

An Assessment of Transport Property Methodologies for Hypersonic Flows

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Abstract

Three different methods of computing mixture viscosity and thermal conductivity are presented and compared under equilibrium and nonequilibrium flow conditions. The three methods are (1) species summation, (2) Wilke's mixing rule, and (3) collision integrals. Under chemical equilibrium conditions at temperatures below 6000 K, the simple species summation method computed essentially identical values of mixture viscosity and thermal conductivity as the other two methods. When the species summation method was incorporated into a Navier-Stokes analysis of a forebody along a descent trajectory, essentially identical stagnation line and surface temperature profiles were produced as when the other two methods were used at a CPU time reduction of up to 63.8%.

Introduction

The determination of the transport properties of high-temperature gases has been a topic of study for decades. Early researchers determined the transport properties of single or binary gas mixtures from kinetic theory.¹⁻⁴ Subsequent work focused on curve fits or approximations to obtain the mixture viscosity and thermal conductivity of multi-component gas mixtures.^{5-9,11} Gupta^{10,12} presented a rigorous method of computing mixture viscosity and thermal conductivity where these quantities are obtained from the collision integrals of the individual species pairs.

The accurate determination of mixture viscosity and thermal conductivity is a critical component in the computation of hypersonic viscous flows. When nonequilibrium phenomena

is included in the physical model, the determination of viscosity and thermal conductivity can become CPU intensive. This paper presents a new method for computing mixture viscosity and thermal conductivity, called species summation, that maintains the accuracy of more rigorous methods at a significant reduction in computational expense. The species summation method is compared against two popular methods for calculating viscosity and thermal conductivity under both equilibrium and non-equilibrium conditions.

Nomenclature

$$\begin{aligned} \overset{\circ}{A} &= 1.0 \times 10^{-8} \text{ cm} \\ k &= \text{Boltzmann constant, } 1.38054 \times 10^{-23} \frac{\text{J}}{\text{K}} \\ m_i &= \text{mass of species i, } \frac{\text{gm}}{\text{particle}} \\ M_i &= \text{mass of species i, } \frac{\text{gm}}{\text{mole}} \\ N_A &= \text{Avogadros number, } 6.0225 \times 10^{23} \frac{\text{particles}}{\text{mole}} \\ R &= \text{Universal Gas Constant, } 8.3144 \frac{\text{J}}{\text{mole} \cdot \text{K}} \\ T &= \text{temperature, K} \\ x_i &= \text{species mole fraction} \\ \kappa &= \text{thermal conductivity, } \frac{\text{J}}{\text{m} \cdot \text{s} \cdot \text{K}} \\ \mu &= \text{viscosity, } \frac{\text{N} \cdot \text{s}}{\text{m}^2} \\ \pi \bar{\Omega}_{ii}^{(2,2)} &= \text{average collision cross section, } \overset{\circ}{A}^2 \end{aligned}$$

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Governing Equations

Species viscosity

Derived from kinetic theory, the expression to determine the viscosity of gas species i can be assumed to be a function of temperature only and is given by²

$$\mu_i = \frac{5}{16} \frac{\sqrt{\pi m_i k T}}{\pi \bar{\Omega}_{ii}^{(2,2)}} = 8.3861 \times 10^{-6} \frac{\sqrt{M_i T}}{\pi \bar{\Omega}_{ii}^{(2,2)}} \frac{N-s}{m^2}$$

Gupta¹⁰ evaluated the collision integrals, $\pi \bar{\Omega}_{ii}^{(2,2)}$, by curve fit relations. The curve fits presented in Ref. 10 have been modified for greater computational efficiency by replacing the exponential leading term in the Gupta curve fits with the quantity, d_i , and take the following form:

$$\pi \bar{\Omega}_{ii}^{(2,2)} = d_i T^{[a_i (\ln T)^2 + b_i \ln T + c_i]} \quad \text{A}^2$$

Values for the coefficients in the above expression for 11 species air, $[N, O, NO, N_2, O_2, NO^+, N_2^+, O_2^+, O^+, N^+]$, can be found in appendix A.

Mixture Viscosity - Species Summation

The first method used to obtain mixture viscosity is called the species summation method. The mixture viscosity is computed by summing the product of the species mole fractions and species viscosities.

$$\mu = \sum_{i=1}^{nspc} x_i \mu_i \quad \frac{N-s}{m^2}$$

This method assumes no interaction between the various species.

Mixture Viscosity - Wilke's Mixing Rule

The second method considered in this study uses kinetic theory with some simplifying assumptions to compute mixture viscosity. The method is called Wilke's mixing rule^{5,11} and expresses the mixture viscosity as

$$\mu = \sum_{i=1}^{nspc} \frac{x_i \mu_i}{\phi_i} \quad \frac{N-s}{m^2}$$

The quantity ϕ_i is defined as

$$\phi_i = \sum_{j=1}^{nspc} \frac{x_j \left[1 + \sqrt{\frac{\mu_i}{\mu_j} \left(\frac{M_j}{M_i} \right)^{\frac{1}{4}}} \right]^2}{\sqrt{8 \left(1 + \frac{M_i}{M_j} \right)}} = \sum_{j=1}^{nspc} \frac{x_j \left[1 + \sqrt{\frac{\pi \bar{\Omega}_{jj}^{(2,2)}}{\pi \bar{\Omega}_{ii}^{(2,2)}}} \right]^2}{\sqrt{8 \left(1 + \frac{M_i}{M_j} \right)}}$$

If the equivalent species viscosity is defined as

$$\bar{\mu}_i = \frac{\mu_i}{\phi_i} \quad \frac{N-s}{m^2}$$

then the equation for total viscosity can be written as

$$\mu = \sum_{i=1}^{nspc} x_i \bar{\mu}_i \quad \frac{N-s}{m^2}$$

which is similar in form to the species summation method.

Mixture Viscosity - Collision Integrals

The third and most rigorous method for obtaining mixture velocity uses an approximation to the Chapman-Enskog formula.¹⁰

$$\mu = \sum_{i=1}^{nspc} \left[\frac{\frac{M_i}{N_A} x_i}{\sum_{j=1}^{nspc} x_j \Delta_{ij}^{(2)}} \right] \frac{N-s}{m^2}$$

where $\Delta_{ij}^{(2)}$ is defined as

$$\Delta_{ij}^{(2)} = \frac{16}{5} \left[\frac{2 M_i M_j}{\pi N_A k T (M_i + M_j)} \right]^{\frac{1}{2}} \pi \bar{\Omega}_{ij}^{(2,2)} \quad \text{cm-s}$$

The equation for total viscosity can be re-written as

$$\mu = \sum_{i=1}^{nspc} \left[\frac{x_i}{\sum_{j=1}^{nspc} x_j \frac{N_A}{M_i} \Delta_{ij}^{(2)}} \right] = \sum_{i=1}^{nspc} \left[\frac{x_i}{\sum_{j=1}^{nspc} x_j \bar{\Delta}_{ij}^{(2)}} \right] \frac{N-s}{m^2}$$

where $\bar{\Delta}_{ij}^{(2)}$ is defined in mks units as

$$\bar{\Delta}_{ij}^{(2)} = \frac{1}{8.3861 \times 10^{-6}} \left[\frac{2M_j}{TM_i(M_i + M_j)} \right]^{\frac{1}{2}} \pi \bar{\Omega}_{ij}^{(2,2)} \quad \frac{m^2}{N-s}$$

It is interesting to note that if $i = j$, then the quantity $\bar{\Delta}_{ii}^{(2)}$ is equivalent to the inverse of the species viscosity. Defining the quantity μ_{ij} as

$$\mu_{ij} = \frac{1}{\bar{\Delta}_{ij}^{(2)}} = 8.3861 \times 10^{-6} \left[\frac{TM_i(M_i + M_j)}{2M_j} \right]^{\frac{1}{2}} \frac{1}{\pi \bar{\Omega}_{ij}^{(2,2)}} \quad \frac{N-s}{m^2}$$

The equation for total viscosity can be written as

$$\mu = \sum_{i=1}^{nspc} \left[\frac{x_i}{\sum_{j=1}^{nspc} \frac{x_j}{\mu_{ij}}} \right] \quad \frac{N-s}{m^2}$$

Curve fits for μ_{ij} for 11 species air are listed in Appendix B. Finally, if the equivalent species viscosity is defined as

$$\bar{\mu}_i = \frac{1}{\sum_{j=1}^{nspc} \frac{x_j}{\mu_{ij}}} \quad \frac{N-s}{m^2}$$

then the equation for total viscosity can be written as

$$\mu = \sum_{i=1}^{nspc} x_i \bar{\mu}_i \quad \frac{N-s}{m^2}$$

which again is similar in form to the species summation method. This final method for computing mixture viscosity will be referred to as the collision integral method.

Thermal Conductivity

Thermal conductivity is made up of translational and internal components. The internal thermal conductivity is comprised of vibrational, rotational, and electronic components.

$$\kappa = \kappa_{tr} + \kappa_{int} = \kappa_{tr} + (\kappa_{rot} + \kappa_{vib} + \kappa_{el})$$

Species thermal conductivity

The translational thermal conductivity of species i is a function of temperature only and is given by the expression²

$$\kappa_{tr,i} = \frac{75}{64} k \frac{\sqrt{\frac{\pi k T}{m_i}}}{\pi \bar{\Omega}_{ii}^{(2,2)}} = \frac{75}{64} \frac{k}{m_i} \frac{\sqrt{\pi m_i k T}}{\pi \bar{\Omega}_{ii}^{(2,2)}} = \frac{15}{4} \frac{R}{M_i} \mu_i \quad \frac{J}{m-s-K}$$

The species internal thermal conductivity is obtained from the expression¹⁰

$$\kappa_{int,i} = \frac{3}{8} \left[\frac{C_{pi}}{R} - \frac{5}{2} \right] k \frac{\sqrt{\frac{\pi k T}{m_i}}}{\pi \bar{\Omega}_{ii}^{(1,1)}} = \frac{C_{pi}}{R} \frac{R}{M_i} \mu_i \frac{6}{5} \frac{\pi \bar{\Omega}_{ii}^{(2,2)}}{\pi \bar{\Omega}_{ii}^{(1,1)}}$$

The quantity, $\frac{C_{pi}}{R}$, is the internal specific heat normalized by the universal gas constant and contains contributions from the rotational, vibrational, and electronic energy modes. It is equal to the total species specific heat, $\frac{C_{pi}}{R}$, minus the normalized translational component. If the species Schmidt number is defined as¹⁰

$$Sc_{ii} = \frac{\mu_i}{\rho D_{ii}} = \frac{\frac{5}{16} \frac{\sqrt{\pi m_i k T}}{\pi \bar{\Omega}_{ii}^{(2,2)}}}{\rho \frac{3 \sqrt{\pi m_i k T}}{8} \frac{1}{\pi \bar{\Omega}_{ii}^{(1,1)}} \frac{1}{\rho}} = \frac{5}{6} \frac{\pi \bar{\Omega}_{ii}^{(1,1)}}{\pi \bar{\Omega}_{ii}^{(2,2)}}$$

where D_{ii} is the coefficient of self-diffusion, then the expression for species internal thermal conductivity becomes

$$\kappa_{int,i} = \frac{C_{pi}}{R} \frac{R}{M_i} \mu_i \frac{1}{Sc_{ii}} \quad \frac{J}{m-s-K}$$

The total species thermal conductivity is the sum of the translational and internal components and is given by

$$\kappa_i = \frac{R}{M_i} \mu_i \left[\frac{15}{4} + \frac{1}{Sc_{ii}} \frac{C_{pi}}{R} \right] \quad \frac{J}{m-s-K}$$

Mixture Thermal Conductivity - Species Summation

The methods investigated in this study to compute mixture thermal conductivity parallel those used to compute mixture viscosity. The first method to obtain mixture thermal conductivity, called species summation, consists of summing the product of the species mole fractions and species thermal conductivities.

$$\kappa = \sum_{i=1}^{nspc} x_i \kappa_i \quad \frac{J}{m-s-K}$$

This method assumes no interaction between the species.

