AD-A133213

TECHNICAL
LIBRARY

AD A-133 213

TECHNICAL REPORT ARBRL-TR-02512

TRANSPORT ALGORITHMS FOR METHANE FLAMES

Joseph M. Heimerl
Terence P. Coffee

July 1983

US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

Approved for public release; distribution unlimited.

Destroy this report when it is no longer needed.
Do not return it to the originator.

Additional copies of this report may be obtained from the National Technical Information Service, U. S. Department of Commerce, Springfield, Virginia 22161.

The findings in this report are not to be construed as an official Department of the Army position, unless so designated by other authorized documents.

The use of trade names or manufacturers' names in this report does not constitute indorsement of any commercial product.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER
TECHNICAL REPORT ARBRL-TR-02512

2. GOVT ACCESSION NO.

3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle)
TRANSPORT ALGORITHMS FOR METHANE FLAMES

5. TYPE OF REPORT & PERIOD COVERED
Final

6. PERFORMING ORG. REPORT NUMBER

7. AUTHOR(s)
Joseph M. Heimerl
Terence P. Coffee

8. CONTRACT OR GRANT NUMBER(s)

9. PERFORMING ORGANIZATION NAME AND ADDRESS
US Army Ballistic Research Laboratory
ATTN: DRDAR-BLI
Aberdeen Proving Ground, MD 21005

10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
1L161102AH43

11. CONTROLLING OFFICE NAME AND ADDRESS
US Army Armament Research & Development Command
US Army Ballistic Research Laboratory (DRDAR-BLA-S)
Aberdeen Proving Ground, MD 21005

12. REPORT DATE
July 1983

13. NUMBER OF PAGES
33

14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)

15. SECURITY CLASS. (of this report)
Unclassified

15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)
Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Laminar Flames	Multicomponent Transport Algorithms
Steady-State Flames	Diffusion Velocity Approximations
Premixed Flames	Thermal Diffusion Approximations
One-Dimensional Flames	Methane Flames

Flames

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) meg

The effects of three different methods of approximating multispecies transport phenomena in models of premixed, laminar, steady-state flames have been studied. The most precise, the most simple and a compromise transport algorithm were used to model methane-oxygen flames at one atmosphere with diluents of nitrogen, argon or helium. The thermodynamic and Lennard-Jones (Stockmayer) coefficients for individual species were held fixed together with the kinetic network and rate coefficients. Only the (CONT'D)

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

20. Abstract (Cont'd):

computational algorithms were changed. Within factors of 10-20% we found that the computed flame speeds and species and temperature profiles were independent of the algorithm employed. Since we had previously reported a similar independence for hydrogen-oxygen-nitrogen flames, we infer that this result is a general one.

TABLE OF CONTENTS

Page

I. INTRODUCTION.....5

II. THE FLAME EQUATIONS.....6

III. INPUT COEFFICIENTS.....6

IV. APPROXIMATION METHODS.....7

A. Method I.....8
B. Method V.....9
C. Method VI.....11

V. RESULTS AND DISCUSSION.....12

REFERENCES.....19

APPENDIX A.....21

GLOSSARY.....25

DISTRIBUTION LIST.....27

I. INTRODUCTION

We have been concerned with the modeling of premixed, laminar, steady-state flames.[1] In a previous paper,[2] hereinafter called paper I, we studied a set of five H_2-O_2-N_2 flames and found that the species profiles were very nearly independent of the transport algorithms used to describe the multispecies transport phenomena. The computed flame speeds corresponding to this set span a range of more than a factor of 60 in magnitude. Because no exceptions could be found we surmised that this independence of transport algorithm (not of transport parameters) was of a general nature. We wished to verify this inference by performing a similar computer study for the methane-air flame. The results are reported here.

Methane-air was selected because there is sufficient information to model it and because the species therein form a significant subset of the modeling of higher hydrocarbon flames.[3] The method of approach is to select and fix input parameters for CH_4-air mixtures and then vary the mathematical approximations to the multicomponent transport properties. We consider only flames whose total pressure is one atmosphere and whose unburned gas temperature is 298K.

In paper I we employed six methods of approximating transport. Five of these methods encompassed the range of approximations commonly found in the literature. The sixth is a method we developed that is computationally efficient and provides results extremely close to the most precise method. Because of our previous experience, (paper I) we elected here to use only the most precise, the most simple and our best compromise transport methods. They are, in the notation of paper I: Method I, Method V and Method VI, respectively.

To provide as great a range of flame speeds as possible, we have also examined the stoichiometric methane-oxygen system in buffer gases of argon and helium.

The remainder of this paper consists of four sections. Section II briefly recalls the appropriate flame equations. Section III lists the input parameters used. Section IV reviews the approximate transport methods, and the results and discussion are found in Section V.

---

[1] *J.M. Heimerl and T.P. Coffee, "The Detailed Modeling of Premixed, Laminar Steady-State Flames. I. Ozone,"* Combustion and Flame, *Vol. 39, pp. 301-315, 1980.*

[2] *T.P. Coffee and J.M. Heimerl, "Transport Algorithms for Premixed, Laminar Steady-State Flames,"* Combustion and Flame, *Vol. 43, pp. 273-289, 1981.*

[3] *J. Warnatz, "The Structure of Laminar Alkane-, Alkene-, and Acetylene Flames," Proceedings of 18th Symposium (International) on Combustion, pp. 369-384, 1981.*

II. THE FLAME EQUATIONS

In this section the equations that describe a one-dimensional, laminar, premixed flame that propagates in an unbounded ideal gas are recalled. 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[4] are:*

Overall Continuity:

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

Continuity of Species:

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

and Conservation of Energy:

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

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

$$T = T_u \text{ and } Y_i = Y_{iu} \; (i=1,\ldots N), \tag{4}$$

and for $x = \infty$;

$$\frac{\partial T}{\partial x} = \frac{\partial Y_i}{\partial x} = 0 \; (i=1,\ldots N). \tag{5}$$

The transport properties that are of interest are the diffusion velocities V_i and the heat flux q.

III. INPUT COEFFICIENTS

Thermodynamic, kinetic and transport coefficients are required to obtain solutions to the flame equations of Section II. The enthalpy, entropy and heat capacity for each species are functions of temperature. Over the range $300 \leq T \leq 3000$ K they are adequately described by the polynominal fits of Gordon and McBride.[5]

---

[4] *F.A. Williams, Combustion Theory, Addison-Wesley, Reading, MA, 1965.*

**The terms are defined in the glossary.*

[5] *S. Gordon and B.J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouquet Detonations," NASA-SP-273, 1980 program version.*

The kinetic network, consisting of 14 species and 33 reversible reactions, is taken from Table 1 of Dixon-Lewis.[6] His network is designed for lean to slightly rich flames; we have adopted it and his forward rate coefficients uncritically. (Where there are two entries for forward rate coefficients, we have taken those not enclosed by parentheses.) The rate coefficients for CHO reacting with O_2, H, OH and O are not listed in his table. We take Dixon-Lewis'[6] suggested values of 3.0, 40.0, 5.0 and 10.0 x 10^{12} cm^3 $mole^{-1}s^{-1}$, respectively. Expressions for the reverse rate coefficients were computed from the forward rate coefficients and the corresponding equilibrium constants. These constants were determined from Gibbs free energy functions.

