PROGRAM LOAD (INPUT, OUTPUT, TAPE4=INPUT, TAPE6=OUTPUT,
2      * TAPE3, TAPE9, TAPE15)
3      C LOAD CREATES THE SUBROUTINE F IN FLSC.
4      DIMENSION I1(72)
5      DIMENSION I11(44)
6      DIMENSION LB(25), W(25), AU(7,25), AL(7,25)
7      DIMENSION ALD(25), RLU(25), ARD(25,25), RHU(25,25)
8      DIMENSION AV(25), RV(25)
9      DIMENSION LBPR(25)
10     WRITE(3,1000)
11     FORMAT(1HC,2X,63HFOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT T
12     *HE U VALUES OR)
13     WRITE(3,1005)
14     FORMAT(1HC,2X,62HTHEIR FIRST DERIVATIVES TO BE ZERO. THIS CAN LEA
15     *D TO DIVISION)
16     WRITE(3,1010)
17     FORMAT(1HC,2X,8HHY ZERO.)
18     WRITE(3,1012)
19     FORMAT(6X,14HDO 5 K=1,NPDEM)
20     WRITE(3,1014)
21     FORMAT(6X,32HF(ABS(U(K)).LT.SMALL)U(K)=SMALL)
22     WRITE(3,1016)
23     FORMAT(1X,1H5,4X,36HF(ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL)
24     READ(5,12)NLINE
25     C NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
26     DO 20 K=1,NLINE
27     READ(5,22)I1
28     WRITE(3,22)I1
29     CONTINUE
30     FORMAT(72A1)
31     FORMAT(/1X,72A1/)
32     READ(5,12)NSPC
33     NM=NSPC-1
34     LHM=IH-
35     LBU=2HU(
36     LHP=1H)
37     WRITE(3,1020)((LHM,LHU,K,LHP),K=1,NM)
38     FORMAT(6X,6HYN=1.0,R(A1,A2,12,A1),A1,2(/5X,IH*,1X,
39     * R(A2,12,A1,A1)) )
40     WRITE(3,1025)
41     FORMAT(6X,33HCALL RT(U,YN,R,NPDE,KPUE,IC,KSKH) )
42     WRITE(3,18)NSPC
43     FORMAT(6X,4HIST=.12,7H*(IC-1) )
44     DO 30 K=1,NSPC
45     READ(5,32)LB(K),W(K)
46     WRITE(6,34)K,LB(K),W(K)
47     READ(15,36)(AU(L,K),L=1,5),(I11(L),L=1,5)
48     WRITE(6,36)(AU(L,K),L=1,5),(I11(L),L=1,5)
49     READ(15,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(I11(L),L=1,5)
50     WRITE(6,36)(AU(L,K),L=6,7),(AL(L,K),L=1,3),(I11(L),L=1,5)
51     READ(15,37)(AL(L,K),L=4,7),(I11(L),L=1,20)
52     WRITE(6,37)(AL(L,K),L=4,7),(I11(L),L=1,20)
53     CONTINUE
54     FORMAT(A5,7F7.0)
55     FORMAT(/2X,14,4X,A5,4X,F8.2/)
56     FORMAT(5E15,8,5A1)
57
58

```

```

37 FORMAT(4E15.8,20A1)
   READ(5,232)TPN,PHN,1MN
60    FORMAT(1P3E12.4)
      WRITE(3,27)
27  FORMAT(6X,22HIF(KSKI,GT,1)GO TO 100)
      WRITE(3,28)
28  FORMAT(6X,22HIF(KSKR,GT,1)GO TO 125 )
      HEAD(5,12)NLINE
        DO 40 K=1,NLINE
          HEAD(5,22)11
          WRITE(3,22)11
        CONTINUE
70 C *****
C ENTHALPIES AND HEAT CAPACITIES.
C *****
      WRITE(3,42)
42  FORMAT(6X,24HIF(T,GT,1000.)GO TO 2000)
      DO 50 K=1,NSPC
        WRITE(3,52)K,AL(1,K),AL(2,K)
        WRITE(3,54)(AL(L,K),L=3,5)
        WRITE(3,62)K,AL(6,K),AL(1,K)
        WRITE(3,64)AL(2,K),AL(3,K)
        WRITE(3,66)AL(4,K),AL(5,K)
      CONTINUE
80    50 CONTINUE
      52 FORMAT(6X,1HC,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
      54  FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8,5H))))))
        WRITE(3,56)
      56  FORMAT(6X,10HG0 TO 3000)
        WRITE(3,58)
      58  FORMAT(4H2000.,2X,8HCCONTINUE)
      DO 60 K=1,NSPC
        WRITE(3,52)K, AU(1,K),AU(2,K)
        WRITE(3,54)(AU(L,K),L=3,5)
        WRITE(3,62)K,AU(6,K),AU(1,K)
        WRITE(3,64)AU(2,K),AU(3,K)
        WRITE(3,66)AU(4,K),AU(5,K)
      CONTINUE
90    60 CONTINUE
      62 FORMAT(6X,1HH,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
      64  FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/2.0,4H+T*(,1PE16.8,4H/3.0)
      66  FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/4.0,4H+T*(,1PE16.8,
      * 4H/5.0,6H))))))
        WRITE(3,68)
      68  FORMAT(4H3000.,2X,8HCCONTINUE)
        WRITE(3,134)
134  FORMAT(1HC,2X,39HSPECIFIC HEATS AND SPECIFIC ENTHALPIES. )
      DO 140 K=1,NSPC
        WRITE(3,142)K,K,W(K)
        WRITE(3,144)K,K,W(K)
      CONTINUE
105    140 CONTINUE
      142 FORMAT(6X,6HC(1ST.,12,3H)=C,12,1H/,F6.2)
      144  FORMAT(6X,6HH(1ST.,12,3H)=H,12,1H/,F6.2)
        WRITE(3,146)
110    146  FORMAT(1X,3H125.,2X,8HCCONTINUE)
C *****
C THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
C HEAD IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
C COEFFICIENTS FROM A FILE CREATED BY VALUES, CY=6.

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04/15/80 14.10.20

FTN 4.8+498

PROGRAM LOADF 76/76 OPT=I ROUNO=-*/ TRACE

```

115 C *****
      READ(5,12)NLINE
      DO 72 K=1,NLINE
120      READ(5,22)I1
        WRITE(6,22)I1
121      WRITE(3,22)I1
122      FORMAT(1HC,5X,IHV,12,IH=,1PE14.6,5H*(T**,1PE14.6,IH) )
123      READ(5,12)NLINE
124      DO 70 K=1,NLINE
125      READ(5,22)I1
        WRITE(3,22)I1
        WRITE(6,22)I1
126      CONTINUE
127      DO 80 K=1,NSPC
128      READ(9,82)AV(K),BV(K),I1I
129      WRITE(6,84)K,LB(K),AV(K),BV(K),I1I
130      READ(9,82)ALD(K),BLD(K),I1I
131      WRITE(6,84)K,LB(K),ALD(K),BLD(K),I1I
132      CONTINUE
133      FORMAT(1P2E14.6,44A1)
134      DO 78 K=1,NSPC
135      READ(1,2X,I4,4X,A4,4X,1P2E14.6,44A1/)
        DO 78 K=1,NSPC
136      WRITE(3,79)K,AV(K),BV(K)
137      CONTINUE
138      DO 90 K=1,NSPC
139      WRITE(3,92)K,ALD(K),BLD(K)
140      CONTINUE
141      FORMAT(6X,2HRL,12,IH=,1PE14.6,5H*(T**,1PE14.6,IH) )
142      READ(5,12)NLINE
143      DO 100 K=1,NLINE
144      READ(5,22)I1
145      WRITE(3,22)I1
        WRITE(6,22)I1
146      CONTINUE
147      NM=NSPC-1
148      DO 110 I=1,NSPC
149      DO 110 J=1,NSPC
150      READ(9,82)ABD(I,J),HBD(I,J),I1I
151      WRITE(6,112)I,J,LB(I),LB(J),ABD(I,J),HBD(I,J),I1I
152      CONTINUE
153      FORMAT(1P2E14.6,44A1/)
154      READ(5,114)PRESS
155      FORMAT(F6.0)
156      WRITE(3,116)PRESS
157      FORMAT(1HC,2X,7HPRESS =,F6.2)
158      DO 120 I=1,NM
159      IP=I+1
160      DO 120 J=IP,NSPC
161      ABD(I,J)=ABD(I,J)/PRESS
162      WRITE(3,122)I,J,ABD(I,J),HBD(I,J)
163      CONTINUE
164      FORMAT(1HC,5X,IHV,12,IH=,1PE14.6,5H*(T**,1PE14.6,IH) )
165      C *****
166      C SPACE DERIVATIVES.
167      C *****
168      LPL=1H+
169      WRITE(3,I4R)
170

```

```

175      148  FORMAT(IHC,2X,IHSPACE DERIVATIVE,S.)
          NS=NSPC+1
          WRITE(3,I49)NS
180      149  FORMAT(6X,4HYS=Y,I2)
          DO 150 K=1,NSPC
          WRITE(3,I52)K,K
185      150  CONTINUE
          FORMAT(6X,IHX,I2,2H=Y,I2,3H/Y,S)
          DO 160 K=1,NM
          WRITE(3,I62)K,K
          WRITE(3,I64)K,K
          WRITE(3,I66)K,K
          CONTINUE
          FORMAT(6X,IHU,I2,3H=U(I2,IH))
          FORMAT(6X,2HUU,I2,5H=UPH(I2,IH))
          FORMAT(6X,3HDDU,I2,6H=UPH2(I2,IH))
          LHU=IHU
          WRITE(3,I72)NSPC,((LBM,LBU,K),K=1,NM)
          FORMAT(6X,IHU,I2,4H=1.0,8(A1,A1,I2),A1,2(/5X,IH*,IX,
190      172  * 8(A1,I2,A1)) )
          LBDU=2HUU
          WRITE(3,I74)NSPC,((LBM,LBDU,K),K=1,NM)
          FORMAT(6X,2HUU,I2,IH=,8(A1,A2,I2),A1,2(/5X,IH*,IX,
195      174  * 8(A2,I2,A1)) )
          LHDDU=3HDDU
          WRITE(3,I76)NSPC,((LBM,LHDDU,K),K=1,NM)
          FORMAT(6X,3HDDU,I2,IH=,8(A1,A3,I2),A1,2(/5X,IH*,IX,
200      176  * 8(A3,I2,A1)) )
          DO 180 K=1,NSPC
          WRITE(3,I82)K,K,K,K
          CONTINUE
          FORMAT(6X,2HDY,I2,3H=DU,I2,IH=/f6.2)
          LBU=2HDY
          WRITE(3,I86)((LHPL,LBDY,K),K=1,IUSPC)
          FORMAT(6X,4HDYS=,8(A1,A2,I2),A1,2(/5X,IH*,IX,8(A2,I2,A1)) )
          PSR=PRESS/82.05
          WRITE(3,I234)IPN,PHN,IMN
          WRITE(6,I234)IPN,PHN,IMN
          FORMAT(IHC,2X,5HTPN =,IPEI2.4,6X,5HPHN =,IPEI2.4,6X,
210      234  * 5HTMN =,IPEI2.4)
          WRITE(3,I226)IPN
          FORMAT(6X,I3HOT=UPH(NPDE)*,IPEI2.4)
          WRITE(3,I242)PSR
          FORMAT(6X,5HDRH=,IPEI8.10,2IH*(U/T+DYS/Y,S)/(T*YS))
          DO 800 K=1,NSPC
          A=ALD(K)*BLD(K)
          H=BLD(K)-I.0
          WRITE(3,I803)K,A,H
          CONTINUE
          FORMAT(6X,3HDL,I2,IH=,IPEI6.8,HH*(T**((IPEI6.8,5H)))*DT)
          DO 805 K=1,NSPC
          A=I.0/ALD(K)
          H=-BLD(K)
          WRITE(3,I808)K,A,H
          CONTINUE
          FORMAT(6X,2HVL,I2,IH=,IPEI6.8,HH*(T**((IPEI6.8,2H)) )
          DO 809 K=1,NSPC

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04/15/80 14.10.20

FTN 4.8*49H

OPT=1 ROUND=+-*/ TRACE

75/76

PROGRAM LOADF

```

230      A=1.0/ALD(K)
231      H=-BLD(K)
232      A=A*B
233      H=B-1.0
234      WRITE(3,813)K,A,H
235      CONTINUE
236      FORMAT(6X,3HVD,2I2,1H=,1PE16.8,6H*(T**(.1PE16.8,5H))*DT)
237      DO 815 I=1,NSPC
238      DO 815 J=1,NSPC
239      IF(1.EQ.J)GO TO 815
240      A=1.0/ABD(1,J)
241      H=-BRD(1,J)
242      WRITE(3,818)I,J,A,B
243      CONTINUE
244      FORMAT(6X,2HVD,2I2,1H=,1PE16.8,6H*(T**(.1PE16.8,2H)) )
245      DO 820 I=1,NSPC
246      DO 820 J=1,NSPC
247      IF(1.EQ.J)GO TO 820
248      A=1.0/ABD(1,J)
249      H=-BRD(1,J)
250      A=A*B
251      H=B-1.0
252      WRITE(3,822)I,J,A,B
253      CONTINUE
254      FORMAT(6X,3HVD,2I2,1H=,1PE16.8,6H*(T**(.1PE16.8,5H))*DT)
255      C *****
256      C SPECIFIC HEAT OF THE MIXTURE.
257      C *****
258      WRITE(3,124)
259      FORMAT(1HC,2X,44HSPECIFIC HEAT OF THE MIXTURE. NTIS FORMULA. )
260      LBC=6HC(1ST+
261      LBU=3H)*U
262      WRITE(3,132)((LHPL,LBC,K,LBU,K),K=1,NSPC)
263      FORMAT(6X,7HCM(1C)=,4(A1,A6,12,A3,12),A1,
264      * 4(/5X,1H*,1X,4(A6,12,A3,12,A1)) )
265      C *****
266      C THERMAL CONDUCTIVITY OF THE MIXTURE.
267      C *****
268      WRITE(3,272)
269      WRITE(3,274)
270      FORMAT(1HC,2X,36HTHERMAL CONDUCTIVITY OF THE MIXTURE.)
271      FORMAT(1HC,2X,46HAVERAGE OF LINEAR AND RECIPROCAL MIXING RULES. )
272      LHX=1HX
273      LHPL=1H+
274      LRL=3H*RL
275      LBMIX=5HRLSUM
276      WRITE(3,260)LBMIX,((LHPL,LHX,K,LRL,K),K=1,NSPC)
277      FORMAT(6X,A5,1H=,6(2A1,12,A3,12),A1,2(/5X,1H*,1X,
278      * 8(A1,12,A3,12,A1)) )
279      LBSRL=3H*VL
280      LBMIX=5HRLSIV
281      WRITE(3,260)LBMIX,((LHPL,LHX,K,LRL,K),K=1,NSPC)
282      WRITE(3,265)
283      FORMAT(6X,15HRLSIV=1.0/RLSIV )
284      WRITE(3,270)
285      FORMAT(6X,21HRLM=0.5*(RLSUM+RLSIV) )
286      WRITE(3,306)

```

