

Define  $\Delta x_a(t_N) \triangleq \Phi_{N,0} \Delta x_a(0)|_N$ . Then Eq. (17a) gives

$$\Delta x_a(t_N) = \Phi_{N,N-1} \Phi_{N-1,0} \Delta x_a(0)|_{N-1} + \Phi_{N,0} P_{N-1} \Phi_{N,0}^T \times$$

$$\left( \frac{\partial g_a}{\partial x_a} \right)^T \left[ \left( \frac{\partial g_a}{\partial x_a} \right) \Phi_{N,0} P_{N-1} \Phi_{N,0}^T \left( \frac{\partial g_a}{\partial x_a} \right)^T + W^{-1} \right]^{-1} \times$$

$$\left[ \Delta y_N - \left( \frac{\partial g_a}{\partial x_a} \right) \Phi_{N,0} \Delta x_a(0)|_{N-1} \right] = \overline{\Delta x_a}(t_N) +$$

$$M_N \left( \frac{\partial g_a}{\partial x_a} \right)^T \left[ \left( \frac{\partial g_a}{\partial x_a} \right) M_N \left( \frac{\partial g_a}{\partial x_a} \right)^T + W^{-1} \right]^{-1} \times$$

$$\left[ \Delta y_N - \left( \frac{\partial g_a}{\partial x_a} \right) \overline{\Delta x_a}(t_N) \right] \quad (18a)$$

where

$$\overline{\Delta x_a}(t_N) \triangleq \Phi_{N,N-1} \Delta x_a(t_{N-1})$$

$$M_N \triangleq \Phi_{N,0} P_{N-1} \Phi_{N,0}^T = \Phi_{N,N-1} \tilde{P}_{N-1} \Phi_{N,N-1}^T \quad (18b)$$

$$\tilde{P}_{N-1} = \Phi_{N-1,0} P_{N-1} \Phi_{N-1,0}^T$$

Using Eq. (17b) and the last equation of (18b), the following relationship is established:

$$\tilde{P}_N = M_N - M_N \left( \frac{\partial g_a}{\partial x_a} \right)^T \times$$

$$\left[ \left( \frac{\partial g_a}{\partial x_a} \right) M_N \left( \frac{\partial g_a}{\partial x_a} \right)^T + W^{-1} \right]^{-1} \left( \frac{\partial g_a}{\partial x_a} \right) M_N \quad (19)$$

Equations (18) and (19) are precisely a version of extended Kalman filtering<sup>7</sup> if the Jacobians  $\partial g_a/\partial x_a$ ,  $\partial f_a/\partial x_a$  and the computed output  $g(x,t)$  are evaluated using the previous nominal trajectory rather than using the trajectory updated at each data point (the usually extended Kalman filtering<sup>7</sup>), and if  $W^{-1} = R$ , the covariance matrix of  $v$ . Note that  $\tilde{P}_N$  corresponds to the covariance matrix of the error of the estimate.

### Conclusions

It has been established that, in the absence of process noise, the method of quasi-linearization is in fact equivalent to a version of extended Kalman filtering. The relationship between the sensitivity matrices of the augmented and un-augmented states with respect to the parameters helps clarify the two approaches. The recurrence relationship for the method of quasilinearization developed in this Note is of considerable value when the number of unknown parameters is much larger than the dimension of the output vector.

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## Approximate Transport Calculations for High-Temperature Air

LYNN H. BLAKE\*

Lockheed Palo Alto Research Laboratory,  
Palo Alto, Calif.

### Nomenclature

- $C$  = mass fraction (subscript  $i$  refers to species;  $e$ , to element)  
 $C_p$  = specific heat at constant pressure  
 $D_e$  = equivalent binary diffusion coefficient  
 $h$  = enthalpy  
 $j$  = species mass flux  
 $M$  = molecular weight  
 $p$  = pressure  
 $R$  = universal gas constant  
 $T$  = temperature  
 $x$  = mole fraction  
 $\eta$  = viscosity coefficient  
 $\lambda$  = thermal conductivity  
 $\nu$  = number of components in gas mixture

### Introduction

THE continued interest in atmospheric heating of re-entry vehicles has motivated a more complete investigation of the thermodynamic and transport properties of high-temperature air. A full description of a partially ionized and dissociated air system is very complex because of the large number of species present ( $N_2$ ,  $O_2$ ,  $NO$ ,  $O$ ,  $N$ ,  $O^+$ ,  $e^-$ , etc.). Two problems have plagued attempts to analytically predict the transport properties of such a system: 1) the complexity of the Chapman-Enskog equations<sup>1</sup> describing the transport in a general multicomponent system and 2) the lack of collision cross-section data for the species involved. These complexities have led to the development of two approximate

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\* Research Scientist.

descriptions of the thermal and viscous transport in gaseous mixtures: 1) series truncation of the Chapman-Enskog equations and 2) empirical correlation of the limited experimental data.