For the present purposes we have kept the kinetic parameters constant, i.e., independent of stoichiometry and of the nature of the buffer gas.

To describe the transport properties of the individual species, we have adopted the Lennard-Jones (or Stockmayer) formalism. The transport parameters for the 14 species are taken from Warnatz.[3] The Lennard-Jones parameters, (σ, ε/k), for argon and helium are taken to be (35.42 nm, 93.3 K) and (25.51 nm, 10.22 K), respectively.[7]

IV. APPROXIMATION METHODS

In this section we review the three approximations, Methods I, V and VI, to the multicomponent, polyatomic formalism, based on the theory of Wang Chang and Uhlenbeck.[8-12] We begin with the most accurate, Method I, which is the

---

[6] *G. Dixon-Lewis, "Aspects of the Kinetic Modeling of Methane Oxidation In Flames," Proceedings of the 1st Specialist Meeting (International) of the Combustion Institute, Universite' de Bordeaux, France, Paper No. 49, pp. 284-289, 20-24 July 1981.*

[7] *R.C. Reid, J.M. Prausnitz, and T.K. Sherwood, The Properties of Gases and Liquids, McGraw-Hill, NY, 3rd Ed., p. 678, 1977.*

[8] *J.O. Hirschfelder, C.F. Curtiss, and R.B. Bird, Molecular Theory of Gases and Liquids, 2nd printing, corrected with notes, John Wiley and Sons, NY, 1964.*

[9] *C.S. Wang Chang, G.E. Uhlenbeck, and J. de Boer, Studies in Statistical Mechanics, Vol. 2, John Wiley and Sons, NY, 1964.*

[10] *L. Monchick, R.J. Munn, and E.A. Mason, "Thermal Diffusion in Polyatomic Gases: A Generalized Stefan-Maxwell Diffusion Equation," J. Chem. Phys., Vol. 45, pp. 3051-3058, 1966.*

[11] *L. Monchick, A.N.G. Pereira, and E.A. Mason, "Heat Conductivity in Polyatomic and Polar Gases and Gas Mixtures," J. Chem. Phys., Vol. 42, pp. 3241-3256, 1965.*

[12] *L. Monchick, K.S. Yun, and E.A. Mason, "Formal Kinetic Theory of Transport Phenomena in Polyatomic Gas Mixtures," J. Chem. Phys., Vol. 39, pp. 654-669, 1963.*

three-term Sonine approximation to the formalism. Dixon-Lewis[13] gives a discussion of this approximation, and we have generally followed his approach. Method V discusses the case of constant transport parameters. In Method VI we employ a simplified form of the Stefan-Maxwell equations that accounts for molecular diffusion and we provide a procedure that accounts for thermal diffusion.

In each case we determine the diffusion velocities V_i, $i = 1, 2, \ldots N$, and the heat flux q.

A. Method I

Following Dixon-Lewis,[13] we can write

$$q = \sum_{i=1}^{N} \rho Y_i V_i h_i - \lambda_o \frac{\partial T}{\partial x} - \sum_{i=1}^{N} \frac{RTD_i^T}{M_i Y_i} \frac{\partial X_i}{\partial x} \tag{6}$$

and

$$V_i = \frac{1}{X_i} \sum_{j=1}^{N} \frac{Y_j}{X_j} D_{ij} \frac{\partial X_j}{\partial x} - \frac{D_i^T}{\rho Y_i} \frac{\partial}{\partial x} (\ln T). \tag{7a}$$

or

$$V_i = \mathcal{V}_i + \mathcal{W}_i, \tag{7b}$$

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

$$D_{ij} = X_i \frac{16T}{25p} \frac{\sum_{k=1}^{N} M_k X_k}{M_j} c_{i00}^{lji} \tag{8}$$

and

$$D_i^T = \frac{8}{5} \frac{M_i X_i}{R_a} a_{i00}^{1} . \tag{9}$$

Substituting Equations (8) and (9) into Equation (7) we find

$$V_i = \frac{16T}{25p} \sum_{j=1}^{N} \left(c_{i00}^{lji} \frac{\partial X_j}{\partial x}\right) - \frac{8T}{5p} a_{i00}^{1} \frac{\partial}{\partial x} (\ln T). \tag{10}$$

Similary, we can write

$$\lambda_o = \lambda_{o,tr} + \lambda_{o,int} = -4 \sum_{i=1}^{N} X_i a_{i10}^{1} - 4 \sum_{i=1}^{N} X_i a_{i01}^{1} . \tag{11}$$

---

[13] *G. Dixon-Lewis, "Flame Structure and Flame Reaction Kinetics. II. Transport Phenomena in Multicomponent Systems,"* Proc. Roy. Soc., *Vol. A307, pp. 111-135, 1968.*

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

$$(L)\ (a^1_{100} \cdots a^1_{N00},\ a^1_{110} \cdots a^1_{N10},\ a^1_{101} \cdots a^1_{N01})^T \tag{12}$$

and $$= (0 \ldots 0, X_1 \ldots X_N, X_1 \ldots X_N)^T$$

$$(L)\ (c^{1hk}_{100} \cdots c^{1hk}_{N00},\ c^{1hk}_{110} \cdots c^{1hk}_{N10},\ c^{1hk}_{101} \cdots c^{1hk}_{N01})^T \tag{13}$$

$$= (\delta_{1h} - \delta_{1k} \ldots \delta_{Nh} - \delta_{Nk},\ 0 \ldots 0,\ 0 \ldots 0)\ h,k=1\ldots N.$$

The elements of the 3N by 3N matrix (L) have been given in paper I and elsewhere.[13] The procedures we have used for computing these elements have been discussed by us in paper I.

From Equation (13), it appears that we must solve N^2 sets of equations to obtain the c^{1ji}_{i00}. In fact, it has been recommended[3,8,12] that only the a terms be computed using this level of approximation, and that the c terms be computed using a one-term expansion. (Such a procedure, in fact, yields the Stefan-Maxwell equations.)

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 (13) to a vector whose elements are in fact the V_i by multiplying each equation of (13) by $\frac{16T}{25p}\frac{\partial Xh}{\partial x}$ and then summing over h. After some algebra we find

$$(L)\ (V_1 \ldots V_N, \ldots\ldots)^T = \left(\frac{16T}{25p}\frac{\partial X_1}{\partial x} \ldots, \frac{16T}{25p}\frac{\partial X_N}{\partial x}, 0 \ldots 0, 0 \ldots 0\right)^T. \tag{14}$$

Equation (14) 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.