```

306  FORMAT(6X,15HRHLM(IC)=RH*RLM)
C *****
C  DERIVATIVE OF THE THERMAL CONDUCTIVITY OF THE MIXTURE.
C *****
290  WRITE(3,312)
312  FORMAT(1HC,2X,40HSPACE DER OF DENSITY TIMES THERMAL COND.)
745  WRITE(3,745)
      FORMAT(6X,16HDYSY=DYS/(YS*YS) )
      DO 750 K=1,NSPC
750  WRITE(3,752)K,K,K
752  CONTINUE
      FORMAT(6X,2HDX,12,3H=0Y,12,5H/Y5-Y,12,5H*UYSY )
      LBDR=4H*DRL
      LHD=2HDX
      LHM1X=5HDLSUM
      WRITE(3,760)LM1X,((LBPL,LBX,K,LHDRL,K,LBPL,LBDX,K,LBRL,K),
      * K=1,NSPC)
760  FORMAT(6X,A5,1H=,2(2A1,12,A4,12,A1,A2,12,A3,12),A1,
      * 6(/5X,1H*,1X,3(A1,12,A4,12,A1,A2,12,A3,12,A1)) )
      LBPAR=1H)
      LBMI1X=5HDLSIV
      LBVDL=4H*DVL
      WRITE(3,765)LBMI1X,((LBPL,LBDX,K,LBSRL,K,LBPL,LBX,K,LBDVL,K),
      * K=1,NSPC)
765  FORMAT(6X,A5,1H=,2(A1,A2,12,A3,12,2A1,12,A4,12),A1,
      * 6(/5X,1H*,1X,3(A2,12,A3,12,2A1,12,A4,12,A1)) )
      WRITE(3,770)
770  FORMAT(6X,24HDLSIV=-RLSIV*RLSIV*ULSIV )
      WRITE(3,775)
775  FORMAT(6X,22HDLRM=0.5*(DLSUM*ULSIV) )
      WRITE(3,778)
778  FORMAT(6X,25HDLHLM(IC)=DRH*RLM*RH*DRLM)
C *****
C  SOLVE FOR UV.
C  HIRSHFELDER AND CURTISS APPROXIMATION.
C  THE VELOCITY OF THE LAST SPECIES IS DETERMINED ONLY BY THE RELATION
C  SUM Y1*V1 = 0.0
C *****
400  WRITE(3,400)
      FORMAT(1HC,2X,13HSOLVE FOR UV.)
      LBX=1HX
      LBVD=3H*VD
      K=1
402  WRITE(3,402)K,((LBPL,LBX,J,LBVD,K,J),J=2,NSPC)
      FORMAT(6X,3HSUM,12,1H=,5(2A1,12,A3,212),A1,
      * 3(/5X,1H*,1X,5(A1,12,A3,212,A1)) )
      IF(NM.EQ.1)GO TO 412
      DO 410 K=2,NM
      KM=K-1
      KP=K+1
      WRITE(3,402)K,((LBPL,LBX,J,LBVD,K,J),J=1,KM),((LBPL,LBX,J,
      * LBVD,K,J),J=KP,NSPC)
      CONTINUE
410  CONTINUE
412  I=0
      DO 415 K=1,NM
      WRITE(3,412)K,K,K,P-IN
      CONTINUE
415  CONTINUE

```

04/15/80 14.10.20

FTN 4.8+498

76/76 OPT=1 KOUND=+*/ IRACE

PROGRAM LOADF

```

345      418  FORMAT(6X,IHB,I2,2H=X,I2,4H=SUM,I2,1H*,1PEI2,4)
          DO 420 K=1,NM
            WRITE(3,422)K,K
          CONTINUE
          420  FORMAT(6X,1HT,I2,11H=-RH*(1.0-U,I2,1H) )
          DO 425 K=1,NM
            WRITE(3,428)K,K,K
          CONTINUE
          425  FORMAT(6X,3HFA, I2,2H=T,I2,2H/B,I2)
          DO 465 K=1,NM
            WRITE(3,468)K,K,K
          CONTINUE
          465  FORMAT(6X,1HV,I2,4H=FA, I2,3H*U,I2)
          DO 470 K=1,NM
            WRITE(3,472)K,K,K
          CONTINUE
          470  FORMAT(6X,2HUV,I2,2H=U,I2,2H*V,I2)
          LBUV=2HUV
          LBM=1H-
          476  WRITE(3,476)NSPC,((LBM,LBUV,K),K=1,NM)
          FORMAT(6X,2HUV,I2,1H=,I0(A1,A2,I2),A1,5X,1H*,1X,I0(A2,I2,A1))
          DO 485 K=1,NSPC
            WRITE(3,488)K,K
          CONTINUE
          485  FORMAT(6X,9HRHUV(1ST,I2,7H)=HH*UV,I2)
          C *****
          C SOLVE FOR THE SPACE DERIVATIVE OF UV.
          C *****
          522  WRITE(3,522)
          FORMAT(1HC,2X,30HSPACE DER OF DENSITY TIMES UV.)
          DO 500 K=1,NSPC
            WRITE(3,502)K,K,W(K)
          CONTINUE
          500  FORMAT(6X,3HDDY,I2,4H=DDU,I2,1H/,F6,2)
          LDDY=3HDDY
          506  WRITE(3,506)((LHPL,LDDY,K),K=1,NSPC)
          FORMAT(6X,5HDDYS=,8(A1,A3,I2),A1,2(/5X,1H*,1X,8(A3,I2,A1)) )
          510  WRITE(3,510)
          FORMAT(6X,18HDYSYSU=(DYS/YS)**2 )
          DO 515 K=1,NSPC
            WRITE(3,518)K,K,K,K,K
          CONTINUE
          515  FORMAT(6X,3HDDX,I2,5H=(DUY,I2,7H-2.0*UY,I2,13H*DYS/YS+2.0*Y,
          * 12,9H*DYSYSO-Y,I2,12H*UDYS/YS)/YS )
          LBDX=2HDX
          LBDV=3H*VD
          LBDVD=4H*DVD
          LBA=1HX
          K=1
          532  WRITE(3,532)K,((LHPL,LHDX,J,LBVU,K,J,LHPL,LHX,J,LBDVD,K,J),J=2,
          * NSPC)
          FORMAT(6X,4HDSUM,I2,1H=,2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,
          * 9(/5X,1H*,1X,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)) )
          IF(NM.EQ.1)GO TO 537
          DO 535 K=2,NM
            KM=K-1
            KP=K+1

```

```

345 418 FORMAT(6X,1H8,I2,2H=X,I2,4H*SUM,I2,1H*,1PEI2,4)
      DO 420 K=1,NM
      WRITE(3,422)K,K
      CONTINUE
420 422 FORMAT(6X,1H7,I2,1H=-RH*(1,0-U,I2,1H) )
      DO 425 K=1,NM
      WRITE(3,428)K,K,K
      CONTINUE
425 428 FORMAT(6X,3H*FAC,I2,2H=T,I2,2H/B,I2)
      DO 465 K=1,NM
      WRITE(3,468)K,K,K
      CONTINUE
465 468 FORMAT(6X,1H7,I2,4H=FAC,I2,3H*U,I2)
      DO 470 K=1,NM
      WRITE(3,472)K,K,K
      CONTINUE
470 472 FORMAT(6X,2HUV,I2,2H=U,I2,2H*V,I2)
      LRV=2HUV
      LHM=1H-
      WRITE(3,476)NSPC,((LHM,LBHV,K),K=1,NM)
476 476 FORMAT(6X,2HUV,I2,1H=,10(A1,A2,I2),A1/5X,1H*,IX,10(A2,I2,A1))
      DO 485 K=1,NSPC
      WRITE(3,488)K,K
      CONTINUE
485 488 FORMAT(6X,9HRHUV(1ST,I2,7H)=RH*UV,I2)
      C *****
      C SOLVE FOR THE SPACE DERIVATIVE OF UV.
      C *****
      WRITE(3,522)
522 522 FORMAT(1H,2X,30HSPACE DER OF DENSITY TIMES UV.)
      DO 500 K=1,NSPC
      WRITE(3,502)K,K,K,K
      CONTINUE
500 502 FORMAT(6X,3HDDY,I2,4H=DDU,I2,1H/,F6.2)
      LDDY=3HDDY
      WRITE(3,506)((LBPL,LDDY,K),K=1,NSPC)
506 506 FORMAT(6X,5HDDYS=8(A1,A3,I2),A1,2/(5X,1H*,IX,8(A3,I2,A1)) )
      WRITE(3,510)
510 510 FORMAT(6X,18HDDYS50=(DYS/YS)**2 )
      DO 515 K=1,NSPC
      WRITE(3,518)K,K,K,K,K
      CONTINUE
515 518 FORMAT(6X,3HDDX,I2,5H=(DDY,I2,7H-2,0*UY,I2,13H*UYS/YS+2,0*Y.
      * 12,9H*DYYS50-Y,I2,12H*DDYS/YS)/YS )
      LBDX=2HDX
      LBVD=3H*VD
      LBVDV=4H*DVD
      LBK=1HX
      K=1
      WRITE(3,532)K,((LBPL,LBDX,J,LBVD,K,J),J=2,
      * NSPC)
532 532 FORMAT(6X,4HDSUM,I2,1H=,2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,
      * 9/(5X,1H*,IX,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)) )
      IF(NM.EQ.1)GO TO 537
      DO 535 K=2,NM
      KM=K-1
      KP=K+1

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MAIN 397

```

400      WRITE(3,532)K,((LHPL,LBDX,J,LHVL,J,K,LBPL,LHX,J,LHDVD,J,K),J=I,KM)
      * ,((LHPL,LBDX,J,LHVL,J,K,LBPL,LHX,J,LHDVD,K,J),J=KP,NSPC)
      CONTINUE
535      CONTINUE
537      CONTINUE
      DO 540 K=I,NM
      WRITE(3,542)K,PHN,K,K,K,K
405      CONTINUE
540      CONTINUE
542      FORMAT(6X,2HDX,I2,IH=,IPEI2,4,4H*(DX,I2,4H*SUM,I2,2H*X,I2,
      * 5H*DSUM,I2,IH) )
      DO 545 K=I,NM
      WRITE(3,548)K,K,K
410      CONTINUE
545      CONTINUE
548      FORMAT(6X,2HDT,I2,12H=-DRH*(I,0-U,I2,7H)*RH*DU,I2)
      DO 550 K=I,NM
      WRITE(3,552) (K,L=I,7)
415      CONTINUE
550      CONTINUE
552      FORMAT(6X,4HDFAC,I2,IH=,2HDT,I2,2H/B,I2,2H-T,I2,3H*DB,I2,
      * 3H/(H,I2,2H*B,I2,IH) )
      DO 590 K=I,NM
      WRITE(3,592)K,K,K,K,K
420      CONTINUE
590      CONTINUE
592      FORMAT(6X,2HDX,I2,5H=DFAC,I2,3H*DX,I2,4H*FAC,I2,4H*DDX,I2)
      DO 595 K=I,NM
      WRITE(3,598)K,K,K,K,K
425      CONTINUE
595      CONTINUE
598      FORMAT(6X,3HDX,I2,3H=DU,I2,2H*V,I2,2H+U,I2,3H*DV,I2)
      LBDV=3HDX
      WRITE(3,802)NSPC,((LBM,LBDV,K),K=I,NM)
      FORMAT(6X,3HDX,I2,IH=,6(AI,A3,I2),AI,2(/5X,1H*,1X,
802      * 9(A3,I2,A1) ) )
      DO 810 K=I,NSPC
      WRITE(3,812)K,K,K
430      CONTINUE
810      CONTINUE
812      FORMAT(6X,10HDRV(I2,*,I2,8H)=10H*UV,I2,7H*RH*DUV,I2)
      C *****
      C FIND THE TIME DERIVATIVES.
      C *****
      WRITE(3,612)
612      FORMAT(1H,2X,26HFIND THE TIME DERIVATIVES.)
      WRITE(3,622)
622      FORMAT(6X,15HSP=ASP+RSP*TIME)
      TMSPH2=TMN/(PHN*PHN)
      WRITE(3,628)
628      FORMAT(1X,3HI00,2X,RHCONTINUE)
      WRITE(3,632)
632      FORMAT(6X,25HIF(KPDE,EQ.NPDE)GO TO I50)
      WRITE(3,636)TMN
636      FORMAT(6X,3HRY=,IPE20,I0,8H*H(KPDE) )
      TMSPH=TMN/PHN
      WRITE(3,638)TMSPH
445      FORMAT(6X,4HDX=,IPE20,I0,16H*RH*UV(I2,*,KPDE) )
      WRITE(3,642)
642      FORMAT(6X,23HFVAL=SP*UPH(KPDE)*11Y+RY)
      WRITE(3,646)
646      FORMAT(6X,6HRETUHI)
      WRITE(3,648)
648      FORMAT(1X,3HI50,2X,RHCONTINUE)

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04/15/80 14.10.20

FTN 4.8+49H

PROGRAM LOADF 76/76 OPT=1 KOUND=+--+ / T-ACE