Following the work of Brokaw,<sup>2</sup> the infinite series form of the Chapman-Enskog transport equations have been approximated by the first terms of the series.<sup>3,4</sup> Hansen<sup>5</sup> used a form of this approximation to calculate the transport coefficients of air to 15,000°K. By using the more complete collision cross-sections data of Yun, et al.,<sup>6,7</sup> Yos<sup>8,9</sup> has determined the viscous and thermal transport coefficients of air to 30,000°K. The finite series equations gave results within a few percent of the Chapman-Enskog equations used by Peng and Pindroh.<sup>10</sup>

For the low-temperature gas mixtures, empirical transport equations have been suggested<sup>3,11,12</sup> from correlations of the limited experimental data with approximate forms of the transport equations. The simplicity of these empirical equations has motivated a more complete investigation of their utility to applications of high-temperature systems. Yun<sup>6,7</sup> showed the results of the empirical equations for viscosity and thermal conductivity to be within 10% of his more rigorous analysis for binary systems of N<sub>2</sub> - N, O<sub>2</sub> - O, and H<sub>2</sub> - H. In this Note, the simplified empirical equations for the viscous and thermal transport in gaseous mixtures were applied to high-temperature air and their results compared with the results of Yos<sup>9</sup> and Hansen.<sup>5</sup>

### Formulation

In the finite series, approximation of the Chapman-Enskog transport equations suggested by Brokaw<sup>2</sup> and used by Yos,<sup>9</sup> the description of the interaction of a particle *i* with all other particles *j* is retained. In contrast, the simplified empirical transport equations are obtained from the Chapman-Enskog equations by assuming the collision integral ratio  $A_{ij}^1$  to be a unique constant independent of temperature and the force law between molecules *i* and *j*. For this approximation, the complex transport series equations for gas mixtures reduce to simple forms which have been shown to correlate well with experimental data at near ambient temperatures. The resulting forms of the empirical transport equations are presented below.

From the comparison of extensive experimental data, Buddenberg and Wilke<sup>11</sup> showed the viscosity of gas mixtures could be represented by the following equation ( $\pm 5\%$ ):

$$\eta_m = \sum_{i=1}^v x_i \eta_i \left/ \left( x_i + \frac{2RT}{pM_i} \sum_{j=1, j \neq i}^v \frac{x_j}{D_{ij}} \right) \right. \quad (1)$$

Wilke<sup>12</sup> further simplified Eq. (1) by assuming a rigid sphere form of the binary diffusion coefficient  $D_{ij}$ <sup>13</sup> to obtain a viscosity equation for mixtures that is a function only of the molecular weights, individual species, viscosity coefficients, and the mole fractions, as follows:

$$\eta_m = \sum_{i=1}^v x_i \eta_i \left/ \sum_{j=1}^v x_j \Phi_{ij} \right. \quad (2)$$

$$\Phi_{ij} = \frac{1}{2(2)^{1/2}} \left( 1 + \frac{M_i}{M_j} \right)^{-1/2} \left[ 1 + \left( \frac{\eta_i}{\eta_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4} \right]^2$$

Wilke<sup>12</sup> showed that Eq. (2) correlated well with experimental data of binary as well as general gas mixtures at ambient temperatures. In this Note, the utility of Eq. (2) in describing the viscosity of high-temperature air is investigated.

If thermal and pressure diffusion are neglected and no external force fields are assumed, the energy transfer in a gas mixture is by molecular collision and chemical enthalpy. For a one-dimensional temperature field, the energy flux can be written

$$q_y = -\lambda_{fm} \frac{\partial T}{\partial y} + \sum_{i=1}^v h_i j_i \quad (3)$$

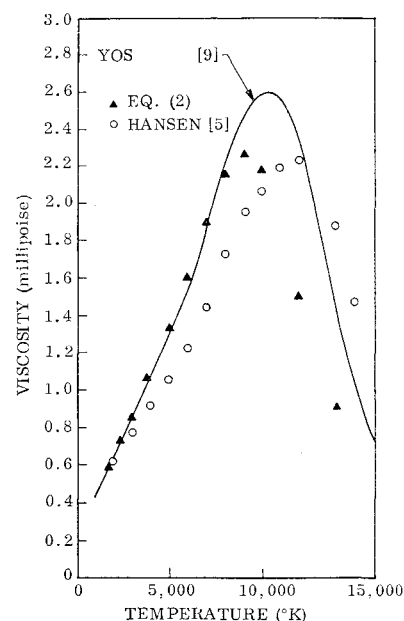


Fig. 1 Viscosity of air vs temperature—1 atm.