B. Method V.

This is the most simple method we have considered. It consists of an empirical formula for the thermal conductivity,

$$\lambda_o = 0.5\ \left[\sum_{i=1}^{N} X_i\lambda_i + \left\{\sum_{i=1}^{N} X_i/\lambda_i\right\}^{-1}\right], \tag{15}$$

and a generalization of Fick's Law for molecular diffusion. Specifically, we have

$$Y_iV_i = -D_{im}\frac{\partial Y_i}{\partial x} \tag{16}$$

where

$$D_{im} = \frac{1 - X_i}{\sum\limits_{j\neq i} \frac{X_j}{\mathcal{D}_{ij}}}. \tag{17}$$

In the Lennard-Jones formalism $\mathcal{D}_{ij} \propto T^{1.5}/\Omega^{(1,1)*}$, where $\Omega^{(1,1)*}$ is approximately proportional to $T^{-0.17}$.[14] Since $\rho \propto T^{-1}$, it is not unreasonable to assume that $\rho^2\mathcal{D}_{ij}$ 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 $\Omega^{(2,2)*} \propto T^{-0.16}$,[14] 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 the constants $(\rho\lambda)$ and $(\rho^2 D_{im})$.

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.,

$$\left(\sum_{i=1}^{N} Y_i h_i\right)_B = \sum_{i=1}^{N} (Y_i h_i)_u , \tag{18}$$

we can compute the adiabatic flame temperature T_B by a numerical trial and error procedure. In this process we also find values for the burned gas mass fractions, Y_{iB}.

At this level of approximation we would like to use an appropriate constant (or "global") c_p. So we will assume that $c_{pi} = c_p$ = constant, i=1 ... 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

$$\sum_{i=1}^{N} Y_i h_i = \sum_{i=1}^{N} Y_i h_i^\circ + c_p (T - T_o). \tag{19}$$

Substituting (19) into (18) we find

$$c_p = \frac{\sum_{i=1}^{N} h_i^\circ (Y_{iu} - Y_{iB})}{T_B - T_u} . \tag{20}$$

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 λ using Equations (17) and (15), respectively. Then $\rho^2 D_{im}$, i=1,2,...N-1, and $\rho\lambda$ are evaluated. The diffusion velocity V_N is found from the constraint

---

[14] *A.A. Westenberg, "Present Status of Information on Transport Properties Applicable to Combustion Research,"* Combustion and Flame, *Vol. 1, pp. 346-358, 1957.*

$$\sum_{i=1}^{N} Y_i V_i = 0. \tag{21}$$

C. Method VI

For the thermal conductivity we use the simplest formula (15), since we have found in paper I that the exact choice is not important. For the molecular diffusion velocities V_i we use the expression based upon the Stefan-Maxwell equations with the additional assumption that all but the ith species move with the same velocity. The result is the formula recommended by Hirshfelder and Curtiss[15]

$$V_i = - \frac{(1 - Y_i)}{X_i \sum_{j \neq i} \frac{X_j}{\mathcal{D}_{ij}}} \frac{\partial X_i}{\partial x} . \tag{22}$$

For flames with low mass species and steep temperature gradients, the neglect of thermal diffusion is often as important as the differences between the computational methods. So we have generated 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 we identify from Equation (7a)

$$W_1 = \frac{-D_1^T}{\rho Y_1} \frac{\partial \ln T}{\partial x} \tag{23}$$

Since the thermal diffusion ratio is defined[8]

$$k_{12} = \frac{X_1 X_2}{\rho Y_1 Y_2} \frac{D_1^T}{\mathcal{D}_{12}} , \tag{24}$$

we can use Equation (22) to recast Equation (23) in terms of known entities; specifically, we have:

$$W_1 = k_{12} V_1 \frac{\partial}{\partial x} (\ln T) / \frac{\partial X_1}{\partial x} . \tag{25}$$

Theoretical expressions for k_{12} have been derived and even in the first approximation the expressions are quite complicated. For the special case of heavy isotopes, however, the first approximation simplifies to[8]

$$k_{12} = \frac{15(2A^* + 5)(6C^* - 5)(M_1 - M_2)}{2A^*(16A^* - 12B^* + 55)(M_1 + M_2)} X_1 X_2 . \tag{26}$$

---

[15] *J.O. Hirschfelder and C.F. Curtiss, "Theory of Propagation of Flames. Part I: General Equations," Proceedings of 3rd Symposium (International) on Combustion, pp. 121-127, 1949.*

Fortunately, Equation (26) reproduces H_2-N_2 thermal diffusion ratios to within 30%, and so we use it as a simple but reasonable approximation for k_{12}. Equation (25) can now be evaluated.

Generalizing Equation (25) we define

$$\mathcal{W}_i = k_{im} \mathcal{V}_i \frac{\partial}{\partial x} (\ln T) / \frac{\partial X_i}{\partial x} \quad , \tag{27}$$

where[16]

$$k_{im} = \sum_{\substack{j=1 \\ i \neq j}}^{N} k_{ij} \quad . \tag{28}$$

The k_{ij} are given by expressions analogous to Equation (26).

From Equation (26) we can see that the influence of $\mathcal{W}_i$ will be the greater the larger the mass differences. Normally, the thermal diffusion ratio does not exceed 0.1 and in practice, we compute $\mathcal{W}_i$ only for the lighter species, i.e., H, H_2, and He.

The resulting diffusion velocities $V_1 = \mathcal{V}_i + \mathcal{W}_i$ do not satisfy Equation (21). One technique to satisfy this constraint is due to Oran and Boris.[17] They note that diffusion velocities enter into the Stefan-Maxwell equations as differences. They then conclude that if a set of diffusion velocities V_i satisfies the Stefan-Maxwell equations, 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 (21) is satisfied.

V. RESULTS AND DISCUSSION

Table 1 shows the computed flame speeds for mixtures of CH_4 and O_2 in buffer gases of N_2, Ar and He for the three transport methods. Quantitatively the buffer gas is defined through the relationship

$$\frac{[O_2]}{[O_2] + [X]} = 0.21, \tag{29}$$

where X = N_2, Ar or He and the brackets indicate concentrations. Only for X = N_2 in Equation (29) are stoichiometries other than unity considered. The span of values for the flame speeds is seen to exceed a factor of seven.

---

[16] *S. Chapman and T.G. Cowling, The Mathematical Theory of Non-Uniform Gases, 3rd Ed., Cambridge University Press, 1970.*

[17] *E.S. Oran and J.P. Boris, "Detailed Modeling of Combustion Systems," Progress in Energy and Combustion Science, Vol. 7, pp. 1-72, 1981.*

The largest difference between Method I, the most complete formulation of the transport, and the other two methods is 11%. Compare Method V and Method I for the case of stoichiometric flame with N_2 as buffer. In paper I, using the kinetics given by Tsatsaronis,[18] we found the same trends for stoichiometric methane-air mixtures.

Table 2 shows a comparison between our results using the most precise transport method and two sets of experimental results that consider all three buffer gases. For stoichiometric methane-air, Andrews and Bradley,[19] Warnatz,[3] and Dixon-Lewis and Islam[20] report experimental flame speeds of 45, 42.5 and 38 $cm\text{-}s^{-1}$, respectively.

For the 6.5% and 13% methane-air cases Warnatz[3] lists experimental values as 19.5 and 16(±5) $cm\text{-}s^{-1}$. The reason for the factor of two discrepancy in the fuel-rich case probably lies in the fact that we uncritically adopted a reaction network designed for lean to slightly rich methane/air flames. Other than for the fuel-rich case, we see that our computed flame speeds are realistic.

The fact that the flame speeds for the three transport methods agree is a necessary but not sufficient condition to judge the relative effectiveness of the methods. The species and temperature profiles must also be examined.