```

460      650 K=1,NM
        WRITE(3,652)K,K
        CONTINUE
        652      FORMAT(6X,2HUU,12,5H=UPH(,12,1H) )
        K=NSPC
        LBUU=2HUU
        656      WRITE(3,656)K,((LHM,LBUU,J),J=1,LHM)
        FORMAT(6X,2HUU,12,1H=,8(A1,A2,12),A1,2(/5X,1H*,1X,8(A2,12,A1)) )
        465      WRITE(3,662)TMSPH2
        662      FORMAT(6X,3HTL=,1PE20,10,1H*)
        664      WRITE(3,664)
        FORMAT(5X,1H*,1X,41H(DRHLM(IC)*UPH(NPUE)+RHLM(IC)*UPH2(NPUE)) )
        LBHL=1H
        470      LHC=6HC(1ST+
        LHRHUV=10H)*RHUV(1ST
        WRITE(3,668)TMSPH,((LBBL,LBPL,LHC,K,LRRHUV,LBPL,K,LBP),K=1,
        * NSPC),LRP
        668      FORMAT(6X,4HTD=,1PE20,10,12H*UPH(NPDE)*(,2A1,A6,12,A10,A1,12,
        * 3A1,10(/5X,1H*,1X,2(A6,12,A10,A1,12,3A1)) )
        TMSPT=TMN/TPN
        LHR=2HR(
        LBH=8H)*H(1ST+
        475      WRITE(3,672)TMSPT,((LBBL,LBPL,LH,K,LHH,K,LBP),K=1,NSPC),LRP
        672      FORMAT(6X,4HTR=,1PE20,10,2H*(,2(2A1,A2,12,A8,12,A1),2A1,
        * 9(/5X,1H*,1X,2(A2,12,A8,12,3A1)) )
        480      WRITE(3,676)
        676      FORMAT(6X,35HVAL=SP*UPH(NPUE)+(TL+TH+TD)/CM(IC) )
        STOP
        END
485

```

PROGRAM WILL BE ENTERED AT LOADF (241)

BLOCK	ADDRESS	LENGTH	FILE
LOADF	110	10331	LGO
/STP.END/	10441	1	SL-FTNL1B
/FCL.C./	10442	30	SL-FTNL1B
/J8.I0./	10472	144	SL-FTNL1B
QENTRY=	10636	4	SL-FTNL1B
COMIO=	10642	10	SL-FTNL1B
FECMSK=	10652	41	SL-FTNL1B
FEIFST=	10713	3	SL-FTNL1B
FLIN=	10716	156	SL-FTNL1B
FLIOUT=	11074	315	SL-FTNL1B
FMTAP=	11411	377	SL-FTNL1B
FORSYS=	12010	300	SL-FTNL1B
FORUTL=	12310	45	SL-FTNL1B
GETFIT=	12355	54	SL-FTNL1B
INCOM=	12431	144	SL-FTNL1B
INPC=	12575	173	SL-FTNL1B
KODER=	12770	476	SL-FTNL1B
KRAKER=	13466	454	SL-FTNL1B
OUTC=	14142	155	SL-FTNL1B
OUTCOM=	14317	204	SL-FTNL1B
ERRCAP=	14523	317	SL-FTNL1B
FERCAP=	15042	171	SL-FTNL1B
SYSALD=	15233	1	SL-FTNL1B

1 H2 2.00
 .31001901E+01 .5119464E+03 .52644210E-07 -.34909973E-10 .36945345E-14 H2
 -.87738042E+03 -.19629421E+01 .30574451E+01 .26765200E-02 -.58099162E-05 H2
 .55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01 H2

2 N2 28.00
 .28963194E+01 .15154866E-02 -.57235277E-06 .99807393E-10 -.65223555E-14 N2
 -.90586184E+03 .61615148E+01 .36748261E+01 -.12081500E-02 .23240102E-05 N2
 -.63217559E-09 -.22577253E-12 -.10611588E+04 .23580424E+01 N2

VISCOSITY FROM WARMATZ ST PAR.
 LEAST SQUARES FIT, T=300.2000.
 THERMAL CONDUCTIVITIES FROM WARMATZ ST PAR.
 LEAST SQUARES FIT, T=300.2000.

1 H2 2.188700E-06 6.502900E-01 H2 VISCOSITY.
 1 H2 6.357900E-06 7.383300E-01 H2 THERMAL CONDUCTIVITY.
 2 N2 4.266700E-06 6.613600E-01 N2 VISCOSITY.
 2 N2 6.407700E-07 7.999600E-01 N2 THERMAL CONDUCTIVITY.

BINARY DIFFUSION COEFFICIENTS FROM WARMATZ ST PAR.
 LEAST SQUARES FIT, T=300.2000.

1	2	H2	N2	5.951700E-05	1.663800E+00	H2	N2	MINARY DIFFUSION.
2	2	N2	N2	1.537400E-05	1.672900E+00	N2	N2	MINARY DIFFUSION.

TPN = 1.0000E+03 PHIN = 5.0000E-05 TMN = 1.0000E-03

```

1  SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,KPUE,IC,KSKT,KSKR)
   DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
   COMMON/TARAH/ASP,ASP,IPN,PHN,IM3,IMSPH,IMSPH2,IMSTP,TPENT
   COMMON/TARP/PRESS,PSM,NPDEM
   COMMON/TARSM/SMALL
   DIMENSION R(20)
   DIMENSION C(1000),H(1000),RHM(100),DRHLM(100),CM(100)
   COMMON/TABCT/RL,CPMX,H0(20),R2D(20),R2DM(20)
   COMMON/TARMF/RHUV(1000),DRHUV(1000)
   COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
   C AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.
   C FOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT THE U VALUES OR
   C THEIR FIRST DERIVATIVES TO BE ZERO. THIS CAN LEAD TO DIVISION
   C BY ZERO.
   DO 5 K=1,NPDEM
     IF (ABS(U(K)).LT.SMALL)U(K)=SMALL
   5   IF (ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL
   C TEST CASE. BINARY MIX OF H2 AND N2. TRANSPORT WARNATZ PAR.
   C U = MASS FRACTIONS. Y = MASS FRACTIONS / MOLECULAR WEIGHTS.
     YN=1.0-U( 1)
     CALL RT(U,YN,R,NPDE,KPUE,IC,KSKT)
     IST= 2*(IC-1)
     IF (KSKT.GT.1)GO TO 100
     IF (KSKR.GT.1)GO TO 125
   C THIS ENTHALPIES AND HEAT CAPACITIES.
     IF (T.GT.1000.)GO TO 2000
     C 1=1.9872*( 3.05744510E+00+T*( 2.67652000E-03
       *+T*( -5.80991620E-06+T*( 5.52103910E-09+T*( -1.81227390E-12))))))
     H 1=1.9872*( -9.84904740E+02+T*( 3.05744510E+00
       *+T*( 2.67652000E-03+2.0+T*( -5.80991620E-06+3.0
       *+T*( 5.52103910E-09+4.0+T*( -1.81227390E-12+5.0))))))
     C 2=1.9872*( 3.67482610E+00+T*( -1.20815000E-03
       *+T*( 2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13))))))
     H 2=1.9872*( -1.06115880E+03+T*( 3.67482610E+00
       *+T*( -1.20815000E-03+2.0+T*( 2.32401020E-06+3.0
       *+T*( -6.32175590E-10+4.0+T*( -2.25772530E-13+5.0))))))
     GO TO 3000
   2000 CONTINUE
     C 1=1.9872*( 3.10019010E+00+T*( 5.11194640E-04
       *+T*( 5.26442100E-08+T*( -3.49099730E-11+T*( 3.69453450E-15))))))
     H 1=1.9872*( -8.77380420E+02+T*( 3.10019010E+00
       *+T*( 5.11194640E-04+2.0+T*( 5.26442100E-08+3.0
       *+T*( -3.49099730E-11+4.0+T*( 3.69453450E-15+5.0))))))
     C 2=1.9872*( 2.89631940E+00+T*( 1.51548660E-03
       *+T*( -5.72352770E-07+T*( 9.98073930E-11+T*( -6.52235550E-15))))))
     H 2=1.9872*( -9.05861840E+02+T*( 2.89631940E+00
       *+T*( 1.51548660E-03+2.0+T*( -5.72352770E-07+3.0
       *+T*( 9.98073930E-11+4.0+T*( -6.52235550E-15+5.0))))))
   3000 CONTINUE
   C SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
     C(IST+ 1)=C 1/ 2.00
     H(IST+ 1)=H 1/ 2.00
     C(IST+ 2)=C 2/ 24.00
     H(IST+ 2)=H 2/ 24.00
   125 CONTINUE
   C VISCOSITY FROM WARNATZ ST PAR.
   C LEAST SQUARES FIT, I=300,2000.

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60      C THERMAL CONDUCTIVITIES FROM WARMATZ ST PAR.
      C LEAST SQUARES FIT, T=300.2000.
      C V 1= 2.144700E-06*(T** 6.502900E-01)
      C V 2= 4.266700E-06*(T** 6.613600E-01)
      C RL 1= 6.357900E-06*(T** 7.383300E-01)
      C RL 2= 6.407700E-07*(T** 7.999400E-01)
65      C BINARY DIFFUSION COEFFICIENTS FROM WARMATZ ST PAR.
      C LEAST SQUARES FIT, T=300.2000.
      C PRESS = 1.00
      C D 1 2= 5.9517000E-05*(T** 1.46380000E+00)
      C SPACE DERIVATIVES.
      C YS=Y 3
      C X 1=Y 1/YS
      C X 2=Y 2/YS
      C U 1=U( 1)
      C DU 1=UPH( 1)
      C DUU 1=UPH2( 1)
      C U 2=1.0-U 1
      C DU 2=-DU 1
      C DUU 2=-DUU 1
      C DY 1=DU 1/ 2.00
      C DY 2=DU 2/ 28.00
      C DYS=+DY 1+DY 2
80      C TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03
      C DT=UPH(NPDE)* 1.0000E+03
      C DRH=- 1.2187690433E-02*(DT/T+DYS/YS)/(T*YS)
      C DHL 1= 4.69422831E-06*(T**(-2.61670000E-01))*DT
      C DHL 2= 5.12590369E-07*(T**(-2.00040000E-01))*DT
      C VL 1= 1.57284638E+05*(T**(-7.34330000E-01))
      C VL 2= 1.56062238E+06*(T**(-7.99960000E-01))
      C DVL 1= -1.16127967E+05*(T**(-1.73833000E+00))*DT
      C DVL 2= -1.24843548E+06*(T**(-1.79996000E+00))*DT
      C VD 1 2= 1.68019221E+04*(T**(-1.66380000E+00))
      C DVD 1 2= -2.79550381E+04*(T**(-2.66380000E+00))*DT
90      C SPECIFIC HEAT OF THE MIXTURE. NTIS FORMULA.
      C CM(IC)=C(IST+ 1)*U 1+C(IST+ 2)*U 2
      C THERMAL CONDUCTIVITY OF THE MIXTURE.
      C AVERAGE OF LINEAR AND RECIPROCAL MIXING RULES.
      C RLSUM=X 1*RL 1+X 2*VL 2
      C RLSIV=X 1*VL 1+X 2*VL 2
      C RLSIV=1.0/RLSIV
      C RLM=0.5*(RLSUM+RLSIV)
      C RMLM(IC)=RMLM
      C DYSY=DYS/(YS*YS)
100      C SPACE DER OF DENSITY TIMES THERMAL COND.
      C DX 1=DY 1/YS-Y 1*DYSY
      C DX 2=DY 2/YS-Y 2*DYSY
      C DLSUM=X 1*DLR 1+DX 1*RL 1+X 2*DLR 2+DX 2*RL 2
      C DLSIV=DX 1*VL 1+X 1*DLVL 1+DX 2*VL 2+X 2*DLVL 2
      C DLSIV=-RLSIV*RLSIV*DLVL 1
      C DRLM=0.5*(DLSUM+DLSIV)
      C DRMLM(IC)=DRH+RLM+RMLM*DRMLM
110      C SOLVE FOR UV.
      C SUM 1=X 2*VD 1 2
      C H 1=X 1*SUM 1* 5.0000E-05
      C T 1=-H*(1.0-U 1)
      C FAC 1=T 1/R 1