Mixture Thermal Conductivity - Wilke's Mixing Rule

The second method to compute mixture thermal conductivity is Wilke's mixing rule.^{5,11}

$$\kappa = \sum_{i=1}^{nspc} \frac{x_i \kappa_i}{\phi_i} \quad \frac{J}{m-s-K}$$

Using the previously defined quantity ϕ_i , the equivalent species thermal conductivity is defined as

$$\bar{\kappa}_i = \frac{\kappa_i}{\phi_i} \quad \frac{J}{m-s-K}$$

and the equation for total thermal conductivity can be written as

$$\kappa = \sum_{i=1}^{nspc} x_i \bar{\kappa}_i \quad \frac{J}{m-s-K}$$

Mixture Thermal Conductivity - Collision Integrals

Similar to the calculation of mixture viscosity, the collision integral method provides a more rigorous method for the computation of mixture translational thermal conductivity by using an approximation to the Chapman-Enskog formula.¹⁰

$$\kappa_{tr} = \frac{15}{4} k \sum_{i=1}^{nspc} \left[\frac{x_i}{\sum_{j=1}^{nspc} \alpha_{ij} x_j \Delta_{ij}^{(2)}} \right] \quad \frac{J}{m-s-K}$$

where $\Delta_{ij}^{(2)}$ is defined as before. The quantity α_{ij} is defined as

$$\alpha_{ij} = 1 + \left[1 - \frac{M_i}{M_j} \right] \left[0.45 - 2.54 \frac{M_i}{M_j} \right] \left[1 + \frac{M_i}{M_j} \right]^2$$

Using the relations derived for the calculation of mixture viscosity, the equation for mixture translational thermal conductivity can be re-written as

$$\kappa_{tr} = \sum_{i=1}^{nspc} \left[\frac{\frac{15}{4} k \frac{N_A}{M_i} x_i}{\frac{N_A}{M_i} \sum_{j=1}^{nspc} \alpha_{ij} x_j \Delta_{ij}^{(2)}} \right] = \sum_{i=1}^{nspc} \left[\frac{\frac{15}{4} R x_i}{\sum_{j=1}^{nspc} \frac{\alpha_{ij} x_j}{\mu_{ij}}} \right] \quad \frac{J}{m-s-K}$$

Finally, if the equivalent species translational thermal conductivity is defined as

$$\bar{\kappa}_{tr,i} = \frac{\frac{15}{4} R}{\sum_{j=1}^{nspc} \frac{\alpha_{ij} x_j}{\mu_{ij}}} \quad \frac{J}{m-s-K}$$

then the equation for total translational thermal conductivity can be written as

$$\kappa_{tr} = \sum_{i=1}^{nspc} x_i \bar{\kappa}_{tr,i} \quad \frac{J}{m-s-K}$$

The equation for mixture internal thermal conductivity is¹⁰

$$\kappa_{int} = k \sum_{i=1}^{nspc} \left[\frac{\left[\frac{C_{pi}}{R} - \frac{5}{2} \right] x_i}{\sum_{j=1}^{nspc} x_j \Delta_{ij}^{(1)}} \right] = k \sum_{i=1}^{nspc} \left[\frac{\frac{C_{pint,i}}{R} x_i}{\sum_{j=1}^{nspc} x_j \Delta_{ij}^{(1)}} \right] \quad \frac{J}{m-s-K}$$

where $\Delta_{ij}^{(1)}$ is defined as

$$\Delta_{ij}^{(1)} = \frac{8}{3} \left[\frac{2 M_i M_j}{\pi N_A k T (M_i + M_j)} \right]^{\frac{1}{2}} \pi \bar{\Omega}_{ij}^{(1,1)} = \Delta_{ij}^{(2)} \frac{5}{6} \frac{\pi \bar{\Omega}_{ij}^{(1,1)}}{\pi \bar{\Omega}_{ij}^{(2,2)}}$$

The binary Schmidt number, Sc_{ij} , is defined as

$$Sc_{ij} = \frac{5}{6} \frac{\pi \bar{\Omega}_{ij}^{(1,1)}}{\pi \bar{\Omega}_{ij}^{(2,2)}}$$

Curve fits for the binary Schmidt number are listed in appendix C. The equation for mixture internal thermal conductivity can be re-written as

$$\kappa_{int} = \sum_{i=1}^{nspc} \left[\frac{\frac{R}{M_i} \frac{C_{pint,i}}{R} x_i}{\sum_{j=1}^{nspc} x_j \Delta_{ij}^{(2)} Sc_{ij}} \right] = \sum_{i=1}^{nspc} \left[\frac{x_i \frac{R}{M_i} \frac{C_{pint,i}}{R}}{\sum_{j=1}^{nspc} x_j \frac{Sc_{ij}}{\mu_{ij}}} \right] \quad \frac{J}{m-s-K}$$

If the equivalent species internal thermal conductivity is defined as

$$\bar{\kappa}_{\text{int},i} = \frac{R}{M_i} \frac{C_{\text{pint},i}}{\sum_{j=1}^{nspc} x_j \frac{Sc_{ij}}{\mu_{ij}}} \quad \frac{J}{m-s-K}$$

the mixture internal thermal conductivity is

$$\kappa_{\text{int}} = \sum_{i=1}^{nspc} x_i \bar{\kappa}_{\text{int},i} \quad \frac{J}{m-s-K}$$

The expression for total mixture thermal conductivity is therefore

$$\kappa = \kappa_{tr} + \kappa_{\text{int}} = \sum_{i=1}^{nspc} x_i (\bar{\kappa}_{tr,i} + \bar{\kappa}_{\text{int},i}) \quad \frac{J}{m-s-K}$$

Results

Viscosity - Equilibrium Gas

The first series of results presented are to investigate the differences in viscosity produced by the species summation, Wilke's mixing rule, and collision integral methods under equilibrium gas conditions. The species viscosities are a function of temperature only. The equivalent species and mixture viscosities are a function of temperature and species mole fraction. Equilibrium species mole fractions for an eleven species air ($N, O, NO, N_2, O_2, N_2^+, O_2^+, NO^+, N^+, O^+, e$)

chemistry model obtained from a Gibbs free energy minimization are a function of temperature and pressure. In the first series of results, the species mole fractions were computed at two values of pressure at temperatures ranging from 200 to 15000 K.

The mole fractions of the neutral and ionized species at a constant pressure of 1.0 atm are shown in Figs. 1a and 1b. Below 2500 K the gas is essentially diatomic oxygen and nitrogen. The formation of NO begins at 2000 K. The concentration of NO peaks at around 3500 K and then decreases. Oxygen dissociation begins at 2500 K. Significant nitrogen dissociation is not apparent until the temperature reaches 5000 K. Substantial ionization is evident at temperatures above 8000 K.

Figures 2a, 2b, and 2c compare the species viscosity to the equivalent species viscosity from the Wilke's mixing rule and collision integral methods for the neutral diatomic species,

N_2, O_2 , and NO . The three methods compute essentially the same value of viscosity at temperatures below 3500 K. The two equivalent viscosities then begin to diverge from the species viscosity. The equivalent species viscosity from the Wilke's mixing rule and collision integral methods are very close in value until the temperature reaches 8000 K when the equivalent species viscosity from the Wilke's mixing rule decreases. This is because at temperatures above 8000 K the ϕ_i parameter for the neutral diatomic species increases sharply.

The next two plots show species viscosity and the equivalent species viscosity from the Wilke's mixing rule and collision integral methods for the neutral atomic species, N and O . Below 8000 K, the equivalent species viscosity from the Wilke's mixing rule and collision integral methods are very close in value and are less than the species viscosity. This is because the equivalent species viscosities include contributions from the diatomic species which have lower species viscosities in this temperature range. As the temperature increases, the diatomic species dissociate which reduces the impact on the equivalent species viscosity. As was seen before, above 8000 K the equivalent species viscosity from the Wilke's mixing rule decreases. Above 8000 K the equivalent species viscosity from collision integrals for N does follow the species viscosity curve.

Figure 2f shows species viscosity and the equivalent species viscosity from the Wilke's mixing rule and collision integral methods for NO^+ . The equivalent species viscosity from collision integrals is orders of magnitude higher than the species viscosity at temperatures below 8000 K. This is because the equivalent species viscosity from collision integrals includes contributions for the neutral species which have higher species viscosities. The other ionized species viscosity and equivalent species viscosity curves show similar features.

The equivalent species viscosities are functions of species mole fractions which are functions of both temperature and pressure. Figure 3 compares species mole fraction, species viscosity, and equivalent species viscosity from collision integrals for selected species at two levels of pressure, 1.0 and 0.1 atm. At the lower pressure, dissociation and ionization occur at a lower temperature. There is only a slight difference in the equivalent species viscosity curves and virtually no difference below 4000 K.

Figure 4 shows the mixture viscosity computed by the three methods as a function of temperature at constant pressures of 1.0 and 0.1 atm. Also shown on the 1.0 atm plots are data from Gupta¹² and data using Sutherland's law, which is valid only for a perfect gas. The expression for Sutherland's law is

$$\mu = 1.458 \times 10^{-6} \left(\frac{\frac{3}{T^2}}{T+110.4} \right) \quad \frac{N-s}{m^2}$$

For both the 1.0 atm and 0.1 atm plots, viscosity increases with temperature until about 10000 K. This is because species viscosities are an increasing function of temperature and because atomic species have a higher species viscosity than diatomic species and as the temperature increases dissociation occurs. Viscosity drops at temperatures above 10000 K because above this temperature ionized species mole fractions become significant and ionized species have a lower species viscosity than neutral species.

Figure 4a compares total viscosity computed by the different methods as a function of temperature at a constant pressure of 1.0 atm. Below 8000 K, all methods except Sutherland predict essentially the same viscosity. Above 8000 K, the viscosity predicted by Wilke's mixing rule decreases while that predicted by the other methods continues to rise. This is due to the sharp increase in the ϕ_i parameters that begins at around 8000 K. The viscosity computed by Ref. 12, using the collision integral method, begins to decrease at a lower temperature than the present results. This is probably due to a different level of ionized species mole fractions computed by Ref. 12 in this temperature range.

Figure 4b shows the computed mixture viscosity in the low temperature range, below 3000 K. The methods predict essentially identical values of total viscosity. This means that in the low temperature range, which would be expected near a wall where viscous effects are most important, simply summing up the species viscosities to obtain the mixture viscosity gives the same result as the more rigorous and computationally expensive collision integral method. It should be remembered that this result is based on equilibrium species mole fractions.

This fact that the mixture viscosities are the same below 3000 K is not surprising based on the curves shown in Fig. 2. Below 3000 K the gas is mostly N_2 and O_2 with a small amount of NO and O . The equivalent species viscosities for N_2 , O_2 , and NO are essentially the same as the corresponding species viscosities at temperatures less than 3000 K and there is not enough atomic oxygen to cause a significant difference in mixture viscosity.

The mixture viscosity from species summation remains more or less equal to the mixture viscosity from collision integrals in the temperature range of 3000 to 8000 K. Looking at the species and equivalent species viscosity curves in Fig. 2, in this temperature range the neutral diatomic equivalent species viscosity is greater than the neutral diatomic species viscosity. However, the neutral atomic equivalent species viscosity is less than the neutral atomic species viscosity, and the two discrepancies partially cancel out.

Figures 4c and 4d show the results at a constant pressure of 0.1 atm. The behavior is similar to that seen at a constant pressure of 1.0 atm. The uniformity of the mixture viscosity curves is consistent over an order of magnitude change in pressure.

Thermal Conductivity - Equilibrium Gas

Similar to what was done with viscosity, Figure 5 compares the species and equivalent species conductivity as a function of temperature at a constant pressure of 1.0 atm. Figures 5a through 5c show the results for the neutral diatomic species. Below 4000 K, the three curves are essentially identical. Above 4000 K, the equivalent species thermal conductivities are higher than the species thermal conductivity. Above 8000 K, the conductivity predicted by Wilke's mixing rule decreases due to the sharp increase in the ϕ_i parameters that occurs at high temperatures.

The results for the neutral atomic species are shown in Figs. 5d and 5e. Similar to viscosity, the equivalent species conductivities are less than the species conductivity at temperatures below 8000 K due to the influence of the diatomic species. Figure 5f compares the conductivities of nitric oxide ion. As was seen with ionic species viscosity, the equivalent species conductivities are larger than the species conductivity again due to the influence of the other species. The other ionic species conductivity curves are similar in nature.

The effect of pressure on the equivalent species conductivity computed by the collision integral method for diatomic nitrogen and atomic oxygen are shown in Fig. 6. A one order of magnitude change in pressure had very little effect on the equivalent species conductivity especially at temperatures below 6000 K.

Figures 7a and 7b show mixture thermal conductivity computed from species summation, collision integrals, and Wilke's mixing rule as a function of temperature at a constant pressure of 1.0 atm. Also shown on the 1.0 atm figures is data from Gupta.¹² The three curves are nearly identical at temperatures below 6000 K. Above 6000 K, the mixture thermal conductivities from species summation and Wilke's mixing rule continue to match but underpredict the value computed by the collision integral method.

The mixture thermal conductivities computed by the three methods at a constant pressure of 0.1 atm are shown in Figs. 7c and 7d. Similar to the 1.0 atm pressure results, the three curves are nearly identical at temperatures below 6000 K. The mixture thermal conductivities from species summation and Wilke's mixing rule underpredict the value calculated using the collision integral method at temperatures between 6000 and 12500 K.

Effect on Surface Temperature and Heating - Re-entry Forebody Flow

The three methods for determining mixture viscosity and thermal conductivity were incorporated into a 2-D/axisymmetric real-gas flow solver.¹³ Flow solutions were computed over a 2.5 meter radius sphere at several points along a representative

descent trajectory to determine mixture viscosity and thermal conductivity effects on the computed flow properties.

Altitude, (km)	Density (kg/m ³)	Velocity (kg/sec)	Mach No.
75	3.9916e-5	7082.9	24.5
70	7.8825e-5	6361.0	21.5
60	3.0694e-4	5115.3	16.2
50	1.0256e-3	3400.8	10.3

Table One. Freestream conditions

Solutions were computed for the four freestream conditions shown in Table One. These were taken from the descent trajectory of a generic winged body Single-Stage-to-Orbit vehicle that was studied under the Access to Space Reusable Launch Vehicle technology program.¹⁴ Looking at the values in Table One, the solutions cover a two order of magnitude range in freestream density and Mach numbers ranging from 24.5 at 75 km altitude to 10.3 at 50 km altitude.