Using the Lees<sup>14</sup> binary diffusion approximation for a multi-component gas, the energy flux of Eq. (3) can be written as

$$q_y = -\lambda_T \frac{\partial T}{\partial y} - D_{ep} \sum_{e=1}^v \sum_{i=1}^v h_i \frac{\partial C_i}{\partial C_e} \frac{\partial C_e}{\partial y} \quad (4)$$

$$\lambda_T = \lambda_{fm} + \sum_{i=1}^v D_e h_i \frac{\partial C_i}{\partial T}$$

The factor  $\lambda_T$  is considered the total thermal conductivity coefficient and can be identified as the sum of the effects of molecular collision and enthalpy transport.

Mason and Saxena<sup>3</sup> have shown the energy transport due to molecular collisions ( $\lambda_{fm}$  (frozen flow)) can be written in a form similar to the simplified mixture viscosity equation (2), as follows:

$$\lambda_{fm} = \sum_{i=1}^v x_i \lambda_i \left/ \sum_{j=1}^v x_j \Phi_{ij} \right. \quad (5)$$

A comparison of the total thermal conductivity results of Eq. (4) with those of Yos<sup>9</sup> for high-temperature air will be discussed.

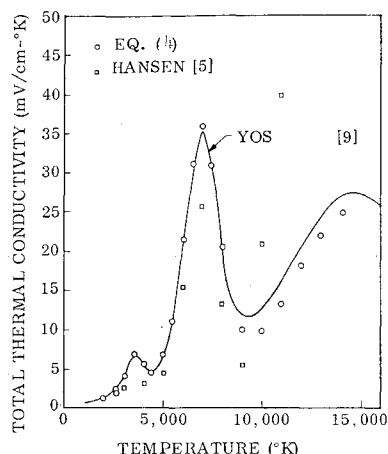
### Discussion

A comparison of the viscosity and thermal conductivity results predicted by the simplified transport Eqs. (2, 4, and 5) was made with the results of Yos<sup>9</sup> and Hansen<sup>5</sup> for high-temperature air. The corresponding Prandtl numbers for the three sets of data are also presented.

The specific heat at constant pressure of the mixture  $C_{pm}$  was determined from the summation

$$C_{pm} = \sum_{i=1}^v (\bar{C}_{p_i} + h_i) \frac{\partial C_i}{\partial T} \quad (6)$$

The specific heat results of Eq. (6) were found to correlate very closely with the results of Predvoditelev<sup>15</sup> and Yos<sup>9</sup> to high temperatures ( $\sim 13,000^\circ\text{K}$ ). The viscosity and conductivity coefficients for the individual species of Yun<sup>6,7</sup> were used. A thermo-chemical computer program (FEMP)<sup>16</sup> was utilized to provide equilibrium compositions for the gaseous mixtures as a function of temperature and pressure. The species concentration gradient with temperature, which appears in the definition of  $C_{pm}$  and  $\lambda_T$ , was obtained by differentiating the equilibrium relations at constant pressure and elemental concentration. Assuming ideal gas relations and the logarithm of the equilibrium constants to be linear