Figure 1 shows the profiles for a stoichiometric flame with helium buffer for the intermediate species H, HO_2, and CH_2O. As can be seen, the shape of each species profile is independent of the transport method. The differences in the peaks are 17%, 12%, and 11% for H, HO_2, and CH_2O, respectively. These differences are typical of the largest found. Most other species profiles show differences less than these. Indeed, the computed temperature profiles for each mixture are nearly identical for each of the three methods.

Figure 2 shows that all three methods produce nearly identical profiles for the intermediate species, H_2. Also seen in Figure 2 are the profiles for fuel CH_4, and oxidizer, O_2. Again, aside from the peaks in the region 0.6 - 1.1 mm, the three transport methods produce nearly identical profiles.

These peaks were observed only in the computations using helium as the buffer gas and they could have three causes. First there are numerical errors. These can be eliminated because, we routinely increase the number of collocation points by 50%, decrease the time step error criterion by a factor of three and increase the total space of the solution interval of 10%, to check the numerical accuracy of the solutions.

---

[18] *G. Tsatsaronis, "Prediction of Propagating Laminar Flames in Methane, Oxygen, Nitrogen Mixtures," Combustion and Flame, Vol. 33, pp. 217-239, 1978.*

[19] *G.E. Andrews and D. Bradley, "Determination of Burning Velocities: A Critical Review," Combustion and Flame, Vol. 18, pp. 133-153, 1972.*

[20] *G. Dixon-Lewis and S.M. Islam, "Flame Modeling and Burning Velocity Measurement," Proceedings of 19th Symposium (International) on Combustion, to be published.*

Second, there is a mass-to-mole conversion that can produce spurious peaks in the mole fraction plots. This phenomenon has been seen and reported earlier.[21] It is briefly discussed in the appendix. A check of all the mass fraction profiles shows the same peaks for O_2 and CH_4 and so we eliminate this as the cause.

Third, there are thermal diffusion effects. Method I implicitly contains the effects of thermal diffusion, Method VI explicitly contains them [Equation (27)] and Method V neglects them entirely. When we set $D^T_{He} = 0$ in Method VI the peaks evident in Figure 2 disappear and the profiles so obtained for O_2 and CH_4 resemble those of Method V. We conclude that the peaks in the O_2 and CH_4 profiles are due to thermal diffusion of helium.

As seen in Section IV, Method VI contains a theoretically crude approximation to thermal diffusion. However, when the results are compared to those of Method I, both here and in paper I, we find quite close agreement. This indicates that, in practice, Method VI is quite precise.

We employ a relaxation technique[1] to find steady state solutions to the flame Equations (1-5), and so we require trial solutions to the profiles. Almost any reasonably well behaved profile will allow Method V to converge rapidly. These solutions are then used as the initial profiles for Method VI. In turn, the solutions for Method VI are used as the trial solutions for Method I. Using this ordering we have found that Method VI required about 3 to 5 times more computational effort than Method V and Method I required 10-25 times more. These values are for the studies presented here and the ranges show that the computational effort can be highly problem dependent.

Based upon these results we recommend Method V as the everyday method of choice and Method VI as the more precise computational method.

In order to emphasize that the choice of transport parameters can be important we examined how the flame speed for the stoichiometric methane-air case is affected by changes in the transport parameters of Method V.[22] We find that a 20% change in $\rho\lambda$ or a 50% change in $\rho^2 D_{O_2 m}$ will change the flame speed by 10%. This change is about the same as the maximum change found between methods in Table 1.

---

[21] *J.M. Heimerl, "A Contribution to the Flat Flame Olympics: Problem B," ARBRL-TR-02416, August 1982. See also: Notes on Numerical Fluid Mechanics, Vol. 6, "Numerical Methods in Laminar Flame Propagation," N. Peters and J. Warnatz, eds., Friedr. Viewag and Son, Braunschweig/Wiesbaden, pp. 71-86, 1982 (AD A119401).*

[22] *T.P. Coffee and J.M. Heimerl, "Sensitivity Analysis For Premixed Laminar, Steady State Flames," ARBRL-TR-02457, January 1983 (AD A123866).*

For the relative tests performed here we have used the same sets of Lennard-Jones (or Stockmayer) parameters for the transport, the same thermodynamic functions and the same kinetic network and parameters. We varied only the transport algorithm and found that within factors of 10 to 20% Method V produces accurate results for both the profiles and the flame speed. Method VI shows even greater accuracy and includes the effect of thermal diffusion. Thus, we have shown that the method used to approximate the multicomponent, polyatomic transport phenomena for methane-oxygen-buffer gas mixtures is not critical. In paper I, we came to the same conclusion for H_2-O_2-N_2 mixtures. Since these two flame types have widely differing properties and since each flame type has been studied over an extensive range of gas mixtures, we infer that this result is a general one.

TABLE 1. CALCULATED FLAME SPEEDS IN CM/S. Stoichiometries other than unity were considered only for the N_2 buffer.

Buffer Gas	Transport Method	%CH_4 6.6	9.5	12 .0
	I	17.6	44.8	31.5
	V	16.0	39.8	28.5
N_2	VI	16.7	43.1	30.6
	I		78.0	
Ar	V		74.2	
	VI		75.0	
	I		131.7	
He	V		131.3	
	VI		133.0	

TABLE 2. COMPARISON OF OUR COMPUTED FLAME SPEEDS WITH THOSE EXPERIMENTAL VALUES THAT CONSIDER ALL THREE BUFFER GASES

Reference/Buffer Gas	N_2	Ar	He
Method I (this paper)	44.8	78.0	131.7
Clingman, et al[23]	40	92	132
Morgan and Kane[24]	38.1	72.8	120.4

---

[23] *W.H. Clingman, R.S. Brokaw, and R.N. Pease, "Burning Velocities of Methane with Nitrogen-Oxygen, Argon-Oxygen and Helium-Oxygen Mixtures," Proceedings of 4th Symposium (International) on Combustion, pp. 310-313, 1953.*

[24] *G.H. Morgan and W.R. Kane, "Some Effects of Inert Diluents on Flame Speeds and Temperatures," Proceedings of 4th Symposium (International) on Combustion, pp. 313-320, 1953.*