The flow solver uses a point implicit solution algorithm where only the chemistry terms are evaluated implicitly. The chemistry models used were 5 and 11 species air. A radiative equilibrium, non-catalytic wall boundary condition was used to determine surface temperature. The solutions were run over a 49x49 grid with a normalized spacing at the wall of 1.0e-4. Second-order Van Leer flux vector splitting with the minmod limiter was used to evaluate the inviscid fluxes. Each of the three solutions was run using the same number of steps at the same time steps for a one-to-one comparison.

The first set of computations used the five species air chemistry model. Figure 8 shows stagnation line and surface radiative equilibrium temperature profiles at the four trajectory points. There is a small oscillation in the surface radiative equilibrium temperatures near the stagnation point and small differences near the bow shock wave, but the simple species summation method for determining mixture viscosity and thermal conductivity yields essentially the same stagnation line and surface temperature profiles as the more complex and more computationally expensive methods over the entire trajectory range.

The computations at the 60 km altitude trajectory point were re-run using the 11 species air chemistry model. Computed stagnation line and surface radiative equilibrium temperatures are shown in Fig. 9. Similar to the five species results, the species summation method results are essentially the same as those from the more complex and computationally expensive Wilke's mixing rule and collision integral methods.

Table two summarizes the Cray C90 computer time required per point per step to evaluate the viscosity and thermal conductivity using each of the three methods. Comparisons of CPU time are computer and algorithm dependent, but under the conditions examined here for the five species model, Wilke's mixing rule required 40.7 % more CPU time to evaluate the viscosity and thermal conductivity than the species summation method. The

collision integral method required 419 % more CPU time to evaluate the viscosity and thermal conductivity than species summation. The computation of viscosity and thermal conductivity using the collision integral method consumed 31% of the total CPU time for each iteration. If the collision integral method is used, 29.3 % more CPU time is required to generate a 5 species air flow solution than if the species summation method is used.

The inclusion of additional species exacerbates the CPU discrepancies between the three methods. Wilke's mixing rule requires almost twice as much CPU time to compute the viscosity and thermal conductivity for 11 species air as the species summation method. The collision integral method requires 8.5 times as much CPU time for 11 species air as compared to the species summation method. When using the collision integral method, 48% of the total CPU time used for each iteration is spent evaluating the viscosity and thermal conductivity. If the collision integral method is used, 63.8 % more CPU time is required to generate an 11 species air flow solution than if the species summation method is used.

	5 species air	11 species air
Species Summation	4.296e-6	8.446e-6
Wilke's Mixing Rule	6.044e-6	1.516e-5
Collision Integrals	1.800e-5	7.184e-5

Table two. Cray C90 computer requirements, sec.

Concluding Remarks

From the results presented in this paper, it would appear that a very simple species summation procedure can be used to compute mixture viscosity and thermal conductivity that maintains accuracy at a significantly reduced computational cost. Under chemical equilibrium conditions, the species summation method yields essentially the same value of mixture viscosity and thermal conductivity as the Wilke's mixing rule and collision integral methods at temperatures below 6000 K. When incorporated into a Navier-Stokes analysis of a forebody at several points along a representative re-entry trajectory, the species summation method yielded essentially identical stagnation line and surface temperature profiles as the more complicated methods with a savings in CPU time per flow solution of up to 63.8%.

References

¹ Curtiss, C. and Hirschfelder, J., "Transport Properties of Multicomponent Gas Mixtures," *J. Chem. Phys.*, Vol. 17, No. 6, 1949, pp. 550-555.

² Hirschfelder, J.O., Curtiss, C.F., and Bird, R.B., "Molecular Theory of Gases and Liquids", John Wiley and Sons, New York, N.Y., 1954.

³ Hirschfelder, J., "Heat Conductivity is Polyatomic or Electronically Excited Gases II," *J. Chem Phys.*, Vol. 26, No. 2, 1957, pp. 282-285.

⁴ Svehla, R., "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA TR-132, 1962.

⁵ Wilke, C.R., "A Viscosity Equation for Gas Mixtures", *J. Chem. Phys.*, Vol. 18, No. 4, 1950, pp. 517-519.

⁶ Mason, E. and Saxena, S., "Approximate Formula for the Thermal Conductivity of Gas Mixtures," *Physics of Fluids*, Vol. 1, No. 5, 1958, pp. 361-369.

⁷ Hanson, C., "Approximations for the Thermodynamic and Transport Properties of High-Temperature Air," NASA TR-50, 1960.

⁸ Viegas, J. and Howe, J., "Thermodynamic and Transport Property Correlation Formulas for Equilibrium Air from 1,000 K to 15,000 K," NASA TN D-1429, 1962.

⁹ Blottner, F., "Chemically Reacting Viscous Flow Program for Multi-Component Gas Mixtures," Sandia Labs Report SC-RR-70-754, 1971.

¹⁰ Gupta, R.N., Yos, J.M., and Thompson, R.A., "A Review of Reaction Rates and Thermodynamic and Transport Properties for the 11 Species Air Model for Chemical and Thermal Nonequilibrium Calculations to 30000 K", NASA TM-101528, 1989.

¹¹ Candler, G., "The Computation of Weakly Ionized Hypersonic Flows in Thermo-Chemical Nonequilibrium, Stanford Phd thesis, 1988, p. 21.

¹²Gupta, R.N., Yos, J.M., Thompson, R.A., and Lee, K., "A Review of Reaction Rates and Thermodynamic Properties for an 11-Species Air Model for Chemical and Thermal Non-equilibrium Calculations to 30000 K", NASA RP-1232, 1990.

¹³Palmer, G. and Venkatapathy, E., "Comparison of Nonequilibrium Solution Algorithms Applied to Chemically Stiff Hypersonic Flows," *AIAA Journal*, Vol. 33, No. 7, pp. 1211-1219.

¹⁴Henline, W.D., Palmer, G.E., Milos, F.S., Olynick, D.R., and Chen, Y.-K., "Aerothermodynamic Heating Analysis and Heatshield Design of an SSTO Rocket Vehicle for Access-to-Space," AIAA Paper 95-2079, June, 1995.

Appendix A

The collision integral used to obtain species viscosity can be obtained by

$$\pi \bar{\Omega}_{ii}^{(2,2)} = d_i T \left[a_i (\ln T)^2 + b_i \ln T + c_i \right]$$

For 11 species air, the coefficients are:

N:	a = 0.0	b = -0.0118	c = -0.096	d = 75.581
O:	a = 0.0	b = -0.0207	c = 0.078	d = 35.368
NO:	a = 0.0	b = -0.0453	c = 0.5624	d = 5.8527
N ₂	a = 0.0	b = -0.0203	c = 0.0683	d = 59.74
O ₂	a = 0.0	b = -0.0485	c = 0.6475	d = 3.5279
ions	a = 0.0	b = 0.0	c = -2.0	d = 3.795e+10
e ⁻	a = 0.0	b = 0.0	c = -2.0	d = 3.795e+10

Appendix B

Curve fits to μ_{ij}

Incorporating the term, $8.3861 \times 10^{-6} \left[\frac{TM_i(M_i + M_j)}{2M_j} \right]^{\frac{1}{2}}$,

into the curve fits for $\pi \bar{\Omega}_{ij}^{(2,2)}$ from NASA RP-1232, it is possible to curve-fit the quantity μ_{ij} as

$$\mu_{ij} = d_{ij} T \left[a_{ij} (\ln T)^2 + b_{ij} \ln T + c_{ij} \right] \frac{N-s}{m^2}$$

The a coefficients for 11 species air are zero with the exception of the following species pairs:

$$\begin{aligned} a(O, e) &= a(e, O) = -0.0164 \\ a(N_2, e) &= a(e, N_2) = -0.1147 \\ a(O_2, e) &= a(e, O_2) = -0.0241 \end{aligned}$$

The b coefficients for the ion-neutral and ion-ion species pairs are zero. The b coefficients for the electron-ion and electron-neutral species pairs are zero with the following exceptions:

$$\begin{aligned} b(O, e) &= b(e, O) = 0.243 \\ b(N_2, e) &= b(e, N_2) = 2.8945 \\ b(O_2, e) &= b(e, O_2) = 0.3467 \end{aligned}$$

The b coefficients for the neutral-neutral species pairs are as follows:

$$\begin{aligned} b(N, N) &= 0.0118 \\ b(N, O) = b(O, N) &= -0.0065 \\ b(N, NO) = b(NO, N) &= 0.0196 \\ b(N, N_2) = b(N_2, N) &= 0.0190 \\ b(N, O_2) = b(O_2, N) &= 0.0203 \end{aligned}$$

$$\begin{aligned} b(O, O) &= 0.0207 \\ b(O, NO) = b(NO, O) &= 0.0203 \\ b(O, N_2) = b(N_2, O) &= 0.0169 \\ b(O, O_2) = b(O_2, O) &= 0.0247 \end{aligned}$$

$$\begin{aligned} b(NO, NO) &= 0.0453 \\ b(NO, N_2) = b(N_2, NO) &= 0.0385 \\ b(NO, O_2) = b(O_2, NO) &= 0.0522 \end{aligned}$$

$$\begin{aligned} b(N_2, N_2) &= 0.0203 \\ b(N_2, O_2) = b(O_2, N_2) &= 0.0558 \end{aligned}$$

$$b(O_2, O_2) = 0.0485$$

The c coefficients for ion-neutral species pairs are 0.9 with the following exceptions:

$$\begin{aligned} c(N, N^+) = c(N^+, N) &= 0.9146 \\ c(O, O^+) = c(O^+, O) &= 0.9235 \end{aligned}$$

The c coefficients for ion-ion and ion-electron species pairs are 2.5. The c coefficients for the neutral-neutral species pairs are as follows:

$$\begin{aligned} c(N, N) &= 0.5960 \\ c(N, O) = c(O, N) &= 0.9467 \\ c(N, NO) = c(NO, N) &= 0.4522 \\ c(N, N_2) = c(N_2, N) &= 0.4761 \\ c(N, O_2) = c(O_2, N) &= 0.4270 \end{aligned}$$

$$\begin{aligned} c(O, O) &= 0.4220 \\ c(O, NO) = c(NO, O) &= 0.4270 \\ c(O, N_2) = c(N_2, O) &= 0.5143 \\ c(O, O_2) = c(O_2, O) &= 0.3217 \end{aligned}$$

$$\begin{aligned} c(NO, NO) &= -0.0624 \\ c(NO, N_2) = c(N_2, NO) &= 0.0774 \\ c(NO, O_2) = c(O_2, NO) &= -0.2045 \end{aligned}$$

$$\begin{aligned} c(N_2, N_2) &= 0.4317 \\ c(N_2, O_2) = c(O_2, N_2) &= -0.2590 \\ c(O_2, O_2) &= -0.1475 \end{aligned}$$

The c coefficients for the electron-neutral species pairs are as follows:

$$\begin{aligned} c(e, N) = c(N, e) &= 0.5 \\ c(e, O) = c(O, e) &= -0.6231 \\ c(e, NO) = c(NO, e) &= 0.5 \\ c(e, N_2) = c(N_2, e) &= -24.008 \\ c(e, O_2) = c(O_2, e) &= -0.889 \end{aligned}$$

The d coefficients for 11 species air are:

$$\begin{array}{ll} d(N, N) = 0.4153e-06 & d(N, O) = 0.7219e-07 \\ d(N, NO) = 0.4737e-06 & d(N, N_2) = 0.4166e-06 \\ d(N, O_2) = 0.5485e-06 & d(N, NO^+) = 0.3066e-07 \\ d(N, N_2^+) = 0.3101e-07 & d(N, O_2^+) = 0.3036e-07 \\ d(N, O^+) = 0.3467e-07 & d(N, N^+) = 0.3139e-07 \\ d(N, e) = 0.7093e-03 & \\ d(O, N) = 0.8246e-07 & d(O, O) = 0.9484e-06 \\ d(O, NO) = 0.6054e-06 & d(O, N_2) = 0.3580e-06 \\ d(O, O_2) = 0.1125e-05 & d(O, NO^+) = 0.3351e-07 \\ d(O, N_2^+) = 0.3392e-07 & d(O, O_2^+) = 0.3314e-07 \\ d(O, O^+) = 0.3817e-07 & d(O, N^+) = 0.3961e-07 \\ d(O, e) = 0.192e-01 & \\ d(NO, N) = 0.1015e-05 & d(NO, O) = 0.1135e-05 \\ d(NO, NO) = 0.7849e-05 & d(NO, N_2) = 0.4031e-05 \\ d(NO, O_2) = 0.1545e-04 & d(NO, NO^+) = 0.5241e-07 \\ d(NO, N_2^+) = 0.5333e-07 & d(NO, O_2^+) = 0.5158e-07 \\ d(NO, O^+) = 0.6284e-07 & d(NO, N^+) = 0.6569e-07 \\ d(NO, e) = 0.1519e-01 & \\ d(N_2, N) = 0.8332e-06 & d(N_2, O) = 0.6268e-06 \\ d(N_2, NO) = 0.3764e-05 & d(N_2, N_2) = 0.7430e-06 \\ d(N_2, O_2) = 0.1755e-04 & d(N_2, NO) = 0.4979e-07 \\ d(N_2, N_2^+) = 0.5064e-07 & d(N_2, O_2^+) = 0.4903e-07 \\ d(N_2, O^+) = 0.5939e-07 & d(N_2, N^+) = 0.6202e-07 \\ d(N_2, e) = 0.129e+28 & \\ d(O_2, N) = 0.1253e-05 & d(O_2, O) = 0.2249e-05 \\ d(O_2, NO) = 0.1648e-04 & d(O_2, N_2) = 0.2005e-04 \\ d(O_2, O_2) = 0.1345e-04 & d(O_2, NO^+) = 0.5501e-07 \\ d(O_2, N_2^+) = 0.5601e-07 & d(O_2, O_2^+) = 0.5412e-07 \\ d(O_2, O^+) = 0.6628e-07 & d(O_2, N^+) = 0.6935e-07 \\ d(O_2, e) = 0.819e-02 & \\ d(NO^+, N) = 0.6569e-07 & d(NO^+, O) = 0.6284e-07 \\ d(NO^+, NO) = 0.5241e-07 & d(NO^+, N_2) = 0.5333e-07 \\ d(NO^+, O_2) = 0.5158e-07 & d(NO^+, NO^+) = 0.1211e-1 \\ d(NO^+, N_2^+) = 0.1232e-14 & d(NO^+, O_2^+) = 0.1192e-14 \\ d(NO^+, O^+) = 0.1451e-14 & d(NO^+, N^+) = 0.1517e-14 \end{array}$$