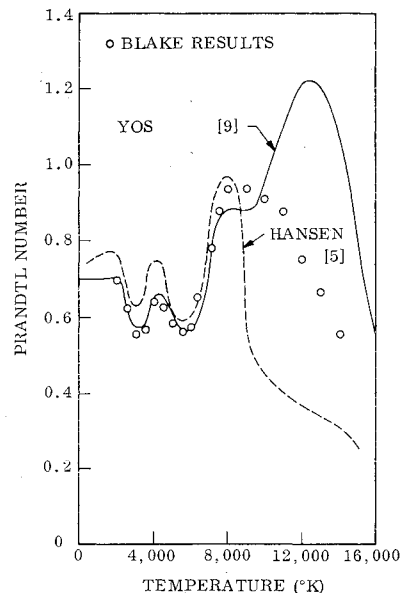


**Fig. 2 Total thermal conductivity of air vs temperature—1 atm.**

functions of temperature, the resulting matrix was solved for the species concentration gradients with temperature. The temperature range (2000–16,000°K) was divided into two regions where the O, O<sup>2</sup>, N, N<sub>2</sub> species were considered in the lower region (2000–6000°K) and O, O<sup>+</sup>, N, N<sup>+</sup>, N<sup>2</sup>, e<sup>-</sup> were considered in the high-temperature range (6000–16,000°K). Finite difference checks with the concentration output of the FEMP program at small-temperature intervals showed a good correlation with the computed concentration gradients.

The theoretical viscosity of air at elevated temperatures is presented in Fig. 1 as obtained from Hansen,<sup>5</sup> Yos,<sup>9</sup> and the approximate viscous transport Equation (2). Equation (2) is shown to correlate well with the Yos data to 9000°K. The breakdown of the simplified model at temperatures greater than 9000°K, the temperature region where significant ionization occurs, is attributed to the inappropriateness of the simple rigid sphere, binary interaction model assumed in Eq. (2). The results of the approximate formulation may be improved by a more realistic diffusion coefficient, e.g., the effective diffusion coefficient suggested by Kendall.<sup>17</sup>

The Hansen<sup>5</sup> data is included for comparison as it has been frequently used in re-entry heating calculations. The difference between the Hansen and Yos data was found to be primarily due to the difference in collision cross-section models and data. This difference was most pronounced in the temperature region where ionization occurs. In this region, the charge-exchange model used by Yos resulted in cross-sectional data one to two orders of magnitude larger than the neutral-neutral cross sections used by Hansen.



**Fig. 3 Prandtl number of air vs temperature—1 atm.**

In order to calculate the enthalpy transport fraction of the total thermal conductivity, an effective diffusion coefficient must be determined. Commensurate with the approximations in the simplified transport equations, the diffusion coefficient used for the air system was that of N<sub>2</sub>—N; thus all molecules in the mixture were assumed to behave like N<sub>2</sub>, and all atoms and ions like N.<sup>18</sup> Electron interactions were not considered in this simple approximation. Therefore, the total thermal conductivity was found for high-temperature air by using the N<sub>2</sub>—N diffusion data of Yun<sup>7</sup> in Eq. (4). A comparison of the total thermal conductivity results from the simplified analysis as shown in Fig. 2 with the results of Yos<sup>9</sup> and Hansen.<sup>5</sup> The results of Eq. (4) correlate well with the Yos data to 9000°K. The significant difference between the Hansen and Yos data at higher temperatures is again attributed to the different collision models and cross-sections data used.

A comparison of the Prandtl number results for air as a function of temperature is shown in Fig. 3 as determined from Hansen, Yos and the simplified equations here discussed. The simplified transport equations yield Prandtl number results which are good to approximately 10,000°K.

In comparison with the more complete descriptions of the viscous and energy transport in high-temperature air, this study has shown the applicability of the simplified transport equations to air systems of temperatures below which appreciable ionization occurs (10,000°K). For this temperature region, the simplified equations give results which correlate well with the more complete analysis of Yos.<sup>9</sup>

These simplified empirical equations can be easily incorporated into analyses of high-temperature air transport such as the hyperbolic re-entry problem. For such calculations the simplified equations provide an accurate property evaluation tool in lieu of the data storage and curve fits used in the past and the more extensive computational requirements of the complete interaction analyses.

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## A Consistent Formulation of Compressible Boundary-Layer Theory with Second-Order Curvature and Displacement Effects

R. T. DAVIS,\* M. J. WERLE,† AND S. F. WORNOM‡  
Virginia Polytechnic Institute, Blacksburg, Va.

### Introduction

RECENTLY, several studies have been made of the compressible boundary-layer equations as modified to directly account for longitudinal surface curvature effects (i.e., Refs. 1 and 2). It is believed that these modified equations are not consistent to second order in boundary-layer theory, and it will be shown here that application of the principles applied in higher-order boundary-layer theory (as recently reviewed by Van Dyke<sup>3</sup>) leads to a somewhat different set of governing equations. The attractive features of this new set of equations are that it, 1) contains all curvature terms (both longitudinal and transverse) normally retained in first- and second-order boundary-layer theory, 2) it straightforwardly reduces to the incompressible set given by Van Dyke<sup>3</sup> and as generalized by Davis, Whitehead, and Wornom,<sup>4</sup> and 3) it clearly shows how displacement speed effects on the viscous flow can be handled as a first-order effect.