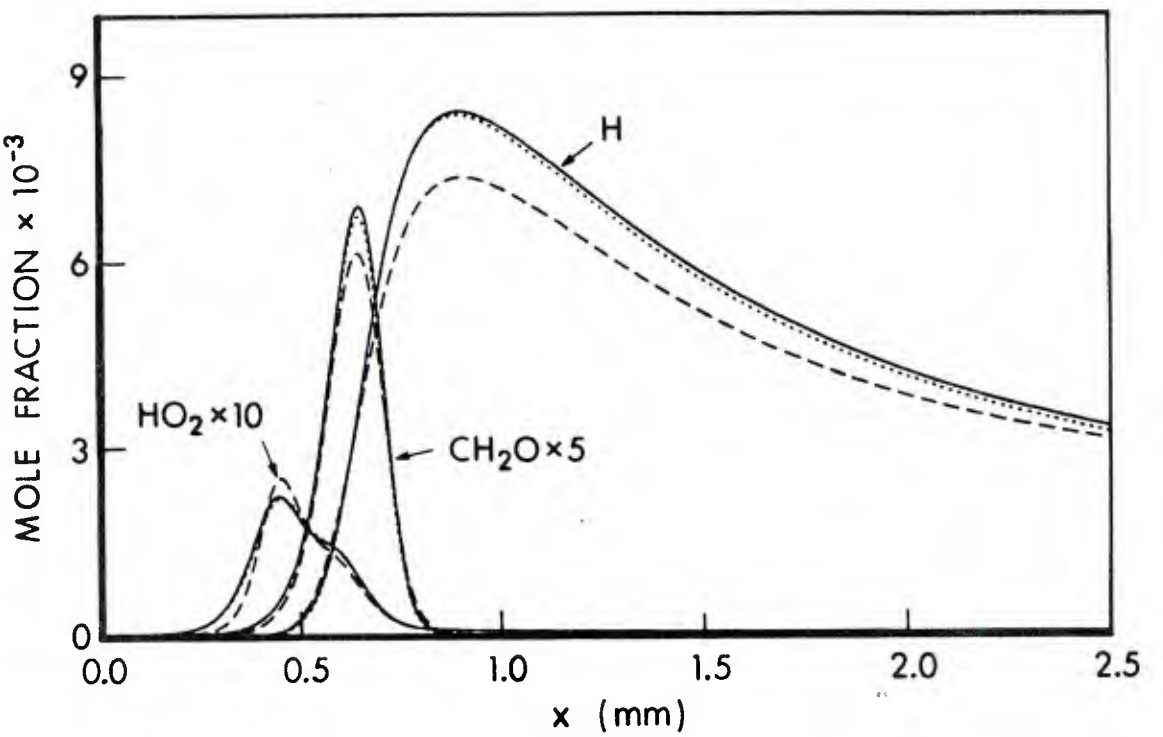

Figure 1. H, HO_2, and CH_2O Species Profiles for a Stoichiometric Flame With Helium Buffer for Transport Method I (line), Method VI (dot), and Method V (dash)

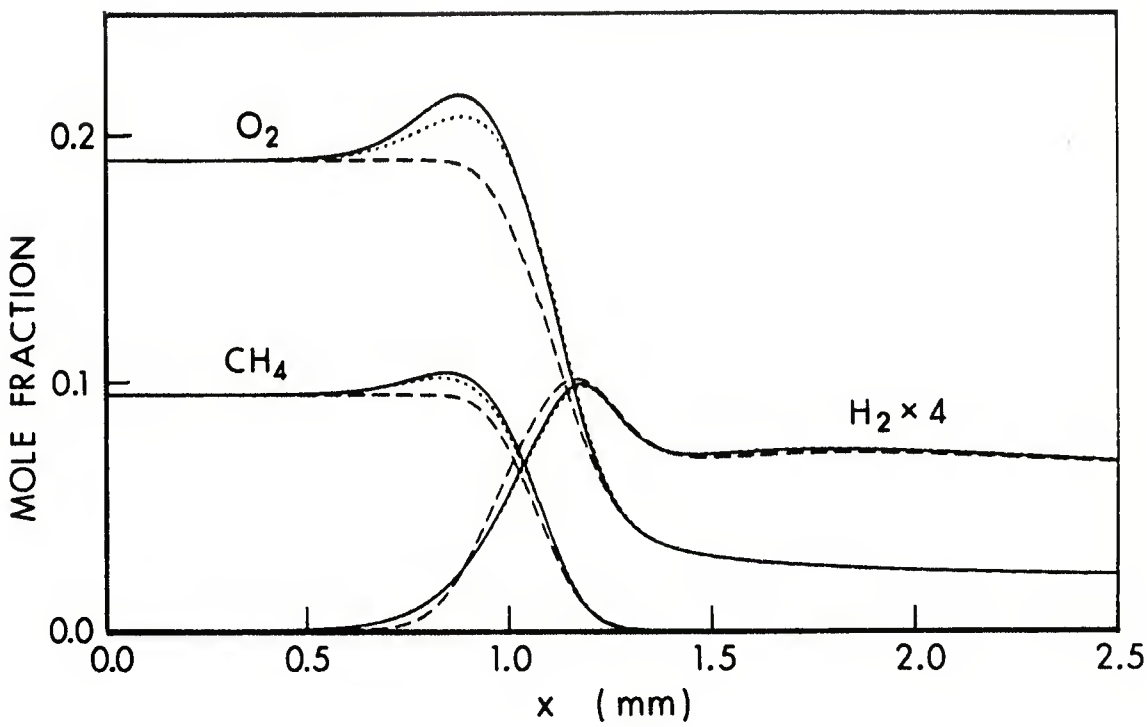

Figure 2. H_2, O_2, and CH_4 Species Profiles for a Stoichiometric Flame With Helium Buffer for Transport Method I (line), Method VI (dot), and Method V (dash)

REFERENCES

1. J.M. Heimerl and T.P. Coffee, "The Detailed Modeling of Premixed, Laminar Steady-State Flames. I. Ozone," Combustion and Flame, Vol. 39, pp. 301-315, 1980.

2. T.P. Coffee and J.M. Heimerl, "Transport Algorithms for Premixed, Laminar Steady-State Flames," Combustion and Flame, Vol. 43, pp. 273-289, 1981.

3. J. Warnatz, "The Structure of Laminar Alkane-, Alkene-, and Acetylene Flames," Proceedings of 18th Symposium (International) on Combustion, pp. 369-384, 1981.

4. F.A. Williams, Combustion Theory, Addison-Wesley, Reading, MA, 1965.

5. S. Gordon and B.J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouquet Detonations," NASA-SP-273, 1980 program version.

6. G. Dixon-Lewis, "Aspects of the Kinetic Modeling of Methane Oxidation In Flames," Proceedings of the 1st Specialist Meeting (International) of the Combustion Institute, Universite' de Bordeaux, France, Paper No. 49, pp. 284-289, 20-24 July 1981.

7. R.C. Reid, J.M. Prausnitz, and T.K. Sherwood, The Properties of Gases and Liquids, McGraw-Hill, NY, 3rd Ed., p. 678, 1977.

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

9. C.S. Wang Chang, G.E. Uhlenbeck, and J. de Boer, Studies in Statistical Mechanics, Vol. 2, John Wiley and Sons, NY, 1964.

10. L. Monchick, R.J. Munn, and E.A. Mason, "Thermal Diffusion in Polyatomic Gases: A Generalized Stefan-Maxwell Diffusion Equation," J. Chem. Phys., Vol. 45, pp. 3051-3058, 1966.

11. L. Monchick, A.N.G. Pereira, and E.A. Mason, "Heat Conductivity in Polyatomic and Polar Gases and Gas Mixtures," J. Chem. Phys., Vol. 42, pp. 3241-3256, 1965.

12. L. Monchick, K.S. Yun, and E.A. Mason, "Formal Kinetic Theory of Transport Phenomena in Polyatomic Gas Mixtures," J. Chem. Phys., Vol. 39, pp. 654-669, 1963.