$$d(NO^+, e) = 0.2002e - 12$$

$$d(N_2^+, N) = 0.6202e - 07$$

$$d(N_2^+, NO) = 0.4979e - 07$$

$$d(N_2^+, O_2) = 0.4903e - 07$$

$$d(N_2^+, N_2^+) = 0.1170e - 14$$

$$d(N_2^+, O^+) = 0.1372e - 14$$

$$d(N_2^+, e) = 0.1869e - 12$$

$$d(O_2^+, N) = 0.6935e - 07$$

$$d(O_2^+, NO) = 0.5501e - 07$$

$$d(O_2^+, O_2) = 0.5412e - 07$$

$$d(O_2^+, N_2^+) = 0.1294e - 14$$

$$d(O_2^+, O^+) = 0.1531e - 14$$

$$d(O_2^+, e) = 0.2135e - 12$$

$$d(O^+, N) = 0.3960e - 07$$

$$d(O^+, NO) = 0.3351e - 07$$

$$d(O^+, O_2) = 0.3314e - 07$$

$$d(O^+, N_2^+) = 0.7834e - 15$$

$$d(O^+, O^+) = 0.8839e - 15$$

$$d(O^+, e) = 0.1067e - 12$$

$$d(N^+, N) = 0.3138e - 07$$

$$d(N^+, NO) = 0.3066e - 07$$

$$d(N^+, O_2) = 0.3036e - 07$$

$$d(N^+, N_2^+) = 0.7162e - 15$$

$$d(N^+, O^+) = 0.8008e - 15$$

$$d(N^+, e) = 0.9344e - 13$$

$$d(e, N) = 0.2778e - 07$$

$$d(e, NO) = 0.2778e - 06$$

$$d(e, O_2) = 0.140e - 06$$

$$d(e, N_2^+) = 0.366e - 17$$

$$d(e, O^+) = 0.366e - 17$$

$$d(e, e) = 0.5176e - 17$$

when $i = j$ the curve fit expression for μ_{ij} is equivalent to that for the species viscosity, μ_i

$$d(N_2^+, O) = 0.5939e - 07$$

$$d(N_2^+, N_2) = 0.5064e - 07$$

$$d(N_2^+, NO^+) = 0.1150e - 14$$

$$d(N_2^+, O_2^+) = 0.1133e - 14$$

$$d(N_2^+, N^+) = 0.1432e - 14$$

$$d(O_2^+, O) = 0.6628e - 07$$

$$d(O_2^+, N_2) = 0.5601e - 07$$

$$d(O_2^+, NO^+) = 0.1271e - 14$$

$$d(O_2^+, O_2^+) = 0.1250e - 14$$

$$d(O_2^+, N^+) = 0.1602e - 14$$

$$d(O^+, O) = 0.3816e - 07$$

$$d(O^+, N_2) = 0.3392e - 07$$

$$d(O^+, NO^+) = 0.7739e - 15$$

$$d(O^+, O_2^+) = 0.7655e - 15$$

$$d(O^+, N^+) = 0.9148e - 15$$

$$d(N^+, O) = 0.3467e - 07$$

$$d(N^+, N_2) = 0.3101e - 07$$

$$d(N^+, NO^+) = 0.7082e - 15$$

$$d(N^+, O_2^+) = 0.7012e - 15$$

$$d(N^+, N^+) = 0.8270e - 15$$

$$d(e, O) = 0.658e - 06$$

$$d(e, N_2) = 0.252e + 23$$

$$d(e, NO^+) = 0.366e - 17$$

$$d(e, O_2^+) = 0.366e - 17$$

$$d(e, N^+) = 0.366e - 17$$

Appendix C

Curve fits to Sc_{ij}

Using the curve fits for $\pi\bar{\Omega}_{ij}^{(2,2)}$ and $\pi\bar{\Omega}_{ij}^{(1,1)}$ from NASA RP-1232 the binary Schmidt number can be curve-fit by

$$Sc_{ij} = \frac{5}{6} \frac{\pi\bar{\Omega}_{ij}^{(1,1)}}{\pi\bar{\Omega}_{ij}^{(2,2)}} = d_{ij} T^{[b_{ij} \ln T + c_{ij}]}$$

For 11 species air, the b coefficients for ion-neutral, ion-ion, electron-neutral, electron-ion, and electron-electron species pairs are zero with the following exceptions:

$$b(N, N^+) = b(N^+, N) = -0.0033$$

$$b(O, O^+) = b(O^+, O) = -0.0034$$

$$b(NO, NO^+) = b(NO^+, NO) = -0.0047$$

The b coefficients for the neutral-neutral species pairs are:

$$b(N, N) = 0.0085$$

$$b(N, O) = b(O, N) = -0.0017$$

$$b(N, NO) = b(NO, N) = 0.0011$$

$$b(N, N_2) = b(N_2, N) = -0.0004$$

$$b(N, O_2) = b(O_2, N) = 0.0024$$

$$b(O, O) = 0.0173$$

$$b(O, NO) = b(NO, O) = 0.0024$$

$$b(O, N_2) = b(N_2, O) = 0.0030$$

$$b(O, O_2) = b(O_2, O) = 0.0021$$

$$b(NO, NO) = 0.0089$$

$$b(NO, N_2) = b(N_2, NO) = 0.0095$$

$$b(NO, O_2) = b(O_2, NO) = 0.0084$$

$$b(N_2, N_2) = 0.0091$$

$$b(N_2, O_2) = b(O_2, N_2) = 0.0093$$

$$b(O_2, O_2) = 0.0075$$

The c coefficients for ion-neutral, ion-ion, electron-neutral, electron-ion, and electron-electron species pairs are zero with the following exceptions:

$$c(N, N^+) = c(N^+, N) = 0.3574$$

$$c(O, O^+) = c(O^+, O) = 0.3663$$

$$c(NO, NO^+) = c(NO^+, NO) = 0.3449$$

The c coefficients for the neutral-neutral species pairs are:

$$\begin{aligned}c(N,N) &= 0.0388 \\c(N,O) = c(O,N) &= 0.0272 \\c(N,NO) = c(NO,N) &= -0.0360 \\c(N,N_2) = c(N_2,N) &= -0.0120 \\c(N,O_2) = c(O_2,N) &= -0.0578\end{aligned}$$

$$\begin{aligned}c(O,O) &= -0.1352 \\c(O,NO) = c(NO, O) &= -0.0578 \\c(O,N_2) = c(N_2,O) &= -0.0682 \\c(O,O_2) = c(O_2,O) &= -0.0483\end{aligned}$$

$$\begin{aligned}c(NO, NO) &= -0.1799 \\c(NO, N_2) = c(N_2, NO) &= -0.1902 \\c(NO, O_2) = c(O_2, NO) &= -0.1693\end{aligned}$$

$$\begin{aligned}c(N_2,N_2) &= -0.1865 \\c(N_2,O_2) = c(O_2,N_2) &= -0.1861\end{aligned}$$

$$c(O_2,O_2) = -0.1498$$

The d coefficients for the ion-neutral species pairs are 0.9012 with the following exceptions:

$$\begin{aligned}d(N,N^+) = d(N^+,N) &= 0.1294 \\d(O,O^+) = d(O^+,O) &= 0.1393 \\d(NO, NO^+) = d(NO^+, NO) &= 0.1244\end{aligned}$$

The d coefficients for the electron-neutral species pairs are 0.8333. The d coefficients for the ion-ion and electron-ion species pairs are 0.4877. The d coefficients for the neutral-neutral species pairs are:

$$\begin{aligned}d(N,N) &= 1.7121 \\d(N,O) = d(O,N) &= 0.6392 \\d(N,NO) = d(NO, N) &= 0.8506 \\d(N,N_2) = d(N_2,N) &= 0.7749 \\d(N,O_2) = d(O_2,N) &= 0.9375\end{aligned}$$

$$\begin{aligned}d(O,O) &= 3.4624 \\d(O,NO) = d(NO, O) &= 0.9375 \\d(O,N_2) = d(N_2,O) &= 0.9769 \\d(O,O_2) = d(O_2,O) &= 0.9069\end{aligned}$$

$$\begin{aligned}d(NO, NO) &= 1.6864 \\d(NO, N_2) = d(N_2, NO) &= 1.7776 \\d(NO, O_2) = d(O_2, NO) &= 1.5985\end{aligned}$$

$$\begin{aligned}d(N_2,N_2) &= 1.7755 \\d(N_2,O_2) = d(O_2,N_2) &= 1.7169\end{aligned}$$

$$d(O_2,O_2) = 1.4728$$

For all neutral-ion pairings, $Sc_{ij} = 0.9102$ except $N - N^+$, $O - O^+$, and $NO - NO^+$ where the Schmidt number ranges from 0.7 to 3.0

For all ion-ion pairings and electron-ion pairings, $Sc_{ij} = 0.48766$

For all electron-neutral pairings, $Sc_{ij} = 0.83333$

The Schmidt number for neutral diatomic-neutral diatomic pairings is approx. 0.7 except at T<1000 where it is slightly higher. Neutral atomic-neutral atomic pairings range from 2.6 to 5.4.

Appendix D

Comparing Wilke's mixing rule and collision integrals

The total viscosity according to Wilke's mixing rule is

$$\mu = \sum_{i=1}^{nspc} \frac{x_i \mu_i}{\phi_i}$$

Using collision integrals, the equation for total viscosity is

$$\mu = \sum_{i=1}^{nspc} x_i \bar{\mu}_i = \sum_{i=1}^{nspc} \left[\frac{x_i}{\sum_{j=1}^{nspc} x_j \bar{\Delta}_{ij}^{(2)}} \right]$$

Equating the terms within the summations of the two expressions gives the expression that must be satisfied for the methods of collision integrals and Wilke's mixing rule to be equivalent.

$$\phi_i = \mu_i \sum_{j=1}^{nspc} x_j \bar{\Delta}_{ij}^{(2)}$$

Substituting the previously described definitions for ϕ_i , μ_i , and $\bar{\Delta}_{ij}^{(2)}$ into the above equation gives

$$\sum_{j=1}^{nspc} \frac{x_j \left[1 + \sqrt{\frac{\pi \bar{\Omega}_{jj}^{(2,2)}}{\pi \bar{\Omega}_{ii}^{(2,2)}}} \right]^2}{\sqrt{8 \left(1 + \frac{M_i}{M_j} \right)}} = \frac{5 \sqrt{\pi m_i k T}}{16 \pi \bar{\Omega}_{ii}^{(2,2)}} \sum_{j=1}^{nspc} x_j \frac{16}{5} \left[\frac{2 N_A M_j}{\pi k T M_i (M_i + M_j)} \right]^{\frac{1}{2}} \pi \bar{\Omega}_{ij}^{(2,2)}$$

Simplifying

$$\sum_{j=1}^{nspc} x_j \left[1 + \sqrt{\frac{\pi \bar{\Omega}_{jj}^{(2,2)}}{\pi \bar{\Omega}_{ii}^{(2,2)}}} \right]^2 = \sum_{j=1}^{nspc} x_j 4 \frac{\pi \bar{\Omega}_{ij}^{(2,2)}}{\pi \bar{\Omega}_{ii}^{(2,2)}}$$

The easiest way to satisfy this is if

$$\pi \bar{\Omega}_{ii}^{(2,2)} = \pi \bar{\Omega}_{ij}^{(2,2)} = \pi \bar{\Omega}_{jj}^{(2,2)}$$

If the collision integrals of the dominant species are roughly equivalent, than Wilke's mixing rule will give roughly the same total viscosity as that found by collision integrals. This is violated somewhat in the 3000-8000 K temperature where the dominant species are N_2 , N , and O and the neutral diatomics have collision integral values approximately 50% higher than neutral atomic species. The agreement begins to fall apart above 8000 K when ionized species mole fractions become significant since the collision integrals of ionized species are orders of magnitude different from neutral species.