### Boundary-Layer Equations

The basic approach taken here is similar to that first set down by Van Dyke<sup>5</sup> except that here no attempt is made to filter out the higher-order effects into separate linear problems. Van Dyke has given a statement of the full Navier Stokes equations for two-dimensional or axisymmetric flow in terms of the usual surface coordinates,  $s$  and  $n$ , with all distances referenced to a length,  $a$ , velocities to  $U_\infty$ , pressure to  $\rho_\infty U_\infty^2$ , density to  $\rho_\infty$ , temperature to  $U_\infty^2/C_p$ , enthalpy to  $U_\infty^2$ , and viscosities to the value of  $\mu$  at  $T = U_\infty^2/C_p$ . With these

definitions the characteristic Reynolds number becomes

$$Re = \rho_\infty U_\infty a / \mu (U_\infty^2 / C_p) = 1/\epsilon^2 \quad (1)$$

For present purposes we approach the full equations with the assumption that in a vanishingly small region near the surface, a region of order  $\epsilon$  thick, all flow properties except the normal velocity component  $v$  are of order one— $v$  itself being of order  $\epsilon$ . Thus, we introduce the stretched normal coordinate

$$N = (1/\epsilon)n \quad (2)$$

and use unsubscripted variables to designate the flow properties in the viscous region according to

$$u_\nu(s, n, \epsilon) = u(s, N, \epsilon) \quad (3a)$$

$$v_\nu(s, n, \epsilon) = \epsilon v(s, N, \epsilon) \quad (3b)$$

$$\rho_\nu(s, n, \epsilon) = \rho(s, N, \epsilon) \quad (3c)$$

$$p_\nu(s, n, \epsilon) = p(s, N, \epsilon) \quad (3d)$$

$$T_\nu(s, n, \epsilon) = T(s, N, \epsilon) \quad (3e)$$

$$H_\nu(s, n, \epsilon) = H(s, N, \epsilon) \quad (3f)$$

and designate the coordinate scale factors as

$$h_1 = (1 + \epsilon \kappa N) = h \quad (4a)$$

$$h_2 = 1 \quad (4b)$$

$$h_3 = (r_0 + \epsilon N \cos \theta)^i = r^i \quad (4c)$$

Introducing these to the full equations and keeping all terms up to second order gives the following:

continuity equation

$$(\partial/\partial s)(\rho r^i u) + (\partial/\partial N)(\rho h r^i v) = 0 \quad (5)$$

$s$ -momentum equation

$$\rho \left( u \frac{\partial u}{\partial s} + v \frac{\partial h u}{\partial N} \right) + \frac{\partial p}{\partial s} = \frac{1}{h r^i} \frac{\partial}{\partial N} (r^i h^2 \tau) \quad (6a)$$

where

$$\tau = \mu [\partial u / \partial N - (h_N/h)u] \quad (6b)$$

$n$ -momentum equation

$$\partial p / \partial N = \rho (h_N/h)u^2 \quad (7)$$

energy equation

$$\rho [u(\partial H / \partial s) + h v(\partial H / \partial N)] = (1/r^i)(\partial/\partial N)[h r^i(q + u\tau)] \quad (8a)$$

where

$$q = (\mu/\sigma)\partial T/\partial N \quad (8b)$$

$$H = T + u^2/2 \quad (8c)$$

and

$$\sigma = \mu C_p/k \quad (8d)$$

state equation

$$p = [(\gamma - 1)/\gamma]\rho T = [(\gamma - 1)/\gamma]\rho(H - u^2/2) \quad (9)$$

It is worthy of note that these equations can be written in several forms all of which are equal through second-order terms. Thus, equivalent forms of the right hand side of Eq. (6a) are

$$1) \text{ R.H.S. Eq. (6a) } = h \frac{\partial}{\partial N} \left( \mu \frac{\partial u}{\partial N} \right) - \epsilon \kappa u \frac{\partial \mu}{\partial N} + \epsilon \left( \kappa + \frac{j \cos \theta}{r_0} \right) \mu \frac{\partial u}{\partial N} \quad (10a)$$

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\* Professor. Department of Engineering Mechanics.

† Assistant Professor. Department of Engineering Mechanics. Associate Member AIAA.

‡ Graduate Research Assistant. Department of Engineering Mechanics.