13. G. Dixon-Lewis, "Flame Structure and Flame Reaction Kinetics. II. Transport Phenomena in Multicomponent Systems," Proc. Roy. Soc., Vol. A307, pp. 111-135, 1968.

14. A.A. Westenberg, "Present Status of Information on Transport Properties Applicable to Combustion Research," Combustion and Flame, Vol. 1, pp. 346-358, 1957.

15. J.O. Hirschfelder and C.F. Curtiss, "Theory of Propagation of Flames. Part I: General Equations," Proceedings of 3rd Symposium (International) on Combustion, pp. 121-127, 1949.

16. S. Chapman and T.G. Cowling, The Mathematical Theory of Non-Uniform Gases, 3rd Ed., Cambridge University Press, 1970.

17. E.S. Oran and J.P. Boris, "Detailed Modeling of Combustion Systems," Progress in Energy and Combustion Science, Vol. 7, pp. 1-72, 1981.

18. G. Tsatsaronis, "Prediction of Propagating Laminar Flames in Methane, Oxygen, Nitrogen Mixtures," Combustion and Flame, Vol. 33, pp. 217-239, 1978.

19. G.E. Andrews and D. Bradley, "Determination of Burning Velocities: A Critical Review," Combustion and Flame, Vol. 18, pp. 133-153, 1972.

20. G. Dixon-Lewis and S.M. Islam, "Flame Modeling and Burning Velocity Measurement," Proceedings of 19th Symposium (International) on Combustion, to be published.

21. J.M. Heimerl, "A Contribution to the Flat Flame Olympics: Problem B," ARBRL-TR-02416, August, 1982. See also: Notes on Numerical Fluid Mechanics, Vol. 6, "Numerical Methods in Laminar Flame Propagation," N. Peters and J. Warnatz, eds., Friedr. Viewag and Son, Braunschweig/Wiesbaden, pp. 71-86, 1982 (AD A119401).

22. T.P. Coffee and J.M. Heimerl, "Sensitivity Analysis For Premixed Laminar, Steady State Flames," ARBRL-TR-02457, January 1983 (AD A123866).

23. W.H. Clingman, R.S. Brokaw, and R.N. Pease, "Burning Velocities of Methane with Nitrogen-Oxygen, Argon-Oxygen and Helium-Oxygen Mixtures," Proceedings of 4th Symposium (International) on Combustion, pp. 310-313, 1953.

24. G.H. Morgan and W.R. Kane, "Some Effects of Inert Diluents on Flame Speeds and Temperatures," Proceedings of 4th Symposium (International) on Combustion, pp. 313-320, 1953.

A-1. G. Dixon-Lewis, M.M. Sutton, and A. Williams, "Some Reactions of Hydrogen Atoms and Simple Radicals at High Temperature," 10th Symposium (International) on Combustion, pp. 495-502, 1965.

APPENDIX A

THE MASS FRACTION TO MOLE FRACTION TRANSFORMATION

APPENDIX A

Because of the conservation of mass, the equation describing a species profile is cast in terms of the mass fraction for that species, Y_i. The solutions of the multispecies equations (and an energy equation) yield values for the Y_i as functions of space. To cast the results into the more familiar mole fractions a transformation $Y_i \rightarrow X_i$ is used. Herein we show how a non-reacting species that has a constant mass fraction profile, e.g., a diluent, can have a mole fraction profile that is quite different in shape.

Given that $Y_i(A) = Y_i(B) = \ldots$, where A,B,... are spatial locations, we ask what is the relationship between say, $X_i(A)$ and $X_i(B)$. In general

$$X_i(A) = (Y_i(A)/M_i)/(\Sigma\ Y_j(A)/M_j). \tag{A-1}$$

Then

$$\begin{aligned} X_i(B) &= (Y_i(B)/M_i)/(\Sigma\ Y_j(B)/M_j) \\ &= (Y_i(A)/M_i)/(\Sigma\ Y_j(B)/M_j) \quad . \end{aligned} \tag{A-2}$$

We require an expression for the denominator of (A-2) in terms of location A. Since

$$\Sigma\ \ Y_j(B)/M_j = \Sigma_{j\neq i}\ \ Y_j(B)/M_j + Y_i(B)/M_i \tag{A-3}$$

and

$$\Sigma\ \ Y_j(A)/M_j = \Sigma_{j\neq i}\ Y_j(A)/M_j + Y_i(A)/M_i\ , \tag{A-4}$$

we can equate $Y_i(B)$ and $Y_i(A)$ given by Equations (A-3) and (A-4) to find that

$$\Sigma\ \ Y_j(B)/M_j = \Sigma_{j\neq i}\ (Y_j(B)-Y_j\ (A))/M_j + \ \Sigma\ Y_j(A)/M_j. \tag{A-5}$$

Substituting (A-5) into (A-2) and using (A-1) we find that

$$X_i(A)/X_i(B) = 1 + \alpha\ , \tag{A-6}$$

where $\alpha = \Sigma_{j\neq i}\ ((Y_j(B)-Y_j(A))/M_j/(\Sigma Y_j(A)/M_j))$. (A-7)

Note that if $|\ \alpha\ | \ll 1$ then $X_i(A) \simeq X_i\ (B)$; if $\alpha \lesseqgtr 0$ then $X_i(A) \lesseqgtr X_i(B)$.

These last inequalities allow the possibility that a flat Y_i profile could be transformed into an X_i profile that is quite different in shape.

Examples of this transformation phenomenon have been found for N_2 and O_2 profiles in an $H_2/O_2/N_2$ flame[21] and for the N_2O profile of an H_2/N_2O flame.[A-1]

[A-1] *G. Dixon-Lewis, M.M. Sutton, and A. Williams, "Some Reactions of Hydrogen Atoms and Simple Radicals at High Temperature," 10th Symposium (International) on Combustion, pp. 495-502, 1965.*

GLOSSARY

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_{pi} = specific heat, cal-gm^{-1}-K^{-1}.

c_p = $\sum_{i=1}^{N} c_{pi} Y_i$, specific heat of mixture, cal-gm^{-1}-K^{-1}.

$\mathcal{D}_{ij}$ = binary diffusion coefficient, cm^2-s^{-1}.

D_{im} = diffusion coefficient of species i into a mixture, cm^2-s^{-1}.

D_{ij} = multicomponent diffusion coefficient, cm^2-s^{-1}.

D_i^T = multicomponent thermal diffusion coefficient, gm-s^{-1}-cm^{-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 cm^3-atm-mole^{-1}-K^{-1}.

t = time, s.

T = temperature, K.

T_u = temperature of unburned mixture, K.

T_B = temperature of burned mixture, K.

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

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

V_i = diffusion velocity due to species gradients, cm-s^{-1}.

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 faction of species i in the burned mixture.

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

σ_i = Lennard-Jones or Stockmayer parameter, Å.

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

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

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

ρ = fluid density, gm-cm^{-3}.