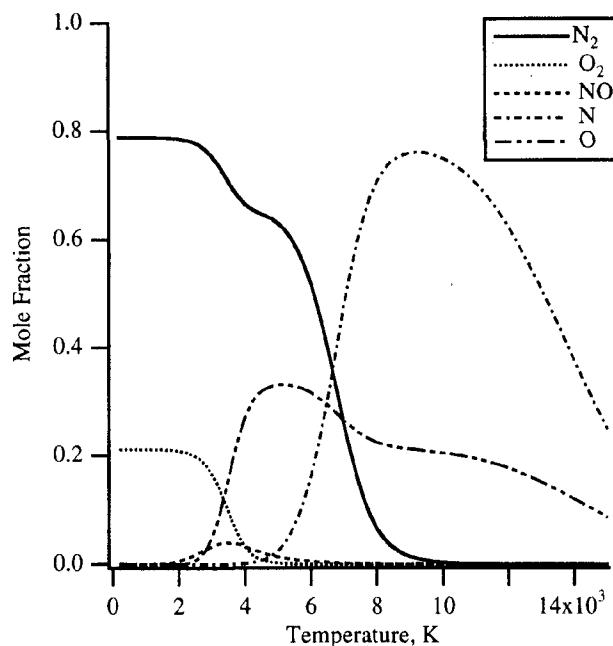


Fig. 1a. Neutral species

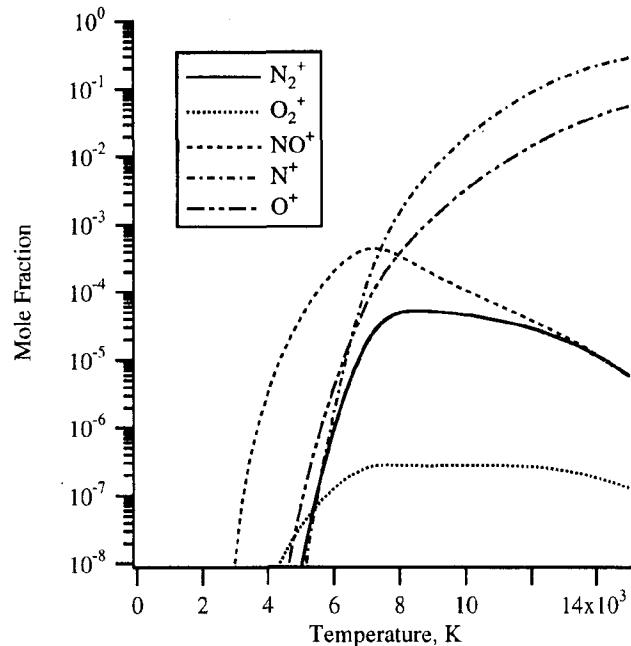


Fig. 1b. Ionized species

Figure 1. Equilibrium species mole fractions, pressure = 1.0 atm

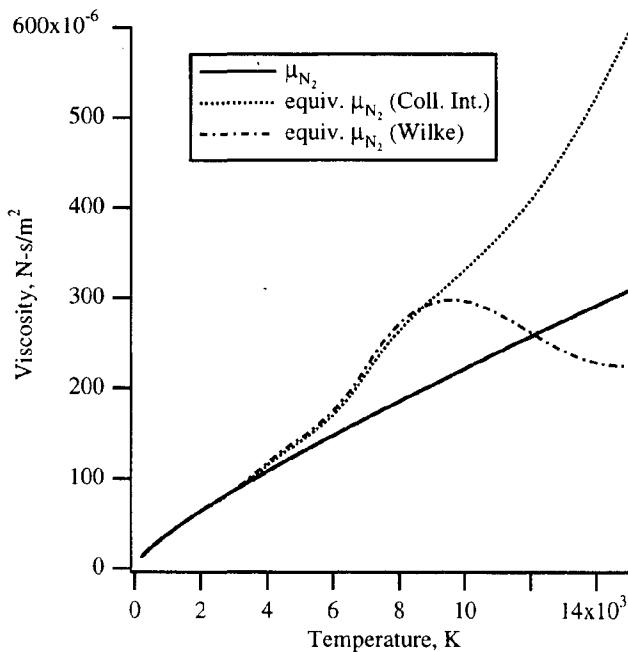


Fig. 2a. Diatomic nitrogen

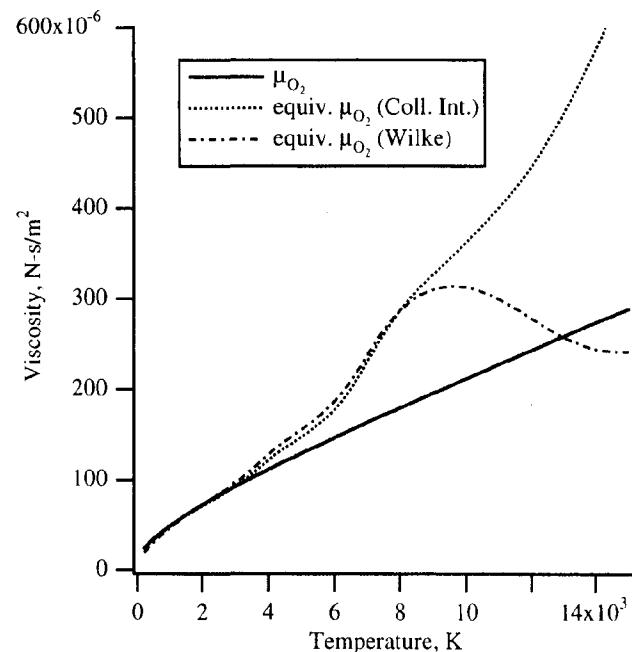


Fig. 2b. Diatomic oxygen

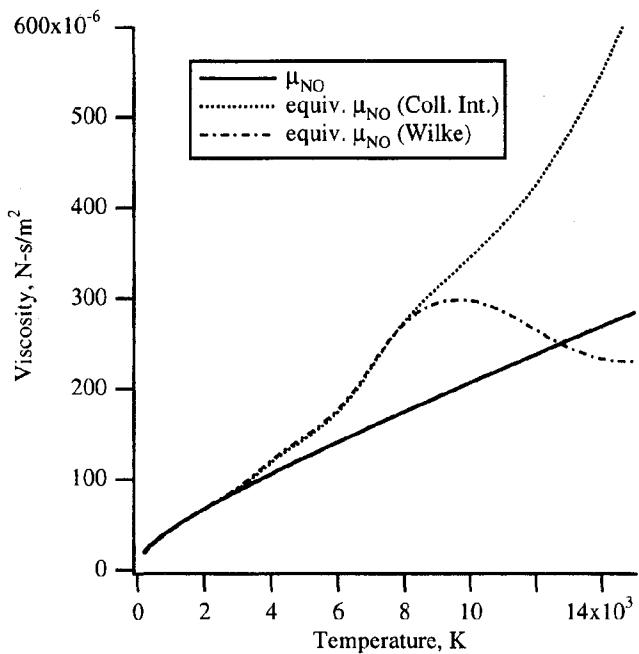


Fig. 2c. Nitric oxide

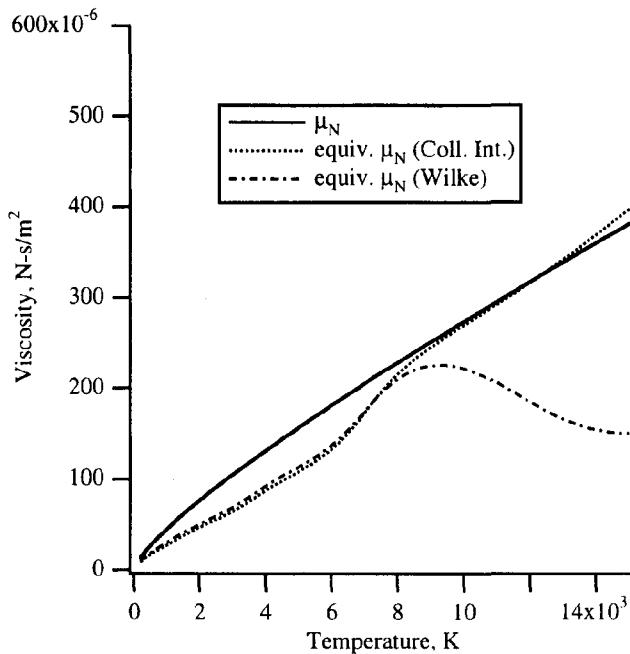


Fig. 2d. Atomic nitrogen

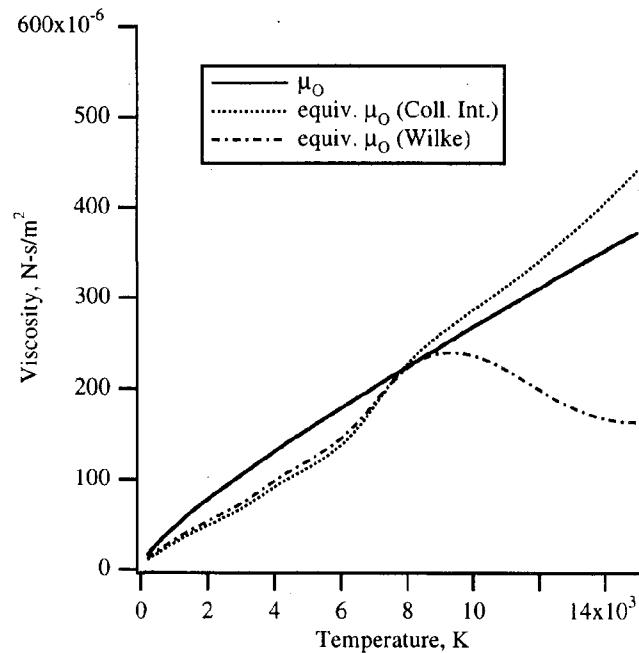


Fig. 2e. Atomic oxygen

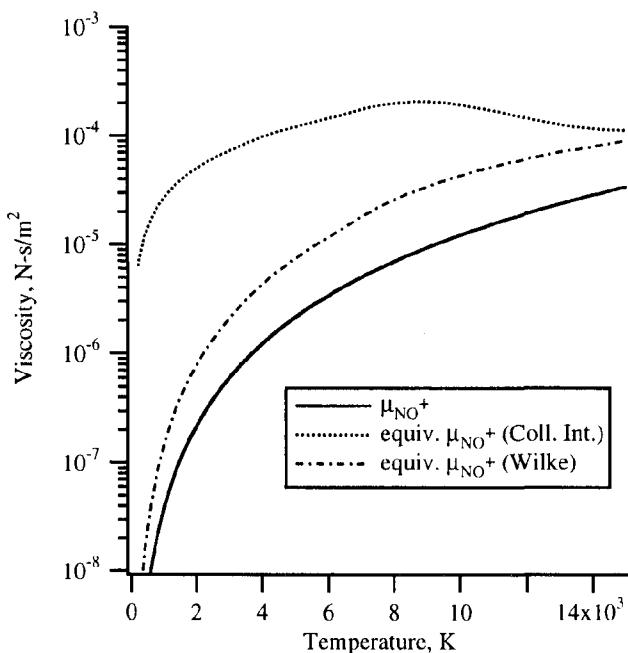


Fig. 2f. Nitric oxide ion

Figure 2. Comparison of species and equivalent species viscosities, pressure = 1.0 atm