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04/15/80 14.10.34

FTN 4.8+498

SUBROUTINE F 76/76 OPT=1 ROUNO=+*/ 1*ACE

```

115      V 1=FAC 1*DX 1
        UV 1=U 1*V 1
        UV 2=-UV 1
        RHUV(1ST+ 1)=RH*UV 1
        RHUV(1ST+ 2)=RH*UV 2
120      C SPACE DER OF DENSITY TIMES UV.
        DDY 1=DDU 1/ 2*00
        DDY 2=DDU 2/ 28*00
        DDYS=+DDY 1+DDY 2
        DYSYSQ=(DYS/YS)**2
        DDY 1=(DDY 1-2*0*DY 1*DYS/YS+2*0*Y 1*DYSYSQ-Y 1*DDYS/YS)/YS
        DDY 2=(DDY 2-2*0*DY 2*DYS/YS+2*0*Y 2*DYSYSQ-Y 2*DDYS/YS)/YS
        USUM 1=+DX 2*VD 1 2+X 2*DVD 1 2
        DB 1= 5*000E-05*(DX 1*SUM 1+X 1*DSUM 1)
        DT 1=-DRH*(1.0-U 1)+RH*DU 1
        DFAC 1=DT 1/8 1-T 1*UH 1/(H 1*B 1)
        DV 1=DFAC 1*DX 1+FAC 1*DDX 1
        DUV 1=DU 1*V 1+U 1*UV 1
        DUV 2=-DUV 1
        DRHUV(1ST+ 1)=DRH*UV 1+RH*DUV 1
        DRHUV(1ST+ 2)=DRH*UV 2+RH*DUV 2
135      C FIND THE TIME DERIVATIVES.
        SP=ASP+BSP*TIME
100      CONTINUE
        IF (KPDE.EQ.NPDE)GO TO 150
        KY= 1.000000000E-03*R(KPDE)
        DY=- 2.000000000E+01*DRHUV(1ST+KPDE)
        FVAL=SP*UPH(KPDE)+DY*RY
        RETURN
150      CONTINUE
        DU 1=UPH( 1)
        DU 2=-DU 1
        TL= 4.000000000E+05*
        * (DRHLM(1C)*UPH(NPDE)+RHLM(1C)*UPH2(NPDE))
        TD=- 2.000000000E+01*UPH(NPDE)*( +C(151+ 1)*RHUV(1ST+ 1) +
        * C(1ST+ 2)*RHUV(1ST+ 2))
        TR=- 1.000000000E-06*( +R( 1)*H(1ST+ 1) +R( 2)*H(1ST+ 2))
        FVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(1C)
        RETURN
        END

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1  PROGRAM LOADF (INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
2  * TAPE3,TAPE9,TAPE15)
3  C  LOADF CREATES THE SUBROUTINE F IN FLSC.
4  DIMENSION I1(72)
5  DIMENSION I11(44)
6  DIMENSION LB(25),W(25),AU(7,25),AL(7,25)
7  DIMENSION LBTHD(25)
8  DIMENSION ESK(25)
9  DIMENSION ALD(25),BLU(25),ABD(25,25),BBU(25,25)
10 DIMENSION AV(25),BV(25)
11 DIMENSION LBPR(25)
12 DIMENSION SGA(25),UM(25),ALP(25)
13 C  BOLIZMAN CONSTANT.
14 RK=1.38054E-16
15 WRITE(3,1000)
16 1000 FORMAT(1HC,2X,63HF, 'THE COMPLETE TRANSPORT CASE. WE DO NOT WANT T
17 *HE U VALUES OR)
18 WRITE(3,1005)
19 1005 FORMAT(1HC,2X,62HTHEIR FIRST DERIVATIVES TO BE ZERO. THIS CAN LEA
20 *D TO DIVISION)
21 WRITE(3,1010)
22 1010 FORMAT(1HC,2X,8HBY ZERO.)
23 WRITE(3,1012)
24 1012 FORMAT(6X,14HDO 5 K=1,NPDEM)
25 1014 FORMAT(6X,32HIF (ABS(U(K)).LT.SMALL)U(K)=SMALL)
26 WRITE(3,1016)
27 1016 FORMAT(1X,1H5,4X,36HIF (ABS(UPH(K)).LT.SMALL)UPH(K)=SMALL)
28 READ(5,12)NLINE
29 12 FORMAT(10I4)
30 C  NLINE IS THE NUMBER OF COMMENT LINES TO BE READ AND PRINTED.
31 DO 20 K=1,NLINE
32 READ(5,22)I1
33 WRITE(3,22)I1
34 CONTINUE
35 20 FORMAT(72A1)
36 22 FORMAT(1X,72A1/)
37 24 READ(5,12)NSPC
38 NM=NSPC-1
39 LBM=1H-
40 LBU=2HU(
41 LBP=1H)
42 WRITE(3,1020)((LBM,LBU,K,LBP),K=1,NM)
43 1020 FORMAT(6X,6HYN=1.0,M(1A1,A2,12,A1),A1,2(/5X,1H*,1X,
44 * 8(A2,12,A1,A1)) )
45 WRITE(3,1025)
46 1025 FORMAT(6X,33HCALL RT(U,YN,R,NPUE,KPUE,IC,KSKR) )
47 WRITE(3,18)NSPC
48 18 FORMAT(6X,4HIST=,12,7H*(IC-1) )
49 DO 30 K=1,NSPC
50 READ(5,32)LB(K),LBTHD(K),W(K),SGA(K),ESK(K),UM(K),ALP(K)
51 32 FORMAT(2A5,1P5E12.4)
52 WRITE(6,34)K,LB(K),LBTHD(K),W(K),SGA(K),ESK(K),UM(K),ALP(K)
53 34 FORMAT(1X,14,2(SX,A5),1P5E12.4/)
54 C  COMPUTE AN APPROXIMATION FOR THERMAL DIFFUSION FOR THOSE SPECIES
55 C  WITH LBTHD = THOFF.
56 READ(15,36)(AU(L,K),L=1,5),(I11(L),L=1,5)
57 36 FORMAT(15,36)
58

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04/15/80 13.55.29

FTN 4.8*498

PROGRAM LOADF 76/76 OPT=I ROUNO=+*/* TRACE

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60      WRITE(6,36) (AU(L,K),L=1,5), (III(L),L=1,5)
        READ(15,36) (AU(L,K),L=6,7), (AL(L,K),L=1,3), (III(L),L=1,5)
        WRITE(6,36) (AU(L,K),L=6,7), (AL(L,K),L=1,3), (III(L),L=1,5)
        READ(15,37) (AL(L,K),L=4,7), (III(L),L=1,20)
        WRITE(6,37) (AL(L,K),L=4,7), (III(L),L=1,20)
        CONTINUE
30      FORMAT(5E15.8,5A1)
36      FORMAT(4E15.8,20A1)
37      READ(5,232) TPN,PHN,TMN
232     FORMAT(1P3E12.4)
        WRITE(3,27)
27      FORMAT(6X,22HIF(KSKI,GT,1)GO TO 100)
        WRITE(3,28)
28      FORMAT(6X,22HIF(KSKR,GT,1)GO TO 125 )
        READ(5,12) NLINE
        DO 40 K=1,NLINE
70      READ(5,22) II
        WRITE(3,22) II
40      CONTINUE
C      *****
C      ENTHALPIES AND HEAT CAPACITIES.
C      *****
80      WRITE(3,42)
42      FORMAT(6X,24HIF(T,GT,1000.)GO TO 2000)
        DO 50 K=1,NSPC
        WRITE(3,52) K,AL(1,K),AL(2,K)
        WRITE(3,54) (AL(L,K),L=3,5)
        WRITE(3,62) K,AL(6,K),AL(1,K)
        WRITE(3,64) AL(2,K),AL(3,K)
        WRITE(3,66) AL(4,K),AL(5,K)
50      CONTINUE
52      FORMAT(6X,1HC,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
54      FORMAT(5X,1H*,1X,3(4H+T*(,1PE16.8,5H))))))
        WRITE(3,56)
56      FORMAT(6X,10HGO TO 3000)
        WRITE(3,58)
58      FORMAT(4H2000,2X,4HCONTINUE)
        DO 60 K=1,NSPC
        WRITE(3,52) K,AU(1,K),AU(2,K)
        WRITE(3,54) (AU(L,K),L=3,5)
        WRITE(3,62) K,AU(6,K),AU(1,K)
        WRITE(3,64) AU(2,K),AU(3,K)
        WRITE(3,66) AU(4,K),AU(5,K)
100     CONTINUE
60      FORMAT(6X,1HH,12,9H=1.9872*(,1PE16.8,4H+T*(,1PE16.8)
62      FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/2.0,4H+T*(,1PE16.8,4H/3.0)
64      FORMAT(5X,1H*,1X,4H+T*(,1PE16.8,4H/4.0,4H+T*(,1PE16.8,
66      * 4H/5.0,6H))))))
        WRITE(3,68)
68      FORMAT(4H3000,2X,4HCONTINUE)
        WRITE(3,134)
134     FORMAT(1HC,2X,3HSPCIFIC HEATS AND SPECIFIC ENTHALPIES. )
        DO 140 K=1,NSPC
        WRITE(3,142) K,K,K(K)
        WRITE(3,144) K,K,K(K)
140     CONTINUE
142     FORMAT(6X,6HC(1ST*,12,3H)=C,12,1H*/F6.2)

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```
115      144  FORMAT(6X,6H(1ST,12,3H)=H,12,1H/,F6.2)
          WRITE(3,146)
120      146  FORMAT(1X,3H125,2X,8HCONTINUE)
          C *****
          C THERMAL CONDUCTIVITIES AND BINARY DIFFUSION COEFFICIENTS.
          C READ IN VISCOSITY, THERMAL CONDUCTIVITY, AND BINARY DIFFUSION
          C COEFFICIENTS FROM A FILE CREATED BY VALUES, CY=6.
          C *****
          READ(5,12)NLINE
          DO 72 K=1,NLINE
125      READ(5,22)I1
          WRITE(6,22)I1
          72  WRITE(3,22)I1
          79  FORMAT(1HC,5X,1HV,12,1H=,1PE14.6,5H*(T**,1PE14.6,1H) )
          READ(5,12)NLINE
          DO 70 K=1,NLINE
130      READ(5,22)I1
          WRITE(3,22)I1
          WRITE(6,22)I1
          70  CONTINUE
          DO 80 K=1,NSPC
          READ(9,82)AV(K),BV(K),I1I
          WRITE(6,84)K,LB(K),AV(K),BV(K),I1I
          READ(9,82)ALD(K),BLD(K),I1I
          WRITE(6,84)K,LB(K),ALD(K),BLD(K),I1I
          80  CONTINUE
          82  FORMAT(1P2E14.6,44AI)
          84  FORMAT(/2X,14,4X,A4,4X,1P2E14.6,44AI/)
          DO 78 K=1,NSPC
          WRITE(3,79)K,AV(K),BV(K)
          78  CONTINUE
          DO 90 K=1,NSPC
          WRITE(3,92)K,ALD(K),BLD(K)
          90  CONTINUE
          92  FORMAT(6X,2HRL,12,1H=,1PE14.6,5H*(T**,1PE14.6,1H))
          READ(5,12)NLINE
          DO 100 K=1,NLINE
          READ(5,22)I1
          WRITE(3,22)I1
          WRITE(6,22)I1
          100 CONTINUE
          NM=NSPC-1
          DO 110 I=1,NSPC
          DO 110 J=1,NSPC
          READ(9,82)ABD(1,J),BBU(1,J),I1I
          WRITE(6,112)I,J,LB(1),LB(J),ABU(1,J),BBU(1,J),I1I
          110 CONTINUE
          112 FORMAT(12X,14,4X,14,4X,A4,4X,1P2E14.6,44AI/)
          READ(5,114)PRESS
          114 FORMAT(F6.0)
          WRITE(3,116)PRESS
          116 FORMAT(1HC,2X,7HPRESS =,F6.2)
          DO 120 I=1,NM
          IP=I+1
          DO 120 J=1P,NSPC
          ABD(1,J)=ABD(1,J)/PRESS
          WRITE(3,122)I,J,ABU(1,J),BBU(1,J)
          170 MAIN
          116 MAIN
          117 MAIN
          118 MAIN
          119 MAIN
          120 MAIN
          121 MAIN
          122 MAIN
          123 MAIN
          124 MAIN
          125 MAIN
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FTN 4.8*498

PROGRAM LOADF 76/76 OPT=1 ROUNDO=**/ TRACE

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175      120      CONTINUE
176      122      FORMAT(1HC,5X,1HD,212,1H=,1PE14.6,5H*(1*,1PE14.6,1H) )
177      READ(5,279)ARTP,CRTP,III
178      WRITE(6,123)ARTP,CRTP,III
179      READ(5,279)ACST,CCST,III
180      WRITE(6,123)ACST,CCST,III
181      FORMAT(1P2E14.6,44A1)
182      123      FORMAT(/2X,1P2E14.6,44A1)
183      C *****
184      C SPACE DERIVATIVES.
185      C *****
186      LBPL=1H*
187      WRITE(3,148)
188      FORMAT(1HC,2X,18HSPACE DERIVATIVES.)
189      NS=NSPC+1
190      WRITE(3,149)NS
191      FORMAT(6X,4HYS=Y,12)
192      DO 150 K=1,NSPC
193      WRITE(3,152)K,K
194      CONTINUE
195      FORMAT(6X,1HX,12,2H=Y,12,3H/Y5)
196      DO 160 K=1,NM
197      WRITE(3,162)K,K
198      WRITE(3,164)K,K
199      WRITE(3,166)K,K
200      CONTINUE
201      FORMAT(6X,1HU,12,3H=U(,12,1H))
202      FORMAT(6X,2HOU,12,5H=UPH(,12,1H))
203      FORMAT(6X,3HODU,12,6H=UPH2(,12,1H))
204      LBU=1HU
205      WRITE(3,172)NSPC,((LBM,LBU,K),K=1,NM)
206      FORMAT(6X,1HU,12,4H=1.0,8(A1,A1,12),A1,2(/5X,1H*,1X,
207      * 8(A1,12,A1)) )
208      LBU=2HOU
209      WRITE(3,174)NSPC,((LBM,LBU,K),K=1,NM)
210      FORMAT(6X,2HOU,12,1H=,8(A1,A2,12),A1,2(/5X,1H*,1X,
211      * 8(A2,12,A1)) )
212      LBU=3HODU
213      WRITE(3,176)NSPC,((LBM,LBU,K),K=1,NM)
214      FORMAT(6X,3HODU,12,1H=,8(A1,A3,12),A1,2(/5X,1H*,1X,
215      * 8(A3,12,A1)) )
216      DO 180 K=1,NSPC
217      WRITE(3,182)K,K,K
218      CONTINUE
219      LBU=2HUY
220      FORMAT(6X,2HUY,12,3H=DU,12,1H=/,6,2)
221      WRITE(3,186)((LBPL,LBU,K),K=1,NM)
222      FORMAT(6X,4HYS=,8(A1,A2,12),A1,2(/5X,1H*,1X,8(A2,12,A1)) )
223      PS=PRESS/82.05
224      WRITE(3,234)TPN,PHN,IMN
225      WRITE(6,234)TPN,PHN,IMN
226      FORMAT(1HC,2X,5HTPN=,1PE12.4,6X,5HPHN=,1PE12.4,6X,
227      * 5HTMN=,1PE12.4)
228      WRITE(3,226)TPN
229      FORMAT(6X,13HDT=UPH(NPDE)*,1PE12.4)
230      WRITE(3,227)TPN
231      FORMAT(6X,15HDT=UPH2(NPDE)*,1PE12.4)

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230	242	WRITE(3,242)PSR FORMAT(6X,5HDRH=-,1PE18.10,21H*(DT/T-DYS/YS)/(T*YS)) DO 807 K=1,NSPC A=1.0/ALD(K) B=-BLD(K) WRITE(3,809)K,A,B CONTINUE
235	807 809	FORMAT(6X,2HVL,12,1H=,1PE16.8,6H*(T**(.1PE16.8,2H))) DO 740 K=1,NSPC A=ALD(K)*BLD(K) B=BLD(K)-1.0 WRITE(3,742)K,A,B CONTINUE
240	740 742	FORMAT(6X,3HDL,12,1H=,1PE14.6,6H*(T**(.1PE14.6,5H))*DT) DO 747 K=1,NSPC A=1.0/ALD(K) B=-BLD(K) A=A*B B=B-1.0 WRITE(3,749)K,A,B CONTINUE
245	747 749	FORMAT(6X,3HVL,12,1H=,1PE14.6,6H*(T**(.1PE14.6,5H))*DT) WRITE(3,745) FORMAT(6X,16HDYS=DYS/(YS*YS)) DO 750 K=1,NSPC WRITE(3,752)K,K,K CONTINUE
250	750 752	FORMAT(6X,2HDX,12,3H=DY,12,5H/YS-Y,12,5H*DY) DO 500 K=1,NSPC WRITE(3,502)K,K,W(K) CONTINUE
255	500 502	FORMAT(6X,3HDDY,12,4H=DDU,12,1H,F6.2) LDDY=3HDDY WRITE(3,506)((LHPL,LDDY,K),K=1,NSPC) FORMAT(6X,5HDDYS=,8(A1,A3,12),A1,2/(5X,1H*,1X,8(A3,12,A1))) WRITE(3,510) FORMAT(6X,18HDYSQ=(DYS/YS)**2) DO 515 K=1,NSPC WRITE(3,518)K,K,K,K,K CONTINUE
260	506 510	FORMAT(6X,3HDDX,12,5H=(DDY,12,7H-2.0*DY,12,13H*DYS/YS+2.0*Y, * 12,9H*DYYSQ-Y,12,12H*DDYS/YS) /YS) DO 815 I=1,NSPC DO 815 J=1,NSPC IF (1.E0,J)GO TO 815 A=1.0/ABD(I,J) H=-BBD(I,J) WRITE(3,818)I,J,A,H CONTINUE
265	515 518	FORMAT(6X,2HVD,212,1H=,1PE16.8,6H*(T**(.1PE16.8,2H))) DO 820 I=1,NSPC DO 820 J=1,NSPC IF (1.E0,J)GO TO 820 A=1.0/ABD(I,J) H=-BBD(I,J) A=A*H H=H-1.0
270	815 818	
275	280	
280	285	