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

DISTRIBUTION LIST

No. Of Copies	Organization
12	Administrator Defense Technical Info Center ATTN: DTIC-DDA Cameron Station Alexandria, VA 22314
1	Commander USA DARCOM ATTN: DRCDMD-ST 5001 Eisenhower Avenue Alexandria, VA 22333
1	Commander USA ARRADCOM ATTN: DRDAR-TDC D. Gyorog Dover, NJ 07801
2	Commander USA ARRADCOM ATTN: DRDAR-TSS Dover, NJ 07801
1	Commander USA ARRCOM ATTN: DRSAR-LEP-L Rock Island, IL 61299
1	Director USA ARRADCOM Benet Weapons Laboratory ATTN: DRDAR-LCB-TL Watervliet, NY 12189
1	Commander USA Aviation Research and Development Command ATTN: DRDAV-E 4300 Goodfellow Blvd. St. Louis, MO 63120
1	Director USA Air Mobility Research and Development Laboratory Ames Research Center Moffett Field, CA 94035
4	Commander US Army Research Office ATTN: R. Girardelli D. Mann R. Singleton D. Squire Research Triangle Park, NC 27709
1	Commander USA Communications Research and Development Command ATTN: DRSEL-ATDD Fort Monmouth, NJ 07703
1	Commander USA Electronics Research and Development Command Technical Support Activity ATTN: DELSD-L Fort Monmouth, NJ 07703
2	Commander USA ARRADCOM ATTN: DRDAR-LCA-G, D.S. Downs J.A. Lannon Dover, NJ 07801
1	Commander USA ARRADCOM ATTN: DRDAR-LC, L. Harris Dover, NJ 07801
1	Commander USA ARRADCOM ATTN: DRDAR-SCA-T, L. Stiefel Dover, NJ 07801
1	Commander USA Missile Command ATTN: DRSMI-R Redstone Arsenal, AL 35898
1	Commander USA Missile Command ATTN: DRSMI-YDL Redstone Arsenal, AL 35898

DISTRIBUTION LIST

No. Of Copies	Organization
1	Commander USA Missile Command ATTN: DRSMI-RK, D.J. Ifshin Redstone Arsenal, AL 35898
1	Commander USA Tank Automotive Command ATTN: DRSTA-TSL Warren, MI 48090
1	Director USA TRADOC Systems Analysis Activity ATTN: ATAA-SL WSMR, NM 88002
2	Commandant US Army Infantry School ATTN: ATSH-CD-CSO-OR Fort Benning, GA 31905
1	Office of Naval Research ATTN: R.S. Miller, Code 432 800 N. Quincy Street Arlington, VA 22217
1	Navy Strategic Systems Project Office ATTN: R.D. Kinert, SP 2731 Washington, DC 20376
1	Commander Naval Air Systems Command ATTN: J. Ramnarace, AIR-54111C Washington, DC 20360
3	Commander Naval Ordnance Station ATTN: C. Irish S. Mitchell P.L. Stang, Code 515 Indian Head, MD 20640

No. Of Copies	Organization
1	Commander Naval Surface Weapons Center ATTN: J.L. East, Jr., G-20 Dahlgren, VA 22448
1	Commander Naval Surface Weapons Center ATTN: G.B. Wilmot, R-16 Silver Spring, MD 20910
4	Commander Naval Weapons Center ATTN: R.L. Derr, Code 388 China Lake, CA 93555
1	Commander Naval Weapons Center ATTN: T. Boggs China Lake, CA 93555
1	Commander Naval Research Laboratory Washington DC 20375
1	Commanding Officer Naval Underwater Systems Center Weapons Dept. ATTN: R.S. Lazar/Code 36301 Newport, RI 02840
1	Superintendent Naval Postgraduate School Dept. of Aeronautics ATTN: D.W. Netzer Monterey, CA 93940
6	AFRPL (DRSC) ATTN: R. Geisler D. George B. Goshgarian J. Levine W. Roe D. Weaver Edwards AFB, CA 93523

DISTRIBUTION LIST

No. Of Copies	Organization
1	AFATL/DLDL ATTN: O.K. Heiney Eglin AFB, FL 32542
1	AFOSR ATTN: L.H. Caveny Bolling Air Force Base Washington, DC 20332
1	NASA Langley Research Center ATTN: G.B. Northam/MS 168 Hampton, VA 23365
4	National Bureau of Standards ATTN: J. Hastie M. Jacox T. Kashiwagi H. Semerjian Washington, DC 20234
1	Aerojet Solid Propulsion Co. ATTN: P. Micheli Sacramento, CA 95813
1	Applied Combustion Technology, Inc. ATTN: A.M. Varney 2910 N. Orange Avenue Orlando, FL 32804
2	Atlantic Research Corp. ATTN: M.K. King 5390 Cherokee Avenue Alexandria, VA 22314
1	Atlantic Research Corp. ATTN: R.H.W. Waesche 7511 Wellington Road Gainesville, VA 22065
1	AVCO Everett Rsch. Lab. Div. ATTN: D. Stickler 2385 Revere Beach Parkway Everett, MA 02149

No. Of Copies	Organization
1	Battelle-Memorial Institute Tactical Technology Center ATTN: J. Huggins 505 King Avenue Columbus, OH 43201
2	Exxon Research & Engineering Co. ATTN: A. Dean M. Chou P.O. Box 45 Linden, NJ 07036
1	Ford Aerospace and Communications Corp. DIVAD Division Div. Hq., Irvine ATTN: D. Williams Main Street & Ford Road Newport Beach, CA 92663
1	General Electric Armament & Electrical Systems ATTN: M.J. Bulman Lakeside Avenue Burlington, VT 05402
1	General Electric Company ATTN: M. Lapp Schenectady, NY 12301
1	General Electric Ordnance Systems ATTN: J. Mandzy 100 Plastics Avenue Pittsfield, MA 01203
1	General Motors Rsch Labs Physics Department ATTN: J.H. Bechtel Warren, MI 48090
3	Hercules, Inc. Alleghany Ballistics Lab. ATTN: R.R. Miller P.O. Box 210 Cumberland, MD 21501

DISTRIBUTION LIST

No. Of Copies	Organization
3	Hercules, Inc. Bacchus Works ATTN: K.P. McCarty P.O. Box 98 Magna, UT 84044
1	Hercules, Inc. AFATL/DLDL ATTN: R.L. Simmons Eglin AFB, FL 32542
1	Honeywell, Inc. Defense Systems Division ATTN: D.E. Broden/ MS MN50-2000 600 2nd Street NE Hopkins, MN 55343
1	IBM Corporation ATTN: A.C. Tam Research Division 5600 Cottle Road San Jose, CA 95193
1	Lawrence Livermore National Laboratory ATTN: C. Westbrook Livermore, CA 94550
1	Lockheed Palo Alto Rsch Lab ATTN: George Lo 3251 Hanover Street Dept. 52-35/B204/2 Palo Alto, CA 94304
1	Los Alamos National Lab ATTN: B. Nichols T7, MS-B284 P.O. Box 1663 Los Alamos, NM 87545