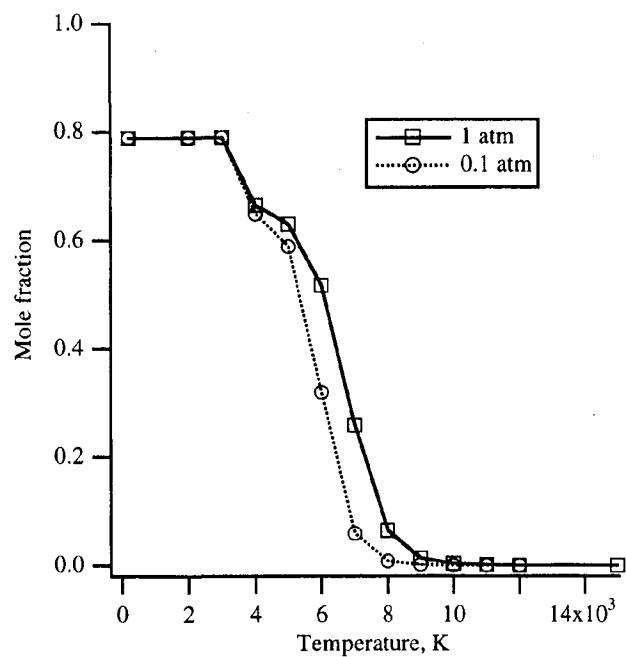


Fig. 3a. Diatomic nitrogen mole fraction

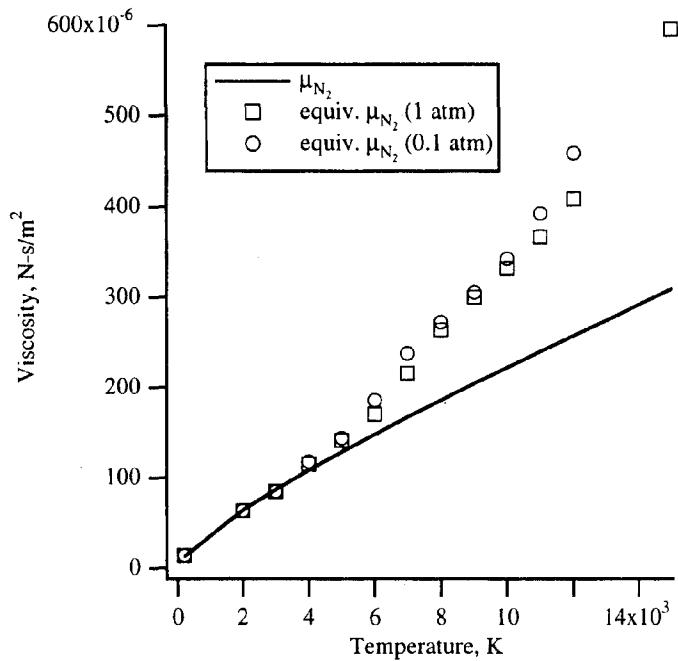


Fig. 3b. Diatomic nitrogen viscosity

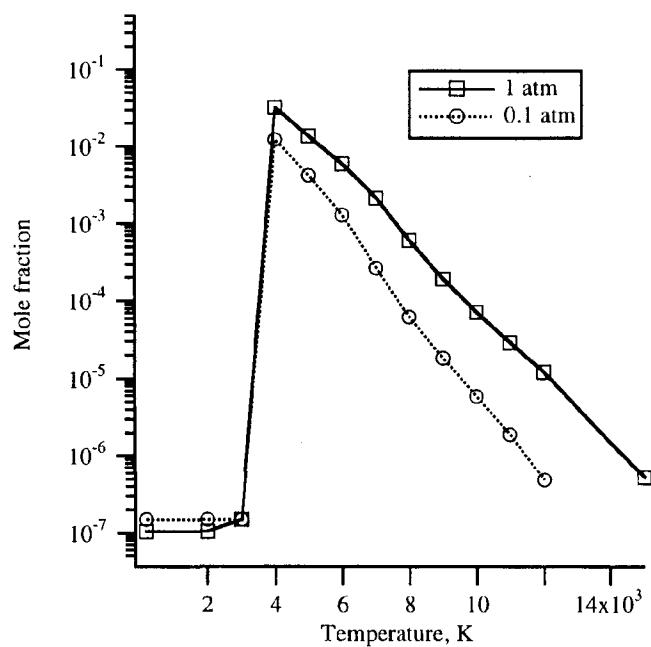


Fig. 3c. Nitric oxide mole fraction

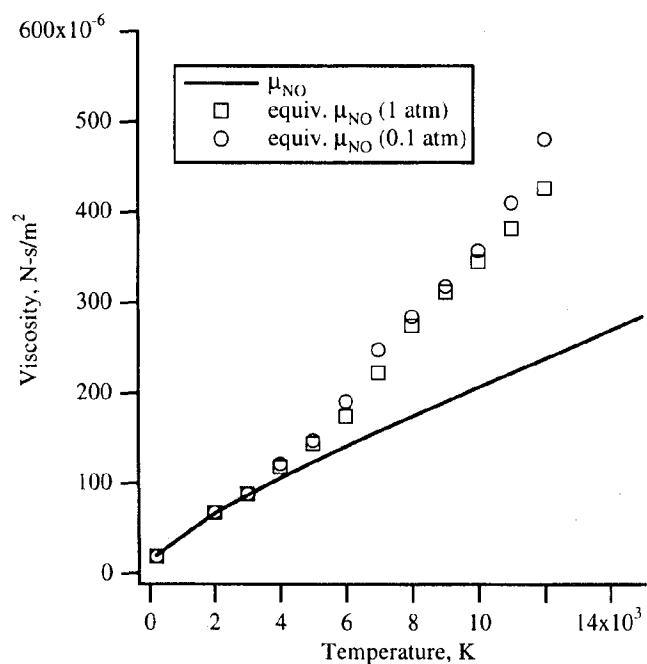


Fig. 3d. Nitric oxide viscosity

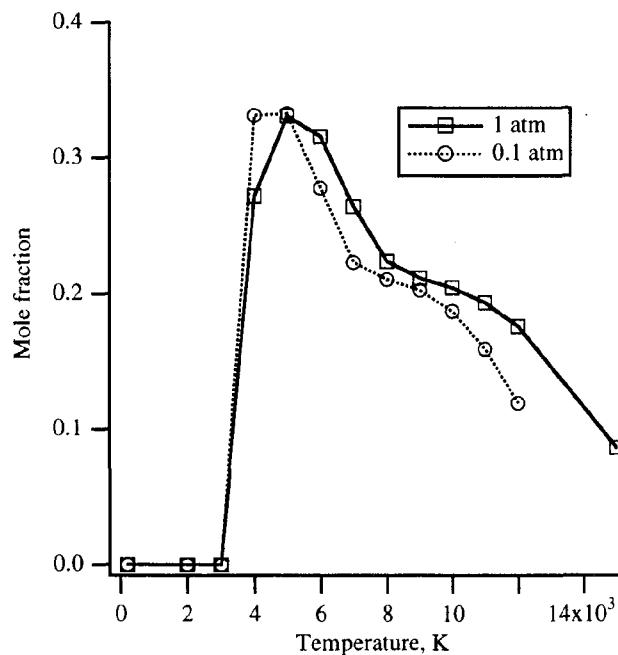


Fig. 3e. Atomic oxygen mole fraction

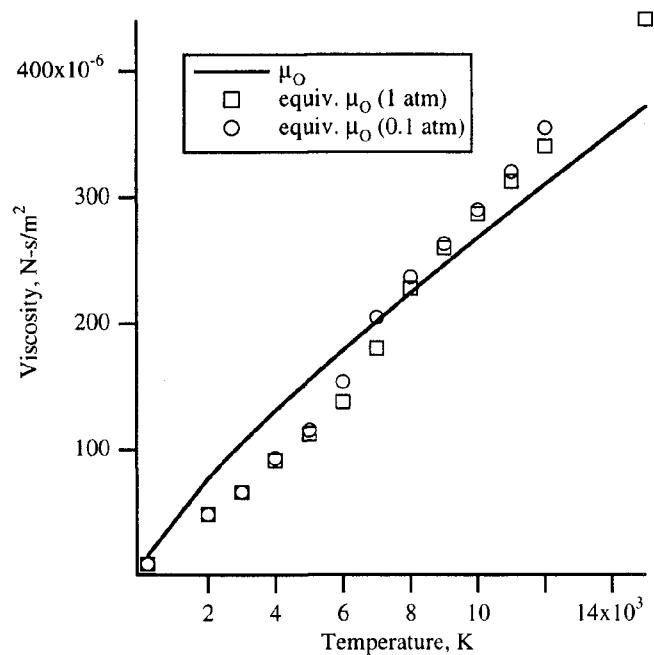


Fig. 3f. Atomic oxygen viscosity

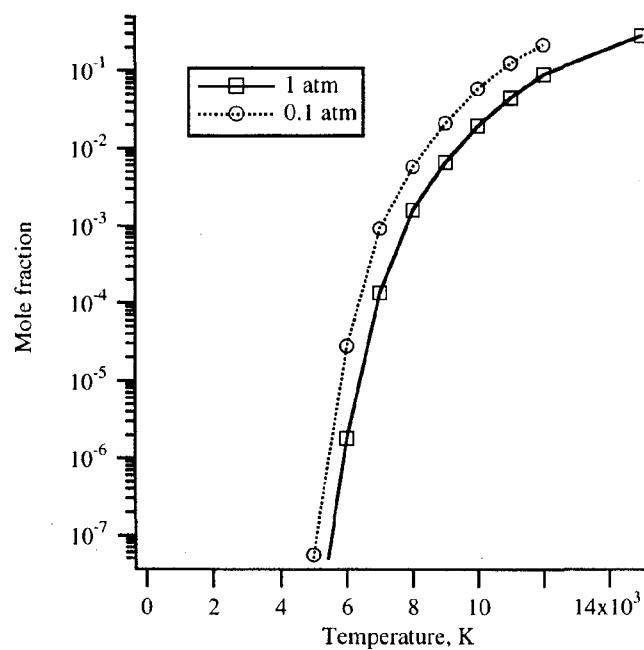


Fig. 3g. Atomic nitrogen ion mole fraction

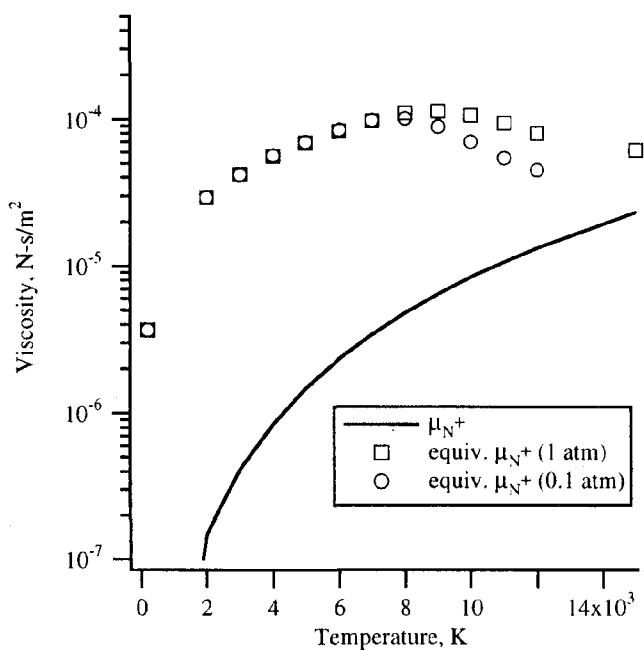


Fig. 3h. Atomic nitrogen ion viscosity

Figure 3. Pressure dependence of species mole fraction and equivalent species viscosity

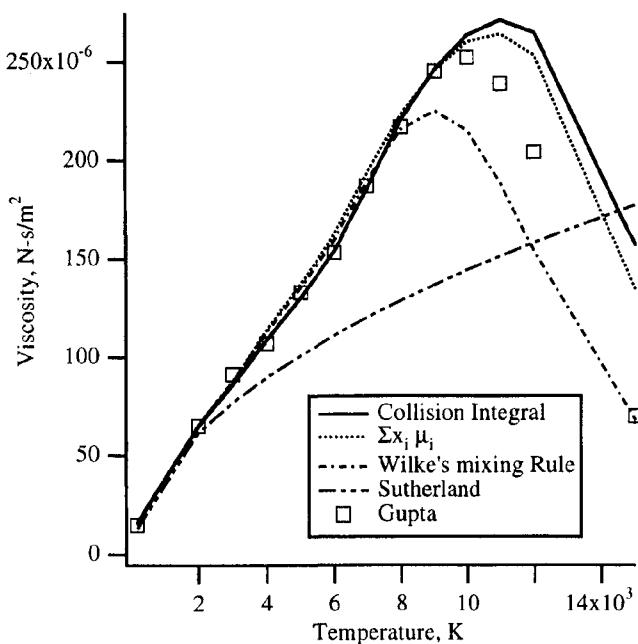


Fig. 4a. Mixture viscosity, $p=1.0$ atm.