```

820 WRITE(3,822)I,J,A,B
821 CONTINUE
822 FORMAT(6X,3HVD,2I2,IH=,IPE16.8,6H*(T**,(IPE16.8,5H))*DI)
C *****
290 C SPECIFIC HEAT OF THE MIXTURE.
C *****
      WRITE(3,I24)
      FORMAT(IHC,2X,4HSPCIFIC HEAT OF THE MIXTURE. NTIS FORMULA. )
      LBC=6HC(IST+
      LHU=3H)*U
295
      WRITE(3,I32)((LBPL,LHC,K,LBU,K),K=1,NSPC)
      FORMAT(6X,7HCM(IC)=*4(A1,A6,I2,A3,I2),A1,
      * 4(/5X,IH*,IX,4(A6,I2,A3,I2,A1)) )
C *****
300 C THERMAL CONDUCTIVITY OF THE MIXTURE.
C *****
      WRITE(3,272)
      WRITE(3,274)
272 FORMAT(IHC,2X,36HTHERMAL CONDUCTIVITY OF THE MIXTURE.)
274 FORMAT(IHC,2X,4HHAVERAGE OF LINEAR AND RECIPROCAL MIXING RULES. )
      LBX=IH*
      LBPL=IH*
      LBRL=3H*RL
      LBMLX=5HRLSUM
310
      WRITE(3,260)LBMLX,((LBPL,LBX,K,LRRL,K),K=1,NSPC)
      FORMAT(6X,A5,IH=,6(2A1,I2,A3,I2) ,A1,2(/5X,IH*,IX,
      * 8(A1,I2,A3,I2,A1)) )
      LRSRL=3H*VL
      LBMLX=5HRLSIV
315
      WRITE(3,265)
      WRITE(3,270)
      FORMAT(6X,I5HRLSIV=I.0/RLSIV )
265
      WRITE(3,270)
      FORMAT(6X,2IHRLM=0.5*(RLSUM*RLSIV))
320
      WRITE(3,306)
      FORMAT(6X,I5HRLM(IC)=RH*RLM )
C *****
C DERIVATIVE OF THE THERMAL CONDUCTIVITY OF THE MIXTURE.
C *****
      WRITE(3,312)
      FORMAT(IHC,2X,40HSPACE DER OF DENSITY TIMES THERMAL COND.)
312
      LBURL=4H*DRL
      LBDX=2HDX
      LBMLX=5HDL SUM
      WRITE(3,760)LBMLX,((LBPL,LBX,K,LHDLR,K,LBPL,LHDX,K,LBRL,K),
      * K=1,NSPC)
      * K=1,NSPC)
760
      FORMAT(6X,A5,IH=,2(2A1,I2,A4,I2,A1,A2,I2,A3,I2),A1,6(/5X,IH*,IX,
      * 3(A1,I2,A4,I2,A1,A2,I2,A3,I2,A1)) )
      LBPAR=IH)
      LBMLX=5HDL SIV
      LBURL=4H*DVL
330
      WRITE(3,765)LBMLX,((LBPL,LHDX,K,LHSLR,K,LBPL,LHX,K,LHDLV,K),
      * K=1,NSPC)
      * K=1,NSPC)
765
      FORMAT(6X,A5,IH=,2(A1,A2,I2,A3,I2,A4,I2,A1,I2,A4,I2),A1,6(/5X,IH*,IX,
      * 3(A2,I2,A3,I2,A1,I2,A4,I2,A1)) )
      WRITE(3,770)
      FORMAT(6X,24HDL SIV=-HLSIV*RLSIV)
770

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PROGRAM	LOADF	76/76	OPT=1	ROUND=+*/	TRACE	FTN	4.8+498	04/15/80	13.55.29	PAGE	8
400	532	* J=2,NSPC)						MAIN	399		
		FORMAT(6X,4HDSUM,I2,1H=,2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,						MAIN	400		
		* 9/(5X,IH*,IX,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)))						MAIN	401		
		1F(NM.EQ.1)GO TO 537						TPC	3		
405		DO 535 K=2,NM						MAIN	402		
		KM=K-1						MAIN	403		
		KP=K+1						MAIN	404		
		WRITE(3,532)K,((LBPL,LHDX,J,LBVD,J,K,LBPL,LBX,J,LBVD,J,K),						MAIN	405		
		* J=1,KM),((LBPL,LHDX,J,LBVD,K,J,LBPL,LBX,J,LBVD,K,J),J=KP,NSPC)						MAIN	406		
410	535	CONTINUE						MAIN	407		
	537	CONTINUE						TPC	4		
		K=NSPC						MAIN	408		
		WRITE(3,532)K,((LBPL,LHDX,J,LBVD,J,K,LBPL,LBX,J,LBVD,J,K),J=1,NM)						MAIN	409		
		DO 540 K=1,NSPC						MAIN	410		
415		WRITE(3,542)K,PHN,K,K,K,K						MAIN	411		
	540	CONTINUE						MAIN	412		
	542	FORMAT(6X,2HDB,I2,1H=,IPEI2,4,4H*(DX,I2,4H*SUM,I2,2H*X,I2,						MAIN	413		
		* 5H*DSUM,I2,IH))						MAIN	414		
		DO 545 K=1,NSPC						MAIN	415		
		WRITE(3,548)K,K,K,K						MAIN	416		
420	545	CONTINUE						MAIN	417		
	548	FORMAT(6X,2HDT,I2,12H=-DRH*(1.0-U,I2,7H)+KH*DU,I2)						MAIN	418		
		DO 550 K=1,NSPC						MAIN	419		
		WRITE(3,552)(K,L=1,7)						MAIN	420		
	550	CONTINUE						MAIN	421		
425	552	FORMAT(6X,4HDFAC,I2,1H=,2HDT,I2,2H/B,I2,2H-T,I2,3H*DB,I2,						MAIN	422		
		* 3H/(8,I2,2H*B,I2,IH))						MAIN	423		
		DO 590 K=1,NSPC						MAIN	424		
		WRITE(3,592)K,K,K,K,K						MAIN	425		
430	590	CONTINUE						MAIN	426		
	592	FORMAT(6X,3HDX,I2,5H=DFAC,I2,3H*DX,I2,4H*FAC,I2,4H*DDX,I2)						MAIN	427		
		DO 595 K=1,NSPC						MAIN	428		
	595	WRITE(3,598)K,K,K,K,K						MAIN	429		
	598	FORMAT(6X,4HDX,I2,3H=DU,I2,3H*VX,I2,2H*U,I2,4H*DVX,I2)						MAIN	430		
435	C	*****						MAIN	431		
	C	USE A BINARY APPROXIMATION FOR THERMAL DIFFUSION FOR THE						MAIN	432		
	C	INDICATED SPECIES.						MAIN	433		
	C	*****						MAIN	434		
	C	WRITE THE NECESSARY ALPHA I J, WHERE I IS A SPECIES WE WANT TO						MAIN	435		
	C	COMPUTE THE THERMAL DIFFUSION FOR.						MAIN	436		
440	C	*****						MAIN	437		
	901	WRITE(3,901)						MAIN	438		
		FORMAT(1HC,2X,40HCOMPUTE ALPHA FOR THE APPROPRIATE PAIRS.)						MAIN	439		
		LHDF=5HTHDF						MAIN	440		
445		DO 900 I=1,NM						MAIN	441		
		IPL=I+1						MAIN	442		
		DO 900 J=1PL,NSPC						MAIN	443		
		IF(LRTHD(I).NE.LHDF.AND.LRTHD(J).NE.LHDF)GO TO 900						MAIN	444		
		IF(LRTHD(I).EQ.LHDF)IP=1						MAIN	445		
		IF(LRTHD(I).EQ.LHDF)JP=J						MAIN	446		
450		IF(LRTHD(I).NE.LHDF)IP=J						MAIN	447		
		IF(LRTHD(I).NE.LHDF)JP=I						MAIN	448		
		I=SQRT(ESK(IP)*ESK(JP))						MAIN	449		
		IF(UM(IP).EQ.0.0.AND.UM(JP).EQ.0.0)GO TO 1302						MAIN	450		
455	C	COMPARING RULF. P. 528, REID AND SHERWOOD.						MAIN	451		
	C	WE ARE ASSUMING AT MOST ONE POLAR SPECIES.						MAIN	452		
		IF(UM(IP).NE.0.0)LP=IP						MAIN	453		

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460      IF (UM(JP),NE,0.0)LP=JP
      IF (LP,EQ,1P)LNP=JP
      IF (LP,EQ,JP)LNP=1P
      UMP=UM(LP)*1.0E-18
      SGC=SGA(LP)*1.0E-8
      TPSTAR=UMP*UMP/(ESK(LP)*RK*SGC*SGC*SGC*SGRT(8.0))
      FC=1.0*(1.0/SQRT(2.0))*(ALP(LNP)*TPSTAR/(SGA(LNP)**3))*SQRT(ESK(
      * LP)/ESK(LNP))
      WRITE(6,1305)IP,JP,LP,LNP,FC
1305      FORMAT(15X,4I6,1PE12.4)
      E=E*FC*FC
      CONTINUE
      WRITE(3,903)E
      FORMAT(6X,5HTS=T/,1PE14.6)
470      LBRTP=3HRTP
      WRITE(3,906)LBRTP,ARTP,CRTP
      FORMAT(6X,A3,1H=,1PE14.6,5H*EXP(,1PE14.6,4H/TS) )
906      LBC=3HCST
      WRITE(3,906)LBC,ACST,CCST
      WRITE(3,909)
      FORMAT(6X,16HCSTP=6.0*CSI-5.0 )
      WM=(W(IP)-W(JP))/W(IP)*W(JP)
      WRITE(3,912)IP,JP,WM
480      FORMAT(6X,2HAL,2I2,1H=,1PE14.6,9H*RTCP*CSST )
      WRITE(3,915)E
      FORMAT(6X,7HOTS=DT/,1PE14.6)
915      A=-ARTP*CRTP
      LBDRTP=4HDRTP
      WRITE(3,918)LBDRTP,A,CRTP
485      FORMAT(6X,A4,1H=,1PE14.6,5H*EXP(,1PE14.6,16H/TS)*DTS/(TS*TS) )
      LBDC=4HDCST
      A=-ACST*CCST
      WRITE(3,918)LBDC,A,CCST
490      WRITE(3,921)
      FORMAT(6X,14HDCSTP=6.0*DCST )
      WRITE(3,924)IP,JP,WM
921      FORMAT(6X,3HDAL,2I2,1H=,1PE14.6,22H*(ORTP*CSST*RTCP*DCSTP) )
924      IF (LBTHD(JP),NE,LBDOFF)GO TO 900
      WRITE(3,927)JP,IP,JP
495      FORMAT(6X,2HAL,2I2,2H=-,2HAL,2I2)
      WRITE(3,930)JP,IP,JP
930      FORMAT(6X,3HDAL,2I2,2H=-,3HDAL,2I2)
900      CONTINUE
      WRITE(3,951)
      FORMAT(1HC,2X,48HCOMPUTE THERMAL DIFFUSION FOR THE GIVEN SPECIES.)
500      LBX=1HX
      LBALP=3H*AL
      LBHX=2HDX
      LBHALP=4H*DAL
      DO 950 1=1,NSPC
      IF (LBTHD(1),NE,LBDOFF)GO TO 950
      IF (1,EQ,1)WRITE(3,933)((LBPL,LBX,J,LHALP,1,J),J=2,NSPC)
933      FORMAT(6X,4HSUM=,4(2A1,I2,A3,2I2),A1,4(15X,1H*,1X,
      * 5(A1,I2,A3,2I2,A1)) )
      IF (1,EQ,NSPC)WRITE(3,933)((LBPL,LBX,J,LHALP,1,J),J=1,NM)
      IF (1,EQ,1.OR,1.EQ,NSPC)GO TO 935
      NM=1-I
510

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515      IP=I+1
      WRITE(3,933)((LBPL,LBX,J,LRALP,I,J),J=1,IM),((LBPL,LBX,J,LRALP,
* I,J),J=IP,NSPC)
      CONTINUE
935      WRITE(3,936)I
      FORMAT(6X,SHRKT=X,I2,4H*SUM )
936      WRITE(3,939)I
      FORMAT(6X,I2HVTOP=PKT*UVX,I2,3H*UT )
939      WRITE(3,942)I
      FORMAT(6X,7HVBOT=DX,I2,2H*U )
942      WRITE(3,945)I
      FORMAT(6X,3HVT,I2,10H=VTOP/VBOT )
945      IF(I.EQ.I)WRITE(3,948)((LBPL,LBX,J,LRALP,I,J,LRPL,LBX,J,LRALP,I,
* J),J=2,NSPC)
      FORMAT(6X,SHDSUM=2(AI,A2,I2,A3,2I2,2AI,I2,A4,2I2),AI,
948      * 8(/5X,IH*,IX,2(A2,I2,A3,2I2,2AI,I2,A4,2I2,AI)) )
      IF(I.EQ.NSPC)WRITE(3,948)((LBPL,LBX,J,LRALP,I,J,LRPL,LBX,
* J,LRALP,I,J),J=I,NM)
      IF(I.EQ.I.OR.I.EQ.NSPC)GO TO 952
      IM=I-1
      IP=I-1
      WRITE(3,948)((LBPL,LBX,J,LRALP,I,J,LRPL,LBX,J,LRALP,I,J),
* J=I,IM),((LBPL,LBX,J,LRALP,I,J,LRPL,LBX,J,LRALP,I,J),J=IP,NSPC)
      CONTINUE
952      WRITE(3,955)I,I
      FORMAT(6X,7HDKT=DX,I2,6H*SUM+X,I2,5H*DSUM )
955      WRITE(3,958)I,I,I
      FORMAT(6X,I4HVTOP=URKT*UVX,I2,12H*UT+RKT*DUVX,I2,
* 11H*DT+RKT*UVX,I2,4H*DDT )
      WRITE(3,961)I,I
      FORMAT(6X,9HVBOT=DDX,I2,5H*U+DX,I2,3H*UT )
961      WRITE(3,964)I
      FORMAT(6X,4HUV,I2,34H=DVTOP/VBOT-VTOP*VBOT/(VBOT*VBOT) )
964      CONTINUE
950      WRITE(3,I129)
      FORMAT(IHC,2X,36HFIND THE FINAL VALUES OF UV AND DUV. )
I129      DO 1130 K=I,NSPC
      IF(LBTHD(K).EQ.LBDOFF)WRITE(3,I132)K,K,K
      IF(LBTHD(K).NE.LBDOFF)WRITE(3,I131)K,K
      CONTINUE
I130      FORMAT(6X,2HUV,I2,4H=UVX,I2)
I131      FORMAT(6X,2HUV,I2,4H=UVX,I2,4H+UV,I2)
I132      DO 1135 K=I,NSPC
      IF(LBTHD(K).EQ.LBDOFF)WRITE(3,I134)K,K,K
      IF(LBTHD(K).NE.LBDOFF)WRITE(3,I137)K,K
      CONTINUE
I133      FORMAT(6X,3HUV,I2,5H=DUVX,I2)
I137      FORMAT(6X,3HUV,I2,5H=DUVX,I2,5H+DUV,I2)
I138      CONTINUE
995      LUV=2HUV
      WRITE(3,I1212)((LHM,LUV,K),K=1,NSPC)
      FORMAT(6X,3HUV=8(AI,A2,I2),AI,2(/5X,IH*,IA,8(A2,I2,AI)) )
      DO 1215 K=1,NSPC
      WRITE(3,I1218)K,K,K
      FORMAT(6X,2HUV,I2,3H=UV,I2,5H+DUV*U,I2)
      LDUV=3HUV
      WRITE(3,I1222)((LHM,LUDUV,K),K=1,NSPC)