No. Of Copies	Organization
1	Olin Corporation Smokeless Powder Operations ATTN: R.L. Cook P.O. Box 222 St. Marks, FL 32355
1	Paul Gough Associates, Inc. ATTN: P.S. Gough 1048 South Street Portsmouth, NH 03801
2	Princeton Combustion Research Laboratories ATTN: M. Summerfield N.A. Messina 1041 US Highway One North Princeton, NJ 08540
1	Hughes Aircraft Company ATTN: T. E. Ward 8433 Fallbrook Avenue Canoga Park, CA 91303
1	Rockwell International Corp. Rocketdyne Division ATTN: J.E. Flanagan/HB02 6633 Canoga Avenue Canoga Park, CA 91304
2	Sandia National Laboratories Combustion Sciences Dept. ATTN: R. Cattolica D. Stephenson Livermore, CA 94550
1	Science Applications, Inc. ATTN: R.B. Edelman 23146 Cumorah Crest Woodland Hills, CA 91364
1	Science Applications, Inc. ATTN: H.S. Pergament 1100 State Road, Bldg. N Princeton, NJ 08540

DISTRIBUTION LIST

No. Of Copies	Organization
1	Space Sciences, Inc. ATTN: M. Farber Monrovia, CA 91016
4	SRI International ATTN: S. Barker D. Crosley D. Golden Tech Lib 333 Ravenswood Avenue Menlo Park, CA 94025
1	Stevens Institute of Tech. Davidson Laboratory ATTN: R. McAlevy, III Hoboken, NJ 07030
1	Teledyne McCormack-Selph ATTN: C. Leveritt 3601 Union Road Hollister, CA 95023
1	Thiokol Corporation Elkton Division ATTN: W.N. Brundige P.O. Box 241 Elkton, MD 21921
3	Thiokol Corporation Huntsville Division ATTN: D.A. Flanagan Huntsville, AL 35807
3	Thiokol Corporation Wasatch Division ATTN: J.A. Peterson P.O. Box 524 Brigham City, UT 84302
1	United Technologies ATTN: A.C. Eckbreth East Hartford, CT 06108
2	United Technologies Corp. Chemical Systems Division ATTN: R.O. McLaren; R. S. Brown P.O. Box 358 Sunnyvale, CA 94086
1	Universal Propulsion Company ATTN: H.J. McSpadden Black Canyon Stage 1 Box 1140 Phoenix, AZ 85029
1	Veritay Technology, Inc. ATTN: E.B. Fisher P.O. Box 22 Bowmansville, NY 14026
1	Brigham Young University Dept. of Chemical Engineering ATTN: M.W. Beckstead Provo, UT 84601
1	Director Jet Propulsion Laboratory ATTN: MS 125/159 4800 Oak Grove Drive Pasadena, CA 91103
1	California Institute of Technology ATTN: F.E.C. Culick/ MC 301-46 204 Karman Lab. Pasadena, CA 91125
1	University of California, Berkeley Mechanical Engineering Dept. ATTN: J. Daily Berkeley, CA 94720
1	University of California Los Alamos National Lab. ATTN: T.D. Butler, P.O. Box 1663, Mail Stop B216 Los Alamos, NM 87545
2	University of California, Santa Barbara Quantum Institute ATTN: K. Schofield M. Steinberg Santa Barbara, CA 93106

DISTRIBUTION LIST

No. Of Copies	Organization
1	University of Southern California Dept. of Chemistry ATTN: S. Benson Los Angeles, CA 90007
1	Case Western Reserve Univ. Div. of Aerospace Sciences ATTN: J. Tien Cleveland, OH 44135
1	Cornell University Department of Chemistry ATTN: E. Grant Baker Laboratory Ithaca, NY 14853
1	Univ. of Dayton Rsch Inst. ATTN: D. Campbell AFRPL/PAP Stop 24 Edwards AFB, CA 93523
1	University of Florida Dept. of Chemistry ATTN: J. Winefordner Gainesville, FL 32611
3	Georgia Institute of Technology School of Aerospace Engineering ATTN: E. Price Atlanta, GA 30332
2	Georgia Institute of Technology School of Aerospace Engineering ATTN: W.C. Strahle B.T. Zinn Atlanta, GA 30332
1	University of Illinois Dept. of Mech. Eng. ATTN: H. Krier MEB, 1206 W. Green St. Urbana, IL 61801
1	Johns Hopkins University/APL Chemical Propulsion Information Agency ATTN: T.W. Christian Johns Hopkins Road Laurel, MD 20707
1	University of Minnesota Dept. of Mechanical Engineering ATTN: E. Fletcher Minneapolis, MN 55455
4	Pennsylvania State University Applied Research Laboratory ATTN: G.M. Faeth K.K. Kuo H. Palmer M. Micci University Park, PA 16802
1	Polytechnic Institute of NY ATTN: S. Lederman Route 110 Farmingdale, NY 11735
2	Princeton University Forrestal Campus Library ATTN: K. Brezinsky I. Glassman P.O. Box 710 Princeton, NJ 08540
1	Princeton University MAE Dept. ATTN: F.A. Williams P.O. Box 710 Princeton, NJ 08544

DISTRIBUTION LIST

No. Of Copies	Organization
2	Purdue University School of Aeronautics and Astronautics ATTN: R. Glick J.R. Osborn Grissom Hall West Lafayette, IN 47907
3	Purdue University School of Mechanical Engineering ATTN: N.M. Laurendeau S.N.B. Murthy D. Sweeney TSPC Chaffee Hall West Lafayette, IN 47906
1	Rensselaer Polytechnic Inst. Dept. of Chemical Engineering ATTN: A. Fontijn Troy, NY 12181
2	Southwest Research Institute ATTN: Robert E. White A.B. Wenzel 8500 Culebra Rd. San Antonio, TX 78228

No. Of Copies	Organization
1	Stanford University Dept. of Mechanical Engineering ATTN: R. Hanson Stanford, CA 94305
2	University of Texas Dept. of Chemistry ATTN: W. Gardiner H. Schaefer Austin, TX 78712
1	University of Utah Dept. of Chemical Engineering ATTN: G. Flandro Salt Lake City, UT 84112
1	Virginia Polytechnical Institute and State University ATTN: J.A. Schetz Blacksburg, VA 24061

Aberdeen Proving Ground

Dir, USAMSAA
ATTN: DRXSY-D
DRXSY-MP, H. Cohen
Cdr, USATECOM
ATTN: DRSTE-TO-F
Dir, USACSL, Bldg. E3516, EA
ATTN: DRDAR-CLB-PA
DRDAR-CLN
DRDAR-CLJ-L

USER EVALUATION OF REPORT

Please take a few minutes to answer the questions below; tear out this sheet, fold as indicated, staple or tape closed, and place in the mail. Your comments will provide us with information for improving future reports.

1. BRL Report Number _____

2. Does this report satisfy a need? (Comment on purpose, related project, or other area of interest for which report will be used.)

_____

_____

_____

3. How, specifically, is the report being used? (Information source, design data or procedure, management procedure, source of ideas, etc.) _____

_____

_____

4. Has the information in this report led to any quantitative savings as far as man-hours/contract dollars saved, operating costs avoided, efficiencies achieved, etc.? If so, please elaborate.

_____

_____

5. General Comments (Indicate what you think should be changed to make this report and future reports of this type more responsive to your needs, more usable, improve readability, etc.) _____

_____

_____

_____

6. If you would like to be contacted by the personnel who prepared this report to raise specific questions or discuss the topic, please fill in the following information.

Name: _____

Telephone Number: _____

Organization Address: _____

_____

_____