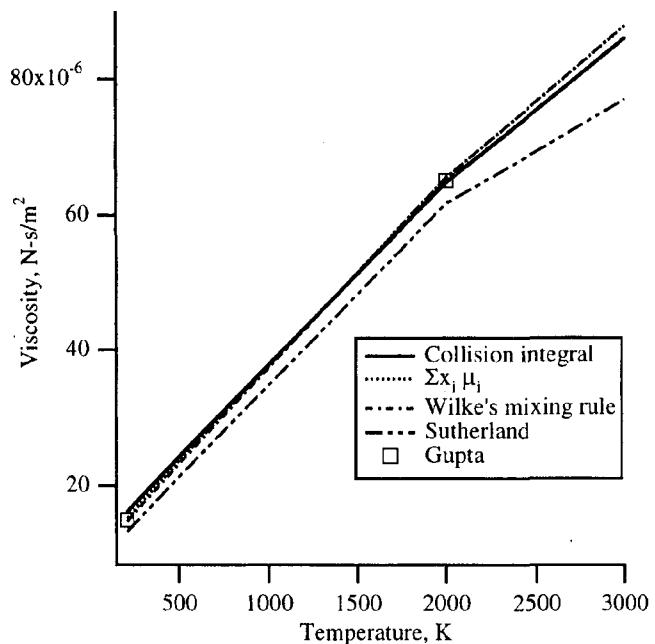


Fig. 4b. Mixture viscosity, $p=1.0$ atm

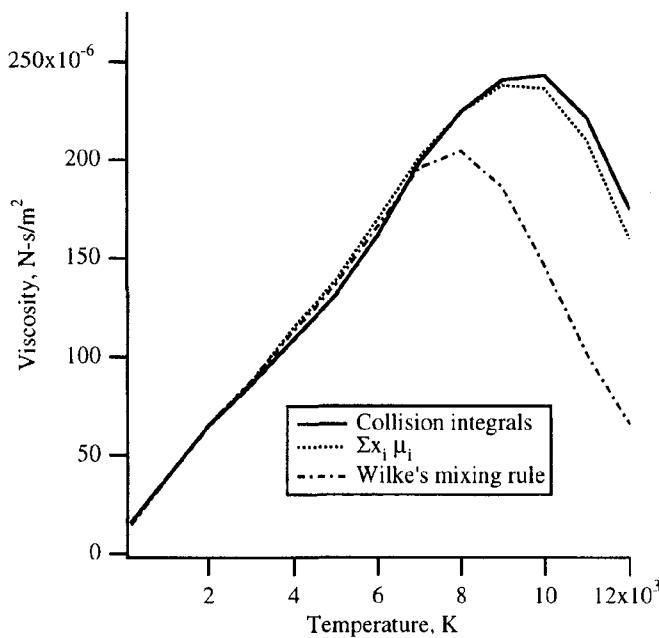


Fig. 4c. Mixture viscosity, $p=0.1$ atm

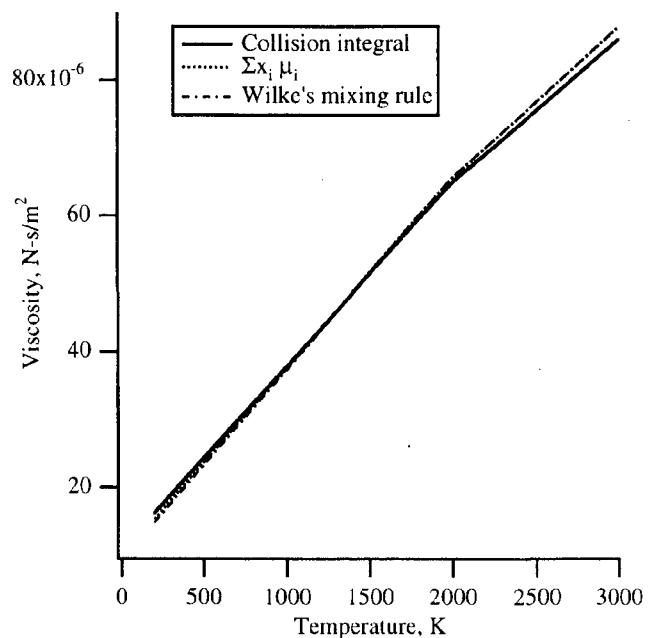


Fig. 4d. Mixture viscosity, $p=0.1$ atm

Figure 4. Comparison of mixture viscosity, 11 Species, equilibrium Air

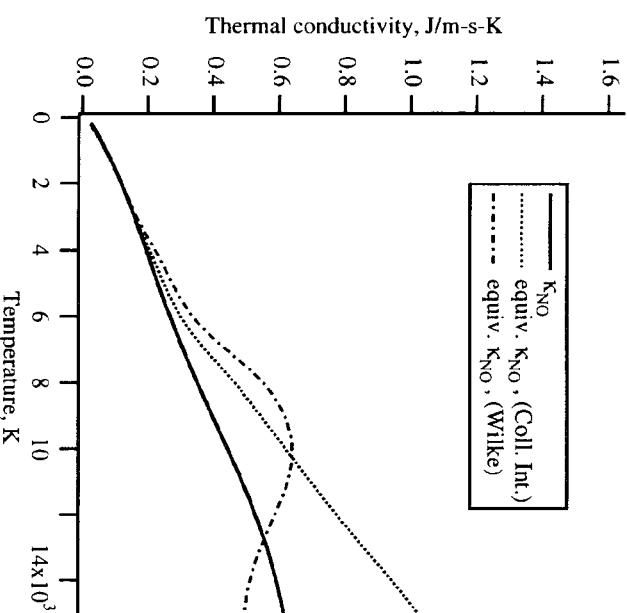


Fig. 5a. Diatomic nitrogen

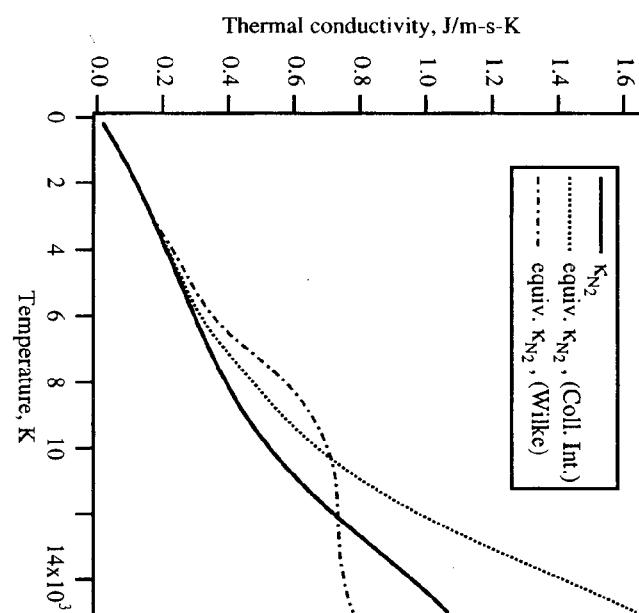


Fig. 5b. Diatomic oxygen

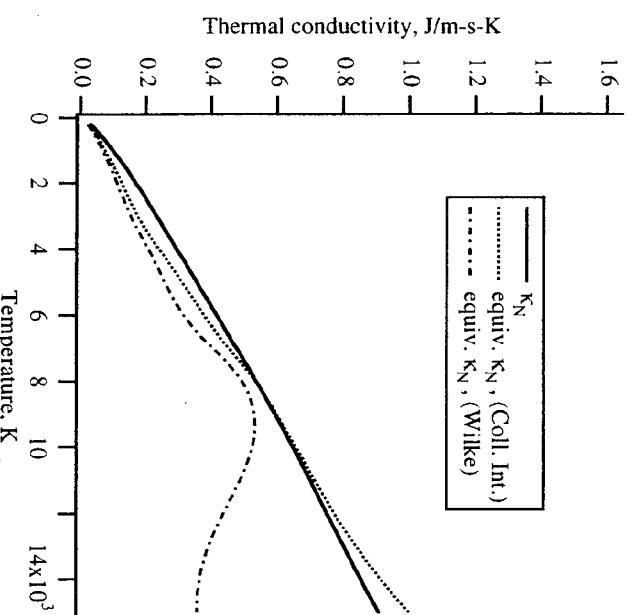


Fig. 5c. Nitric oxide

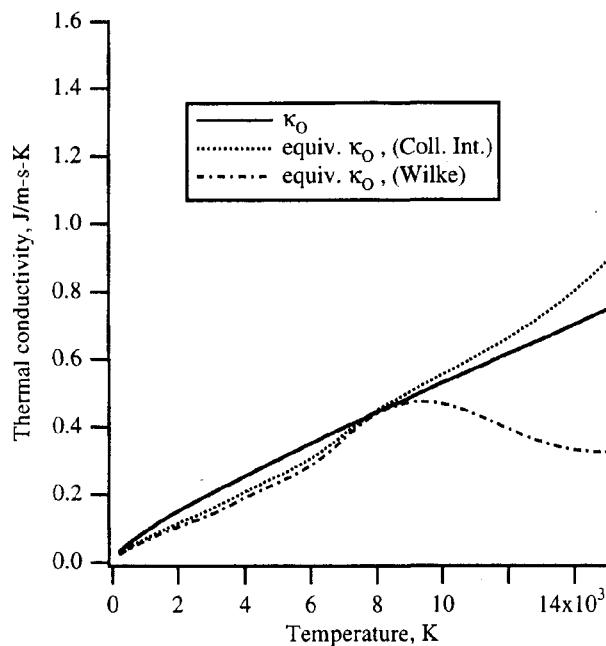


Fig. 5e. Atomic oxygen

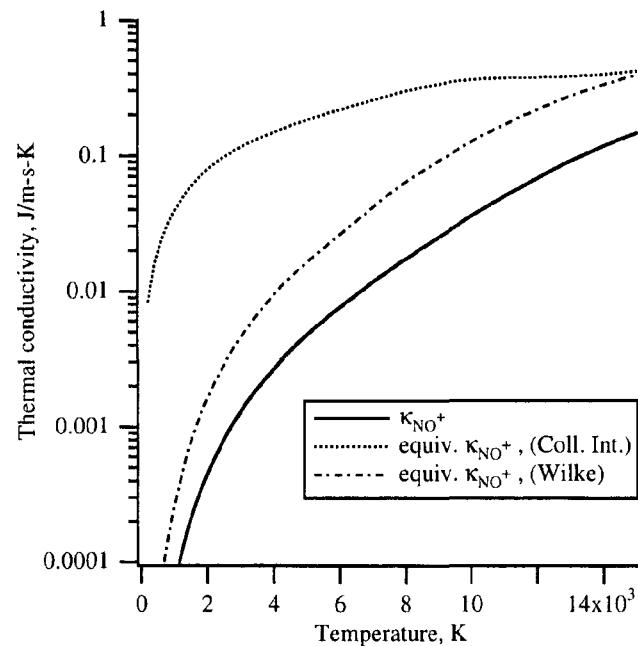


Fig. 5f. Nitric oxide ion

Figure 5. Comparison of species and equivalent species thermal conductivities, pressure = 1.0 atm