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515      1P=1+I
      WRITE(3,933)((LBPL,LBX,J,LBALP,I,J),J=1,IM),((LBPL,LBX,J,LBALP,
      * I,J),J=IP,NSPC)
      CONTINUE
      WRITE(3,936)I
      FORMAT(6X,5HDKT=X,I2,4H*SUM )
      WRITE(3,939)I
      FORMAT(6X,12HVTOP=DKT*UVX,I2,3H*UT )
      WRITE(3,942)I
      FORMAT(6X,7HVBOT=DX,I2,2H* )
      WRITE(3,945)I
      FORMAT(6X,3HUVT,I2,10H=VTOP/VBOT )
      IF(1.EQ.1)WRITE(3,948)((LBPL,LBX,J,LBALP,I,J,LBPL,LBX,J,LBALP,I,
      * J),J=2,NSPC)
      FORMAT(6X,5HDSUM=2(A1,A2,I2,A3,2I2,2A1,I2,A4,2I2),A1,
      * 8(5X,IH*,1X,2(A2,I2,A3,2I2,2A1,I2,A4,2I2,A1)) )
      IF(1.EQ.NSPC)WRITE(3,948)((LBPL,LBX,J,LBALP,I,J,LBPL,LBX,
      * J,LBALP,I,J),J=1,NM)
      IF(1.EQ.1.OR.1.EQ.NSPC)GO TO 952
      IM=I-1
      1P=1+I
      WRITE(3,948)((LBPL,LBX,J,LBALP,I,J,LBPL,LBX,J,LBALP,I,J),
      * J=1,IM),((LBPL,LBX,J,LBALP,I,J,LBPL,LBX,J,LBALP,I,J),J=IP,NSPC)
      CONTINUE
      WRITE(3,955)I,I
      FORMAT(6X,7HDKT=DX,I2,6H*SUM*X,I2,5H*DSUM )
      WRITE(3,958)I,I,I
      FORMAT(6X,14HVTOP=DKT*UVX,I2,12H*DT+DKT*DUVX,I2,
      * 11H*DT+DKT*UVX,I2,4H*DDT )
      WRITE(3,961)I,I
      FORMAT(6X,9HVBOT=DOX,I2,5H*DT+DX,I2,3H*DT )
      WRITE(3,964)I
      FORMAT(6X,4HUVT,I2,34H=DVTOP/VBOT-VTOP*(VBOT*VBOT) )
      CONTINUE
      WRITE(3,1129)
      FORMAT(1HC,2X,36HFIND THE FINAL VALUES OF UV AND DUV. )
      DO 1130 K=1,NSPC
      IF(LBTHD(K).EQ.LBDOFF)WRITE(3,1132)K,K,K
      IF(LBTHD(K).NE.LBDOFF)WRITE(3,1131)K,K,K
      CONTINUE
      1130      FORMAT(6X,2HUV,I2,4H=UVX,I2)
      1131      FORMAT(6X,2HUV,I2,4H=UVX,I2,4H*UVT,I2)
      1132      DO 1135 K=1,NSPC
      IF(LBTHD(K).EQ.LBDOFF)WRITE(3,1134)K,K,K
      IF(LBTHD(K).NE.LBDOFF)WRITE(3,1137)K,K,K
      CONTINUE
      1135      FORMAT(6X,3HDOUV,I2,5H=DOUVX,I2)
      1137      FORMAT(6X,3HDOUV,I2,5H=DOUVX,I2,5H*DOUVT,I2)
      1138      CONTINUE
      995      LUV=2HUV
      WRITE(3,1212)((LHM,LHUV,K),K=1,NSPC)
      1212      FORMAT(6X,3HDOV=8(A1,A2,I2),A1,2(/5X,IH*,1X,8(A2,I2,A1)) )
      DO 1215 K=1,NSPC
      1215      WRITE(3,1218)K,K,K
      1218      FORMAT(6X,2HUV,I2,3H=UV,I2,5H*DUV*U,I2)
      LHUV=3HDOV
      WRITE(3,1222)((LHM,LHDOUV,K),K=1,NSPC)

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1222 FORMAT(6X,4HDDV=,8(A1,A3,I2),A1,2(/5X,1H*,1X,8(A3,I2,A1)) )
1225 DO 1225 K=1,NSPC
1225 WRITE(3,1228)K,K,K
1228 FORMAT(6X,3HDDV,12,4H=DDV,12,6H+DDV*DU,12,6H+DDV*U,12)
575 DO 485 K=1,NSPC
485 WRITE(3,488)K,K
488 FORMAT(6X,9HDDV(1ST+,12,7H)=RH*UV,12)
DO 810 K=1,NSPC
810 WRITE(3,812)K,K,K
812 FORMAT(6X,10HDDV(1ST+,12,8H)=URH*UV,12,7H+RH*DDV,12)
580 C *****
C FIND THE TIME DERIVATIVES.
C *****
612 WRITE(3,612)
612 FORMAT(1HC,2X,26HFIND THE TIME DERIVATIVES.)
622 WRITE(3,622)
622 FORMAT(6X,15HSP=ASP*HSP*TIME)
TMSPH2=TMN/(PHN*PHN)
628 WRITE(3,628)
628 FORMAT(1X,3H100,2X,8HCONTINUE)
632 WRITE(3,632)
632 FORMAT(6X,25HIF (KPE.EQ.NPDE)GO TO 150)
636 WRITE(3,636)TMN
636 FORMAT(6X,3HRY=,1PE20,10,8H*R(KPE) )
TMSPH=TMN/PHN
595 WRITE(3,638)TMSPH
638 FORMAT(6X,4HDI=,1PE20,10,16H*DDHUV(1ST+KPE) )
WRITE(3,642)
642 FORMAT(6X,23HFVAL=SP*UPH(KPE)+UY*RY)
WRITE(3,646)
646 FORMAT(6X,6HRETURN)
648 WRITE(3,648)
648 FORMAT(1X,3H150,2X,8HCONTINUE)
DO 650 K=1,NM
605 WRITE(3,652)K,K
650 CONTINUE
652 FORMAT(6X,2HDD,12,5H=UPH(,12,1H) )
K=NSPC
LDDU=2HDD
610 WRITE(3,656)K,((LBM,LDDU,J),J=1,NM)
610 FORMAT(6X,2HDD,12,1H=,8(A1,A2,I2),A1,2(/5X,1H*,1X,8(A2,I2,A1)) )
WRITE(3,662)TMSPH2
662 FORMAT(6X,3HDL=,1PE20,10,1H*)
664 WRITE(3,664)
664 FORMAT(5X,1H*,1X,4H(DRHLM(1C)*UPH(NPDE)+RHLM(1C)*UPH2(NPDE)) )
LHBL=1H
LHC=6HC(1ST+
LHDDV=10H)*RHUV(1ST
WRITE(3,668)TMSPH,((LHBL,LHPL,LHC,K,LHDDV,LHPL,K,LAP),K=1,
* NSPC),LHP
668 FORMAT(6X,4HDI=,1PE20,10,12H*UPH(NPDE)*(,2A1,A6,12,A10,A1,12,
* 3A1,10(/5X,1H*,1X,2(A6,12,A10,A1,12,3A1)) )
TMSTP=TMN/TPN
LHR=2HPL
620 LHH=RH)*H(1ST+
620 WRITE(3,672)TMSTP,((LHHL,LHPL,LHC,K,LHH,K,LHP),K=1,NSPC),LHP
672 FORMAT(6X,4HDI=,1PE20,10,2PH*(,2(A1,A2,12,AH,12,A1),2A1,

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PROGRAM	LOADF	76/76	OPT=1	ROUND=+-*/	THACE	FIN	4.8+49H	04/15/80	13.55.29	PAGE	12
630		* 9(/5X,IH*1X,2(A2,I2,A8,I2,3A1)))						MAIN	625		
		WRITE(3,676)						MAIN	626		
	676	FORMAT(6X,35HFVAL=SP*UPH(NPDE)*(IL+TR+TD)/CM(IC))						MAIN	627		
		STOP						MAIN	628		
		END						MAIN	629		

HLOCK	ADDRESS	LENGTH	FILE
LOADF	110	12230	LGO
/STP.END/	12340	1	SL-FTNL18
/FCL.C./	12341	30	SL-FTNL18
/Q8.10./	12371	144	SL-FTNL18
Q2NTRY=	12535	4	SL-FTNL18
COMIO=	12541	10	SL-FTNL18
FECMSK=	12551	41	SL-FTNL18
FEIFST=	12612	3	SL-FTNL18
FLIN=	12615	156	SL-FTNL18
FLIOUT=	12773	315	SL-FTNL18
FMATAP=	13310	377	SL-FTNL18
FORSYS=	13707	300	SL-FTNL18
FORUTL=	14207	45	SL-FTNL18
GETFIT=	14254	54	SL-FTNL18
INCOM=	14330	144	SL-FTNL18
INPC=	14474	173	SL-FTNL18
KODER=	14667	476	SL-FTNL18
KRAKER=	15365	454	SL-FTNL18
OUTC=	16041	155	SL-FTNL18
OUTCOM=	16216	204	SL-FTNL18
ERRCAP=	16422	317	SL-FTNL18
FERCAP=	16741	171	SL-FTNL18
EXP.MSG	17132	16	SL-FTNL18
SURT	17150	6	SL-FTNL18
SORT.	17156	32	SL-FTNL18
SYSID=	17210	1	SL-FTNL18
SYS=1ST	17211	65	SL-FTNL18

1 H2 THDFF 2.0000E+00 2.9200E+00 3.8000E+01 0. 7.9000E-01

.31001901E+01 .51119464E-03 .52644210E-07 -.34909973E-10 .36945345E-14 H2
 -.87738042E+03 -.19629421E+01 .30574451E+01 .26765200E-02 -.58099162E-05 H2
 .55210391E-08 -.18122739E-11 -.98890474E+03 -.22997056E+01 H2

2 N2 2.8000E+01 3.6200E+00 9.7500E+01 0. 0.

.28963194E+01 .15154866E-02 -.57235277E-06 .99807393E-10 -.65223555E-14 N2
 -.90586184E+03 .61615144E+01 .36748261E+01 -.12081500E-02 .23240102E-05 N2
 -.63217559E-09 -.22577253E-12 -.10611588E+04 .23580424E+01 N2

VISCOSITY FROM WARNATZ ST PAR.
 LEAST SQUARES FIT, T=300.2000.
 THERMAL CONDUCTIVITIES FROM WARNATZ ST PAR.
 LEAST SQUARES FIT, T=300.2000.

1 H2 2.188700E-06 6.502900E-01 H2 VISCOSITY.

1 H2 6.357900E-06 7.393300E-01 H2 THERMAL CONDUCTIVITY.

2 H2 4.266700E-06 6.613600E-01 N2 VISCOSITY.

2 H2 6.407700E-07 7.999600E-01 N2 THERMAL CONDUCTIVITY.

BINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
 LEAST SQUARES FIT, I=100,300

1	1	H2	H2	1.119300E-04	1.661400E+00	H2	H2	BINARY DIFFUSION.
1	2	H2	N2	5.951700E-05	1.663800E+00	H2	N2	BINARY DIFFUSION.
2	2	N2	N2	1.537400E-05	1.672900E+00	N2	N2	BINARY DIFFUSION.

8.112200E-01 4.866900E-02 RTP=RT/(6C*-5) FIT A*EXP(C/T)

9.542600E-01 -1.435700E-01 C* HCB FIT A*EXP(C/T)

TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03

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1  SUBROUTINE F(TIME,PH,U,UPH,UPH2,FVAL,NPDE,IC,KSKT,KSKP)
   DIMENSION U(NPDE),UPH(NPDE),UPH2(NPDE)
   COMMON/TARAB/ASP,BSP,TPN,PHN,IMN,TMSPH,TMSTP,TPENT
   COMMON/TARP/PRESS,PSR,NPDEM
   COMMON/TARSM/SMALL
5  DIMENSION K(20)
   DIMENSION C(1000),H(1000),RHL(100),DRHLM(100),CM(100)
   COMMON/TABCT/RL,CPMX,H0(20),R2D(20),R2DM(20)
   COMMON/TABMF/RHUV(1000),DRHUV(1000)
10  COMMON/TABRY/T,RH,Y1,Y2,Y3,Y4,Y5,Y6,Y7,Y8,Y9,Y10
   C AT EACH CALL THE TIME RATE OF CHANGE FOR ONE PDE IS RETURNED IN FVAL.
   C FOR THE COMPLETE TRANSPORT CASE, WE DO NOT WANT THE U VALUES OR
   C THEIR FIRST DERIVATIVES TO BE ZERO. THIS CAN LEAD TO DIVISION
   C BY ZERO.
15  DO 5 K=1,NPDEM
   IF(ARS(U(K)),LT,SMALL)U(K)=SMALL
   IF(ARS(UPH(K)),LT,SMALL)UPH(K)=SMALL
5  IF(ARS(UPH(K)),LT,SMALL)UPH(K)=SMALL
   C TEST CASE. BINARY MIX OF H2 AND N2. WARNAT2 TRANSPORT VALUES.
   YN=1.0-U( 1)
   CALL RT(U,YN,R,NPDE,KPDE,IC,KSKP)
20  IST= 2*(IC-1)
   IF(KSKT.GT.1)GO TO 100
   IF(KSKR.GT.1)GO TO 125
   C NT1S ENTHALPIES AND HEAT CAPACITIES.
25  IF(T.GT.1000.)GO TO 2000
   C 1=1.9872*( 3.05744510E+00+T*( 2.67652000E-03
   *+T*( -5.80991620E-06+T*( 5.52103910E-09+T*( -1.81227390E-12))))
   H 1=1.9872*( -9.88904740E+02+T*( 3.05744510E+00
   *+T*( 2.67652000E-03/2.0+T*( -5.80991620E-06/3.0
   *+T*( 5.52103910E-09/4.0+T*( -1.81227390E-12/5.0))))))
30  C 2=1.9872*( 3.67482610E+00+T*( -1.20815000E-03
   *+T*( 2.32401020E-06+T*( -6.32175590E-10+T*( -2.25772530E-13))))
   H 2=1.9872*( -1.06115880E+03+T*( 3.67482610E+00
   *+T*( -1.20815000E-03/2.0+T*( 2.32401020E-06/3.0
   *+T*( -6.32175590E-10/4.0+T*( -2.25772530E-13/5.0))))))
   GO TO 3000
2000 CONTINUE
   C 1=1.9872*( 3.10019010E+00+T*( 5.11194640E-04
   *+T*( 5.26442100E-08+T*( -3.49099730E-11+T*( 3.69453450E-15))))))
40  H 1=1.9872*( -8.77380420E+02+T*( 3.10019010E+00
   *+T*( 5.11194640E-04/2.0+T*( 5.26442100E-08/3.0
   *+T*( -3.49099730E-11/4.0+T*( 3.69453450E-15/5.0))))))
   C 2=1.9872*( 2.89631940E+00+T*( 1.51548660E-03
   *+T*( -5.72352770E-07+T*( 9.98073930E-11+T*( -6.52235550E-15))))))
45  H 2=1.9872*( -9.05861840E+02+T*( 2.89631940E+00
   *+T*( 1.51548660E-03/2.0+T*( -5.72352770E-07/3.0
   *+T*( 9.98073930E-11/4.0+T*( -6.52235550E-15/5.0))))))
3000 CONTINUE
   C SPECIFIC HEATS AND SPECIFIC ENTHALPIES.
50  C(IST+ 1)=C 1/ 2.00
   H(IST+ 1)=H 1/ 2.00
   C(IST+ 2)=C 2/ 28.00
   H(IST+ 2)=H 2/ 28.00
   C(IST+ 3)=C 1/ 2.00
   H(IST+ 3)=H 1/ 2.00
   C(IST+ 4)=C 2/ 28.00
   H(IST+ 4)=H 2/ 28.00
   C(IST+ 5)=C 1/ 2.00
   H(IST+ 5)=H 1/ 2.00
   C(IST+ 6)=C 2/ 28.00
   H(IST+ 6)=H 2/ 28.00
   C(IST+ 7)=C 1/ 2.00
   H(IST+ 7)=H 1/ 2.00
   C(IST+ 8)=C 2/ 28.00
   H(IST+ 8)=H 2/ 28.00
   C(IST+ 9)=C 1/ 2.00
   H(IST+ 9)=H 1/ 2.00
   C(IST+ 10)=C 2/ 28.00
   H(IST+ 10)=H 2/ 28.00
   C(IST+ 11)=C 1/ 2.00
   H(IST+ 11)=H 1/ 2.00
   C(IST+ 12)=C 2/ 28.00
   H(IST+ 12)=H 2/ 28.00
   C(IST+ 13)=C 1/ 2.00
   H(IST+ 13)=H 1/ 2.00
   C(IST+ 14)=C 2/ 28.00
   H(IST+ 14)=H 2/ 28.00
   C(IST+ 15)=C 1/ 2.00
   H(IST+ 15)=H 1/ 2.00
   C(IST+ 16)=C 2/ 28.00
   H(IST+ 16)=H 2/ 28.00
   C(IST+ 17)=C 1/ 2.00
   H(IST+ 17)=H 1/ 2.00
   C(IST+ 18)=C 2/ 28.00
   H(IST+ 18)=H 2/ 28.00
   C(IST+ 19)=C 1/ 2.00
   H(IST+ 19)=H 1/ 2.00
   C(IST+ 20)=C 2/ 28.00
   H(IST+ 20)=H 2/ 28.00
   C(IST+ 21)=C 1/ 2.00
   H(IST+ 21)=H 1/ 2.00
   C(IST+ 22)=C 2/ 28.00
   H(IST+ 22)=H 2/ 28.00
   C(IST+ 23)=C 1/ 2.00
   H(IST+ 23)=H 1/ 2.00
   C(IST+ 24)=C 2/ 28.00
   H(IST+ 24)=H 2/ 28.00
   C(IST+ 25)=C 1/ 2.00
   H(IST+ 25)=H 1/ 2.00
   C(IST+ 26)=C 2/ 28.00
   H(IST+ 26)=H 2/ 28.00
   C(IST+ 27)=C 1/ 2.00
   H(IST+ 27)=H 1/ 2.00
   C(IST+ 28)=C 2/ 28.00
   H(IST+ 28)=H 2/ 28.00
   C(IST+ 29)=C 1/ 2.00
   H(IST+ 29)=H 1/ 2.00
   C(IST+ 30)=C 2/ 28.00
   H(IST+ 30)=H 2/ 28.00
   C(IST+ 31)=C 1/ 2.00
   H(IST+ 31)=H 1/ 2.00
   C(IST+ 32)=C 2/ 28.00
   H(IST+ 32)=H 2/ 28.00
   C(IST+ 33)=C 1/ 2.00
   H(IST+ 33)=H 1/ 2.00
   C(IST+ 34)=C 2/ 28.00
   H(IST+ 34)=H 2/ 28.00
   C(IST+ 35)=C 1/ 2.00
   H(IST+ 35)=H 1/ 2.00
   C(IST+ 36)=C 2/ 28.00
   H(IST+ 36)=H 2/ 28.00
   C(IST+ 37)=C 1/ 2.00
   H(IST+ 37)=H 1/ 2.00
   C(IST+ 38)=C 2/ 28.00
   H(IST+ 38)=H 2/ 28.00
   C(IST+ 39)=C 1/ 2.00
   H(IST+ 39)=H 1/ 2.00
   C(IST+ 40)=C 2/ 28.00
   H(IST+ 40)=H 2/ 28.00
   C(IST+ 41)=C 1/ 2.00
   H(IST+ 41)=H 1/ 2.00
   C(IST+ 42)=C 2/ 28.00
   H(IST+ 42)=H 2/ 28.00
   C(IST+ 43)=C 1/ 2.00
   H(IST+ 43)=H 1/ 2.00
   C(IST+ 44)=C 2/ 28.00
   H(IST+ 44)=H 2/ 28.00
   C(IST+ 45)=C 1/ 2.00
   H(IST+ 45)=H 1/ 2.00
   C(IST+ 46)=C 2/ 28.00
   H(IST+ 46)=H 2/ 28.00
   C(IST+ 47)=C 1/ 2.00
   H(IST+ 47)=H 1/ 2.00
   C(IST+ 48)=C 2/ 28.00
   H(IST+ 48)=H 2/ 28.00
   C(IST+ 49)=C 1/ 2.00
   H(IST+ 49)=H 1/ 2.00
   C(IST+ 50)=C 2/ 28.00
   H(IST+ 50)=H 2/ 28.00
   C(IST+ 51)=C 1/ 2.00
   H(IST+ 51)=H 1/ 2.00
   C(IST+ 52)=C 2/ 28.00
   H(IST+ 52)=H 2/ 28.00
   C(IST+ 53)=C 1/ 2.00
   H(IST+ 53)=H 1/ 2.00
   C(IST+ 54)=C 2/ 28.00
   H(IST+ 54)=H 2/ 28.00
   C(IST+ 55)=C 1/ 2.00
   H(IST+ 55)=H 1/ 2.00
   C(IST+ 56)=C 2/ 28.00
   H(IST+ 56)=H 2/ 28.00
   C(IST+ 57)=C 1/ 2.00
   H(IST+ 57)=H 1/ 2.00
   C(IST+ 58)=C 2/ 28.00
   H(IST+ 58)=H 2/ 28.00
   C(IST+ 59)=C 1/ 2.00
   H(IST+ 59)=H 1/ 2.00
   C(IST+ 60)=C 2/ 28.00
   H(IST+ 60)=H 2/ 28.00
   C(IST+ 61)=C 1/ 2.00
   H(IST+ 61)=H 1/ 2.00
   C(IST+ 62)=C 2/ 28.00
   H(IST+ 62)=H 2/ 28.00
   C(IST+ 63)=C 1/ 2.00
   H(IST+ 63)=H 1/ 2.00
   C(IST+ 64)=C 2/ 28.00
   H(IST+ 64)=H 2/ 28.00
   C(IST+ 65)=C 1/ 2.00
   H(IST+ 65)=H 1/ 2.00
   C(IST+ 66)=C 2/ 28.00
   H(IST+ 66)=H 2/ 28.00
   C(IST+ 67)=C 1/ 2.00
   H(IST+ 67)=H 1/ 2.00
   C(IST+ 68)=C 2/ 28.00
   H(IST+ 68)=H 2/ 28.00
   C(IST+ 69)=C 1/ 2.00
   H(IST+ 69)=H 1/ 2.00
   C(IST+ 70)=C 2/ 28.00
   H(IST+ 70)=H 2/ 28.00
   C(IST+ 71)=C 1/ 2.00
   H(IST+ 71)=H 1/ 2.00
   C(IST+ 72)=C 2/ 28.00
   H(IST+ 72)=H 2/ 28.00
   C(IST+ 73)=C 1/ 2.00
   H(IST+ 73)=H 1/ 2.00
   C(IST+ 74)=C 2/ 28.00
   H(IST+ 74)=H 2/ 28.00
   C(IST+ 75)=C 1/ 2.00
   H(IST+ 75)=H 1/ 2.00
   C(IST+ 76)=C 2/ 28.00
   H(IST+ 76)=H 2/ 28.00
   C(IST+ 77)=C 1/ 2.00
   H(IST+ 77)=H 1/ 2.00
   C(IST+ 78)=C 2/ 28.00
   H(IST+ 78)=H 2/ 28.00
   C(IST+ 79)=C 1/ 2.00
   H(IST+ 79)=H 1/ 2.00
   C(IST+ 80)=C 2/ 28.00
   H(IST+ 80)=H 2/ 28.00
   C(IST+ 81)=C 1/ 2.00
   H(IST+ 81)=H 1/ 2.00
   C(IST+ 82)=C 2/ 28.00
   H(IST+ 82)=H 2/ 28.00
   C(IST+ 83)=C 1/ 2.00
   H(IST+ 83)=H 1/ 2.00
   C(IST+ 84)=C 2/ 28.00
   H(IST+ 84)=H 2/ 28.00
   C(IST+ 85)=C 1/ 2.00
   H(IST+ 85)=H 1/ 2.00
   C(IST+ 86)=C 2/ 28.00
   H(IST+ 86)=H 2/ 28.00
   C(IST+ 87)=C 1/ 2.00
   H(IST+ 87)=H 1/ 2.00
   C(IST+ 88)=C 2/ 28.00
   H(IST+ 88)=H 2/ 28.00
   C(IST+ 89)=C 1/ 2.00
   H(IST+ 89)=H 1/ 2.00
   C(IST+ 90)=C 2/ 28.00
   H(IST+ 90)=H 2/ 28.00
   C(IST+ 91)=C 1/ 2.00
   H(IST+ 91)=H 1/ 2.00
   C(IST+ 92)=C 2/ 28.00
   H(IST+ 92)=H 2/ 28.00
   C(IST+ 93)=C 1/ 2.00
   H(IST+ 93)=H 1/ 2.00
   C(IST+ 94)=C 2/ 28.00
   H(IST+ 94)=H 2/ 28.00
   C(IST+ 95)=C 1/ 2.00
   H(IST+ 95)=H 1/ 2.00
   C(IST+ 96)=C 2/ 28.00
   H(IST+ 96)=H 2/ 28.00
   C(IST+ 97)=C 1/ 2.00
   H(IST+ 97)=H 1/ 2.00
   C(IST+ 98)=C 2/ 28.00
   H(IST+ 98)=H 2/ 28.00
   C(IST+ 99)=C 1/ 2.00
   H(IST+ 99)=H 1/ 2.00
   C(IST+ 100)=C 2/ 28.00
   H(IST+ 100)=H 2/ 28.00
   C(IST+ 101)=C 1/ 2.00
   H(IST+ 101)=H 1/ 2.00
   C(IST+ 102)=C 2/ 28.00
   H(IST+ 102)=H 2/ 28.00
   C(IST+ 103)=C 1/ 2.00
   H(IST+ 103)=H 1/ 2.00
   C(IST+ 104)=C 2/ 28.00
   H(IST+ 104)=H 2/ 28.00
   C(IST+ 105)=C 1/ 2.00
   H(IST+ 105)=H 1/ 2.00
   C(IST+ 106)=C 2/ 28.00
   H(IST+ 106)=H 2/ 28.00
   C(IST+ 107)=C 1/ 2.00
   H(IST+ 107)=H 1/ 2.00
   C(IST+ 108)=C 2/ 28.00
   H(IST+ 108)=H 2/ 28.00
   C(IST+ 109)=C 1/ 2.00
   H(IST+ 109)=H 1/ 2.00
   C(IST+ 110)=C 2/ 28.00
   H(IST+ 110)=H 2/ 28.00
   C(IST+ 111)=C 1/ 2.00
   H(IST+ 111)=H 1/ 2.00
   C(IST+ 112)=C 2/ 28.00
   H(IST+ 112)=H 2/ 28.00
   C(IST+ 113)=C 1/ 2.00
   H(IST+ 113)=H 1/ 2.00
   C(IST+ 114)=C 2/ 28.00
   H(IST+ 114)=H 2/ 28.00
   C(IST+ 115)=C 1/ 2.00
   H(IST+ 115)=H 1/ 2.00
   C(IST+ 116)=C 2/ 28.00
   H(IST+ 116)=H 2/ 28.00
   C(IST+ 117)=C 1/ 2.00
   H(IST+ 117)=H 1/ 2.00
   C(IST+ 118)=C 2/ 28.00
   H(IST+ 118)=H 2/ 28.00
   C(IST+ 119)=C 1/ 2.00
   H(IST+ 119)=H 1/ 2.00
   C(IST+ 120)=C 2/ 28.00
   H(IST+ 120)=H 2/ 28.00
   C(IST+ 121)=C 1/ 2.00
   H(IST+ 121)=H 1/ 2.00
   C(IST+ 122)=C 2/ 28.00
   H(IST+ 122)=H 2/ 28.00
   C(IST+ 123)=C 1/ 2.00
   H(IST+ 123)=H 1/ 2.00
   C(IST+ 124)=C 2/ 28.00
   H(IST+ 124)=H 2/ 28.00
   C(IST+ 125)=C 1/ 2.00
   H(IST+ 125)=H 1/ 2.00
   C(IST+ 126)=C 2/ 28.00
   H(IST+ 126)=H 2/ 28.00
   C(IST+ 127)=C 1/ 2.00
   H(IST+ 127)=H 1/ 2.00
   C(IST+ 128)=C 2/ 28.00
   H(IST+ 128)=H 2/ 28.00
   C(IST+ 129)=C 1/ 2.00
   H(IST+ 129)=H 1/ 2.00
   C(IST+ 130)=C 2/ 28.00
   H(IST+ 130)=H 2/ 28.00
   C(IST+ 131)=C 1/ 2.00
   H(IST+ 131)=H 1/ 2.00
   C(IST+ 132)=C 2/ 28.00
   H(IST+ 132)=H 2/ 28.00
   C(IST+ 133)=C 1/ 2.00
   H(IST+ 133)=H 1/ 2.00
   C(IST+ 134)=C 2/ 28.00
   H(IST+ 134)=H 2/ 28.00
   C(IST+ 135)=C 1/ 2.00
   H(IST+ 135)=H 1/ 2.00
   C(IST+ 136)=C 2/ 28.00
   H(IST+ 136)=H 2/ 28.00
   C(IST+ 137)=C 1/ 2.00
   H(IST+ 137)=H 1/ 2.00
   C(IST+ 138)=C 2/ 28.00
   H(IST+ 138)=H 2/ 28.00
   C(IST+ 139)=C 1/ 2.00
   H(IST+ 139)=H 1/ 2.00
   C(IST+ 140)=C 2/ 28.00
   H(IST+ 140)=H 2/ 28.00
   C(IST+ 141)=C 1/ 2.00
   H(IST+ 141)=H 1/ 2.00
   C(IST+ 142)=C 2/ 28.00
   H(IST+ 142)=H 2/ 28.00
   C(IST+ 143)=C 1/ 2.00
   H(IST+ 143)=H 1/ 2.00
   C(IST+ 144)=C 2/ 28.00
   H(IST+ 144)=H 2/ 28.00
   C(IST+ 145)=C 1/ 2.00
   H(IST+ 145)=H 1/ 2.00
   C(IST+ 146)=C 2/ 28.00
   H(IST+ 146)=H 2/ 28.00
   C(IST+ 147)=C 1/ 2.00
   H(IST+ 147)=H 1/ 2.00
   C(IST+ 148)=C 2/ 28.00
   H(IST+ 148)=H 2/ 28.00
   C(IST+ 149)=C 1/ 2.00
   H(IST+ 149)=H 1/ 2.00
   C(IST+ 150)=C 2/ 28.00
   H(IST+ 150)=H 2/ 28.00
   C(IST+ 151)=C 1/ 2.00
   H(IST+ 151)=H 1/ 2.00
   C(IST+ 152)=C 2/ 28.00
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C LEAST SQUARES FIT, T=300.2000.
C V 1= 2.188700E-06*(T** 6.502900E-01)
C V 2= 4.266700E-06*(T** 6.613600E-01)
C RL 1= 6.357900E-06*(T** 7.383300E-01)
C RL 2= 6.407700E-07*(T** 7.999600E-01)
C HINARY DIFFUSION COEFFICIENTS FROM WARNATZ ST PAR.
C LEAST SQUARES FIT, T=100.300
C PRESS = 1.00
C O 1 2= 5.951700E-05*(T** 1.663800E+00)
C SPACE DERIVATIVES.
YS=Y 3
X 1=Y 1/YS
X 2=Y 2/YS
U 1=U( 1)
DU 1=UPH( 1)
DDU 1=UPH2( 1)
U 2=1.0-U 1
DU 2=-DU 1
DDU 2=-DDU 1
DY 1=DU 1/ 2.00
DY 2=DU 2/ 28.00
DYS=+DY 1+DY 2
C TPN = 1.0000E+03 PHN = 5.0000E-05 TMN = 1.0000E-03
DT=UPH(NPDE)* 1.0000E+03
DRH=- 1.2187690433E-02*(DT/T+DYS/YS)/(T*YS)
VL 1= 1.57284638E+05*(T**(-7.36330000E-01))
VL 2= 1.56062238E+06*(T**(-7.99960000E-01))
DRL 1= 4.694228E-06*(T**(-2.616700E-01))*DT
DRL 2= 5.125904E-07*(T**(-2.000400E-01))*DT
DVL 1= -1.161280E+05*(T**(-1.738330E+00))*DT
DVL 2= -1.248435E+06*(T**(-1.799960E+00))*DT
DYS=DYS/(YS*YS)
DX 1=DY 1/YS-Y 1*DYSY
DX 2=DY 2/YS-Y 2*DYSY
DDY 1=DDU 1/ 2.00
DDY 2=DDU 2/ 28.00
DDYS=+DDY 1+DDY 2
DYSYSQ=(DYS/YS)**2
DDX 1=(DDY 1-2.0*DY 1*DYS/YS+2.0*Y 1*DYSYSQ-Y 1*DDYS/YS)/YS
DDX 2=(DDY 2-2.0*DY 2*DYS/YS+2.0*Y 2*DYSYSQ-Y 2*DDYS/YS)/YS
VD 1 2= 1.68019221E+04*(T**(-1.66380000E+00))
VD 1 2= -2.79550381E+04*(T**(-2.66380000E+00))*DT
C SPECIFIC HEAT OF THE MIXTURE. N15 FORMULA.
CM(IC)=+C(1ST+ 1)*U 1+C(1ST+ 2)*U 2
C THERMAL CONDUCTIVITY OF THE MIXTURE.
C AVERAGE OF LINEAR AND RECIPROCAL MIXING RULES.
RLSUM=+X 1*RL 1+X 2*RL 2
RLSIV=+X 1*VL 1+X 2*VL 2
RLSIV=1.0/RLSIV
RLM=0.5*(PLSUM+RLSIV)
RMLM(IC)=RH*RLM
C SPACE DER OF DENSITY TIMES THERMAL (OND.
DLSUM=+X 1*DRL 1+DX 1*RL 1+X 2*DRL 2+DX 2*RL 2
DLSIV=+DX 1*VL 1+X 1*DVL 1+DX 2*VL 2+X 2*DVL 2
DLSIV=-RLSIV*RLSIV*DLSIV
DRLM=0.5*(DLSUM+DLSIV)

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115      DRHLM(1C)=DRH*RLM+RH*DRLM
      C SOLVE FOR UV.
      SUM 1=X 2*VD 1 2
      SUM 2=X 1*VD 1 2
      H 1=X 1*SUM 1* 5.0000E-05
      B 2=X 2*SUM 2* 5.0000E-05
      T 1=-RH*(1.0-U 1)
      T 2=-RH*(1.0-U 2)
      FAC 1=T 1/R 1
      FAC 2=T 2/R 2
      VX 1=FAC 1*DX 1
      VX 2=FAC 2*DX 2
      UVX 1=U 1*VX 1
      UVX 2=U 2*VX 2
      C SPACE DER OF DENSITY TIMES UV.
      USUM 1=DX 2*VD 1 2+X 2*DVD 1 2
      USUM 2=DX 1*VD 1 2+X 1*DVD 1 2
      DR 1= 5.0000E-05*(UX 1*SUM 1+X 1*DSUM 1)
      DR 2= 5.0000E-05*(UX 2*SUM 2+X 2*DSUM 2)
      DT 1=-DRH*(1.0-U 1)+RH*DU 1
      DT 2=-DRH*(1.0-U 2)+RH*DU 2
      UFAC 1=DT 1/B 1-T 1*UB 1/(B 1*B 1)
      DFAC 2=DT 2/B 2-T 2*UB 2/(B 2*B 2)
      DVX 1=DFAC 1*DX 1+FAC 1*DDX 1
      DVX 2=DFAC 2*DX 2+FAC 2*DDX 2
      DUVX 1=DU 1*VX 1+U 1*DVX 1
      DUVX 2=DU 2*VX 2+U 2*DVX 2
      C COMPUTE ALPHA FOR THE APPROPRIATE PAIRS.
      TS=T/ 6.086871E+01
      RTP= 8.112200E-01*EXP( 4.866900E-02/TS)
      CST= 9.542600E-01*EXP( -1.435700E-01/TS)
      CSTP=6.0*CST-5.0
      AL 1 2= -8.666667E-01*RTP*CSTP
      DTS=DT/ 6.086871E+01
      DRTP= -3.948127E-02*EXP( 4.866900E-02/TS)*DTS/(TS*TS)
      DCST= 1.370031E-01*EXP( -1.435700E-01/TS)*DTS/(TS*TS)
      DCSTP=6.0*DCST
      DUAL 1 2= -8.666667E-01*(DRTP*CSTP+RTP*DCSTP)
      C COMPUTE THERMAL DIFFUSION FOR THE GIVEN SPECIES.
      SUM=X 2*AL 1 2
      RKT=X 1*SUM
      VTOP=RKT*UVX 1*DT
      VBOT=DX 1*T
      UVT 1=VTOP/VBOT
      USUM=X 2*AL 1 2+X 2*DAL 1 2
      DRKT=DX 1*SUM+X 1*USUM
      DVTOP=DRKT*UVX 1*DT+RKT*DUVX 1*DT+RKT*UVX 1*DOT
      DVBOT=DX 1*T+DX 1*DT
      DUVT 1=DVTOP/VBOT-VTOP*DVBOT/(VBOT*VHUT)
      C FIND THE FINAL VALUES OF UV AND DUV.
      UV 1=UVX 1+UVT 1
      UV 2=UVX 2
      DUV 1=DUVX 1+DUVT 1
      DUV 2=DUVX 2
      DV=-UV 1-UV 2
      UV 1=UV 1+DV*U 1
      UV 2=UV 2+DV*U 2

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175      DDV=-DUV 1-DUV 2
          DUV 1=DUV 1+DV*DU 1+DDV*U 1
          DUV 2=DUV 2+DV*DU 2+DDV*U 2
          RHUV(IST+ 1)=RH*UV 1
          RHUV(IST+ 2)=RH*UV 2
          DRHUV(IST+ 1)=DRH*UV 1+RH*DUV 1
          DRHUV(IST+ 2)=DRH*UV 2+RH*DUV 2
      C FIND THE TIME DERIVATIVES.
          SP=ASP+BSP*TIME
180      100 CONTINUE
          IF(KPDE.EQ.NPDE)GO TO 150
          HY= 1.000000000E-03*R(KPDE)
          DY=- 2.000000000E+01*DRHUV(IST+KPDE)
          FVAL=SP*UPH(KPDE)+DY*RY
          RETURN
185      150 CONTINUE
          DU 1=UPH( 1)
          DU 2=-DU 1
          TL= 4.000000000E+05*
          * (DRHLM(IC)*UPH(NPDE)+RHLM(IC)*UPH2(NPDE))
          TD=- 2.000000000E+01*UPH(NPDE)*( +C(IST+ 1)*RHUV(IST+ 1) +
          * C(IST+ 2)*RHUV(IST+ 2))
          TR=- 1.000000000E-06*( +R( 1)*H(IST+ 1) +R( 2)*H(IST+ 2))
          FVAL=SP*UPH(NPDE)+(TL+TR+TD)/CM(IC)
          RETURN
190      198 END
195

```

LIST OF SYMBOLS

- $A_{ij}^* = \Omega_{ij}^{(2,2)*} / \Omega_{ij}^{(1,1)*}$, quotient of collision integrals.
 $B_{ij}^* = [5\Omega_{ij}^{(1,2)*} - 4\Omega_{ij}^{(1,3)*}] / \Omega_{ij}^{(1,1)*}$, quotient of collision integrals.
 $C_{ij}^* = \Omega_{ij}^{(1,2)*} / \Omega_{ij}^{(1,1)*}$, quotient of collision integrals.
 $C_{i,int}$ = internal heat capacity, cal-mole⁻¹-K⁻¹.
 $C_{i,rot}$ = rotational heat capacity, cal-mole⁻¹-K⁻¹.
 $C_{i,tr}$ = translational heat capacity, cal-mole⁻¹-K⁻¹.
 $C_{i,v}$ = heat capacity at constant volume, cal-mole⁻¹-K⁻¹.
 c_{pi} = specific heat, cal-gm⁻¹-K⁻¹.
 $c_p = \sum_{i=1}^N c_{pi} Y_i$, specific heat of the mixture, cal-gm⁻¹-K⁻¹.
 D_{ij} = binary diffusion coefficient, cm²-s⁻¹.
 D_{im} = diffusion coefficient of species i into a mixture, cm²-s⁻¹.
 D_{ij} = multicomponent diffusion coefficient, cm²-s⁻¹.
 D_i^T = multicomponent thermal diffusion coefficient, gm-s⁻¹-cm⁻¹.
 $D_{i,int,j}$ = binary diffusion coefficient for internal energy, cm²-s⁻¹.
 h_i = specific enthalpy, cal-gm⁻¹.
 k = Boltzmann constant = 1.38054X10⁻¹⁶ erg-K⁻¹-molecule⁻¹.
 k_{ij} = thermal diffusion ratio.
 k_{im} = thermal diffusion ratio between species i and the rest of the mixture.
 M_i = molecular weight, gm-mole⁻¹.
 p = pressure, atm.
 q = total energy flux relative to the fluid velocity, cal-cm⁻²-s⁻¹.
 R_i = rate of production of ith species by chemical reaction, mole-cm⁻³-s⁻¹.
 R = gas constant = 1.9872 cal-mole⁻¹-K⁻¹.
 R_a = gas constant = 82.05 cm³-atm-mole⁻¹-K⁻¹.

LIST OF SYMBOLS (Cont'd)

t = time, s.

T = temperature, K.

T_u = temperature of unburned mixture, K.

T_B = temperature of burned mixture, K.

$T_i^* = T/(\epsilon_i/k)$.

$T_{ij}^* = T/(\epsilon_{ij}/k)$.

u = fluid velocity, cm-s^{-1} .

V_i = diffusion velocity, cm-s^{-1} .

$\mathcal{V}_i$ = diffusion velocity due to species gradients, cm-s^{-1} .

$\mathcal{W}_i$ = diffusion velocity due to the temperature gradient, cm-s^{-1} .

x = spatial coordinate, cm.

X_i = mole fraction.

Y_i = mass fraction.

Y_{iu} = mass fraction of species i in the unburned mixture.

Y_{iB} = mass fraction of species i in the burned mixture.

α_i = polarizability, $\text{\AA}^3$.

ϵ_i/k = Lennard-Jones or Stockmayer parameter, K.

η_i = viscosity, poise = $\text{gm-cm}^{-1}\text{-s}^{-1}$.

μ_i = dipole moment, debye = $10^{-18} \text{ gm}^{1/2}\text{-cm}^{5/2}\text{-s}^{-1}$.

σ_i = Lennard-Jones or Stockmayer parameter, $\text{\AA}$.

λ_o = thermal conductivity of the mixtures, neglecting diffusion effects, $\text{cal-cm}^{-1}\text{-s}^{-1}\text{-K}^{-1}$.

$\lambda_{o,tr}$ = thermal conductivity due to translational energy, $\text{cal-cm}^{-1}\text{-s}^{-1}\text{-K}^{-1}$.

$\lambda_{o,int}$ = thermal conductivity due to internal energy, $\text{cal-cm}^{-1}\text{-s}^{-1}\text{-K}^{-1}$.

LIST OF SYMBOLS (Cont'd)

$\lambda_{\text{mix}}^{\text{mon}}$ = thermal conductivity of a mixture of monatomic gases, $\text{cal-cm}^{-1}\text{-s}^{-1}\text{-K}^{-1}$.

$\lambda_{\text{mix}}^{\text{poly}}$ = thermal conductivity of a mixture, $\text{cal-cm}^{-1}\text{-s}^{-1}\text{-K}^{-1}$.

ρ = fluid density, gm-cm^{-3} .

ξ_{ij} = rotational collision numbers.

$\Omega_{ij}^{(1,1)*}; \Omega_{ij}^{(2,2)*}; \Omega_{ij}^{(1,2)*}; \Omega_{ij}^{(1,3)*}$ = collision integral.

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