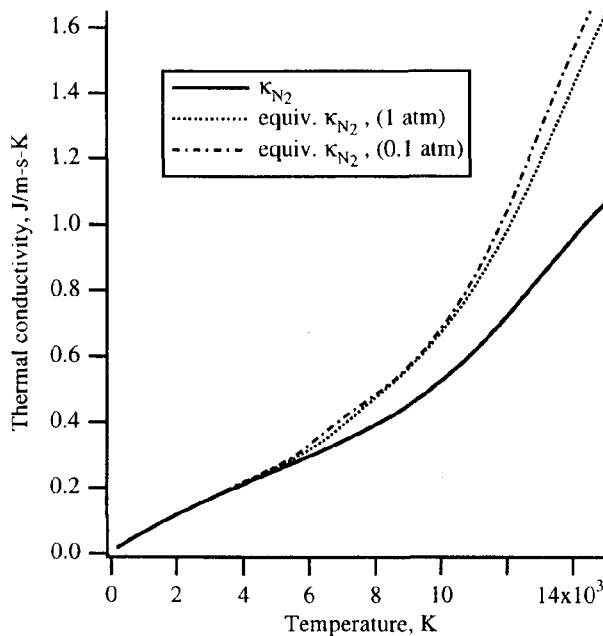


Fig. 6a. Diatomic nitrogen

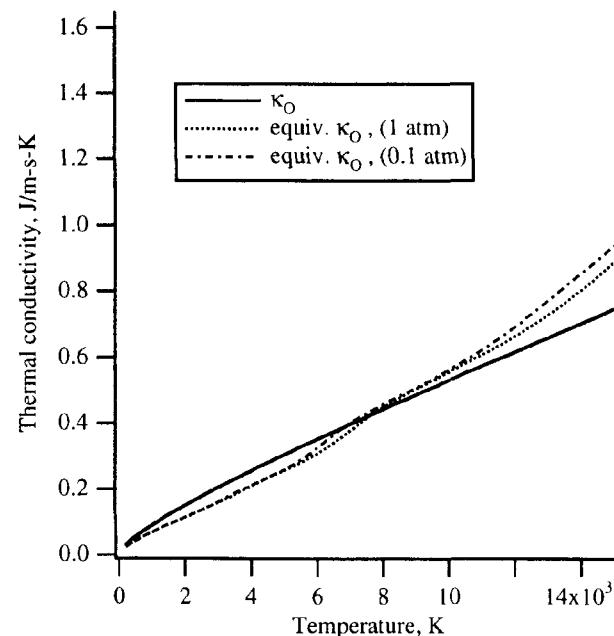


Fig. 6b. Atomic oxygen

Figure 6. Pressure dependence of equivalent species conductivity

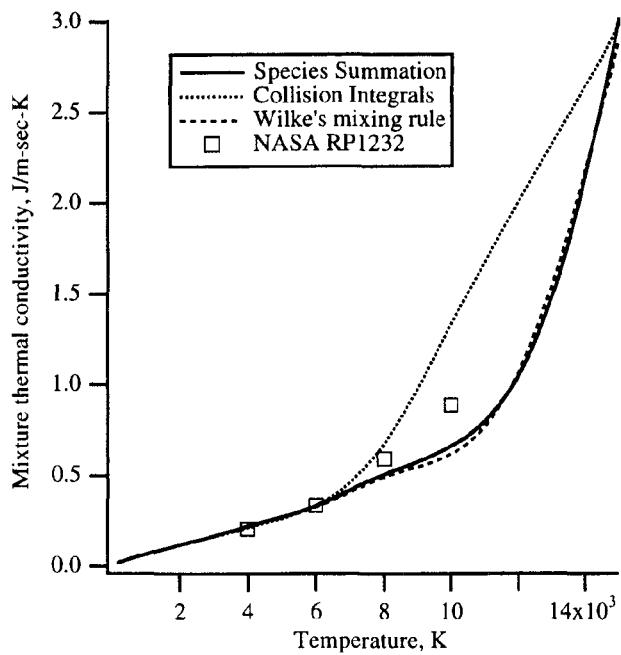


Fig. 7a. Pressure = 1.0 atm

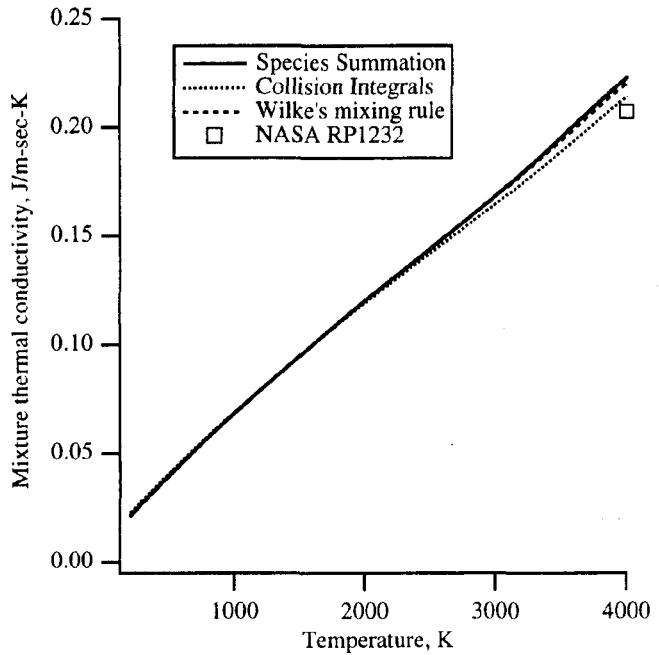


Fig. 7b. Pressure = 1.0 atm, low temperature region

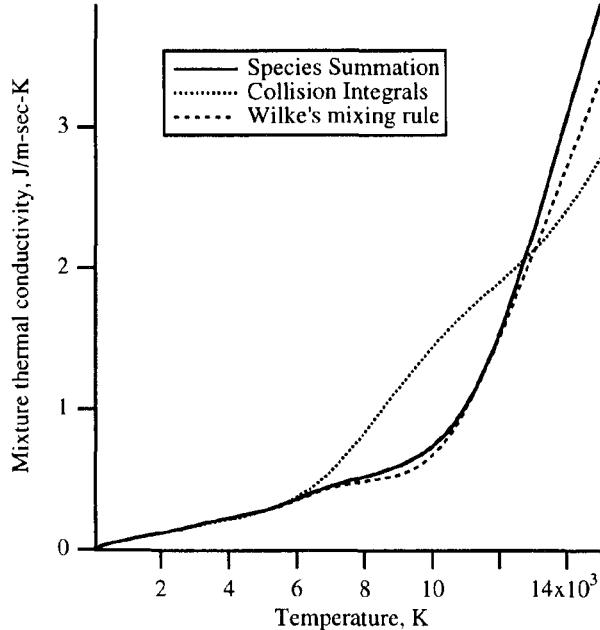


Fig. 7c. Pressure = 0.1 atm

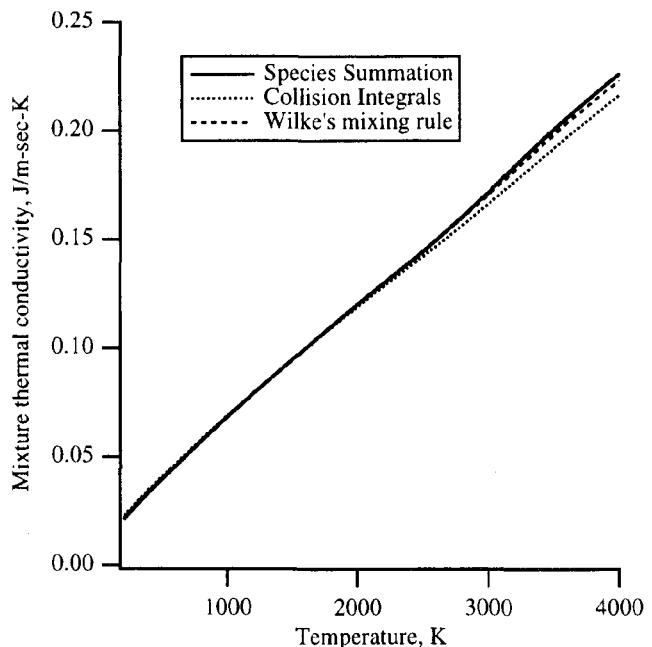


Fig. 7d. Pressure = 0.1 atm, low temperature region

Figure 7. Mixture thermal conductivity comparison

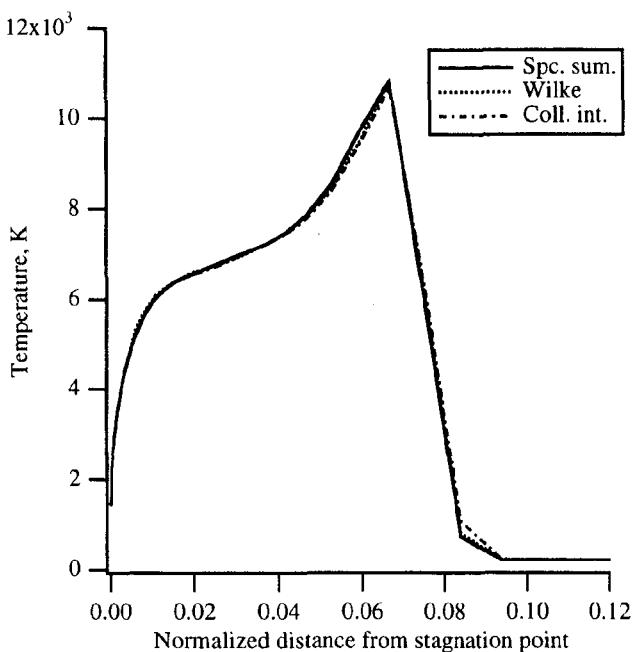


Fig. 8a. Stagnation line temperatures, 75 km

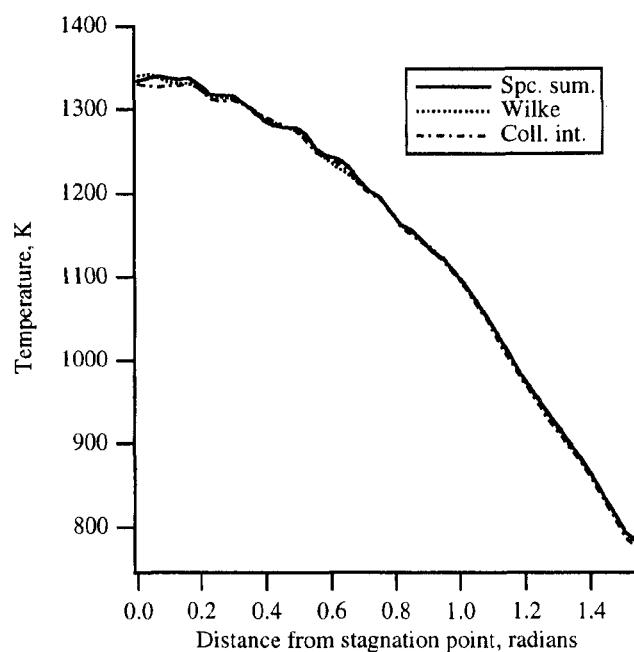


Fig. 8b. Radiative equilibrium surface temperatures, 75km.

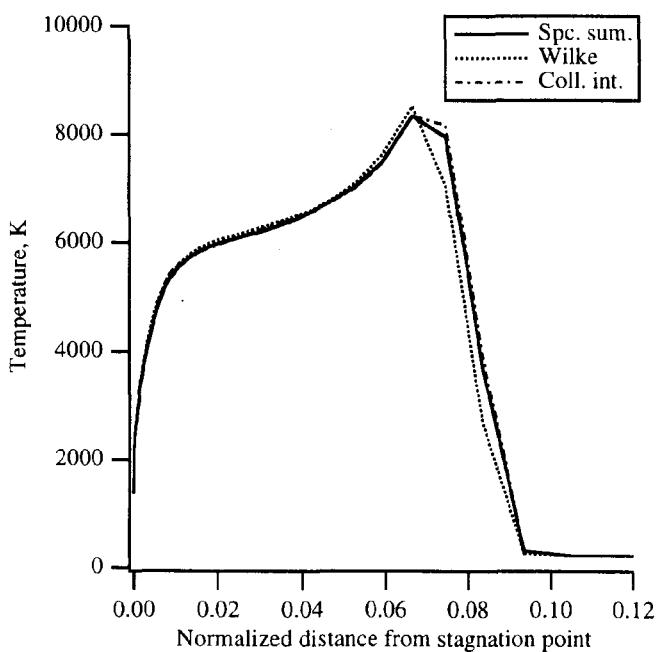


Fig. 8c. Stagnation line temperatures, 70 km.

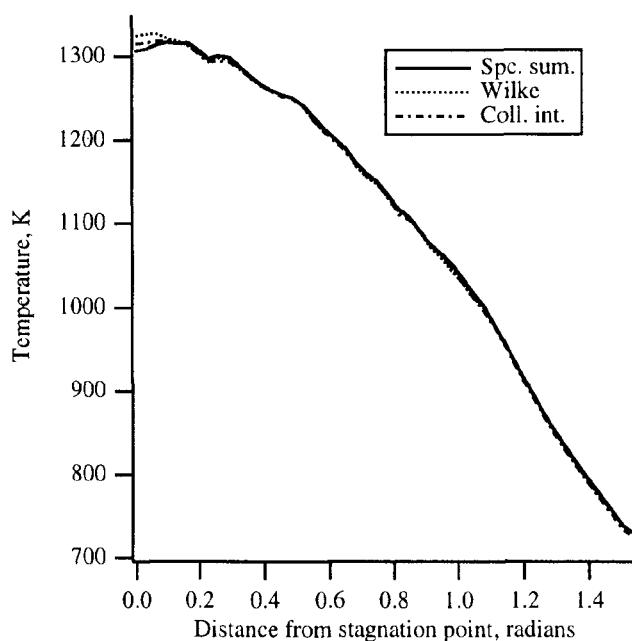


Fig. 8d. Radiative equilibrium surface temperatures, 70 km.

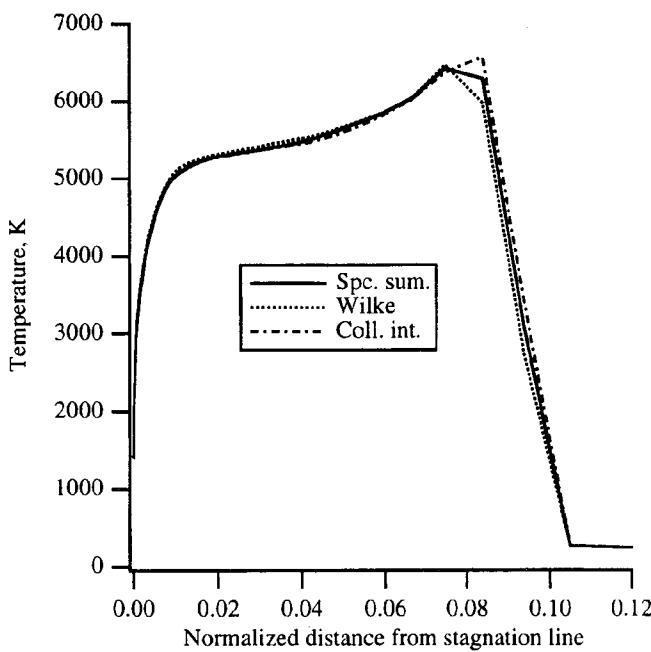


Fig. 8e. Stagnation line temperatures, 60km.

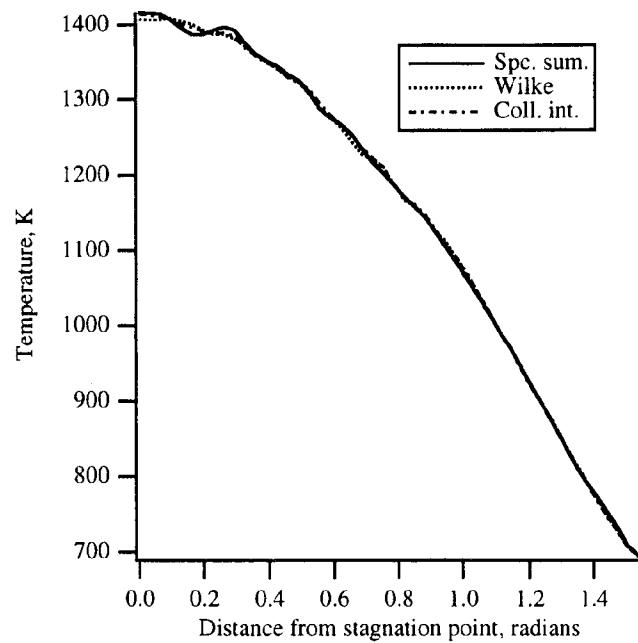


Fig. 8f. Radiative equilibrium surface temperature, 60km.

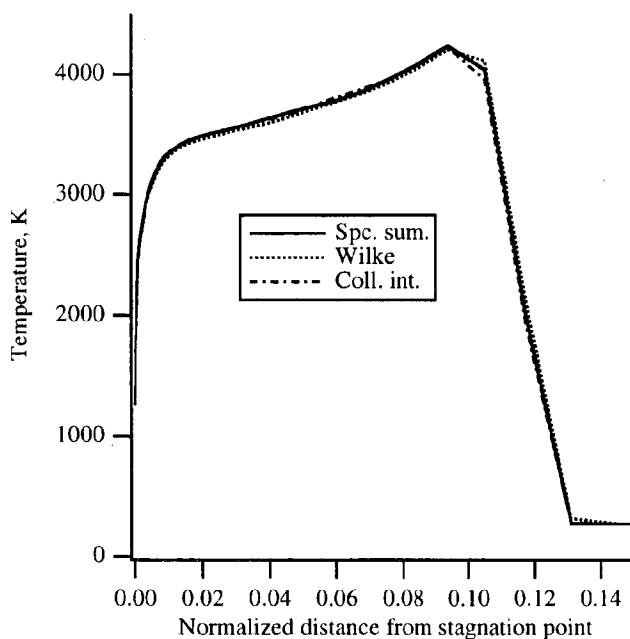


Fig. 8g. Stagnation line temperatures, 50km.

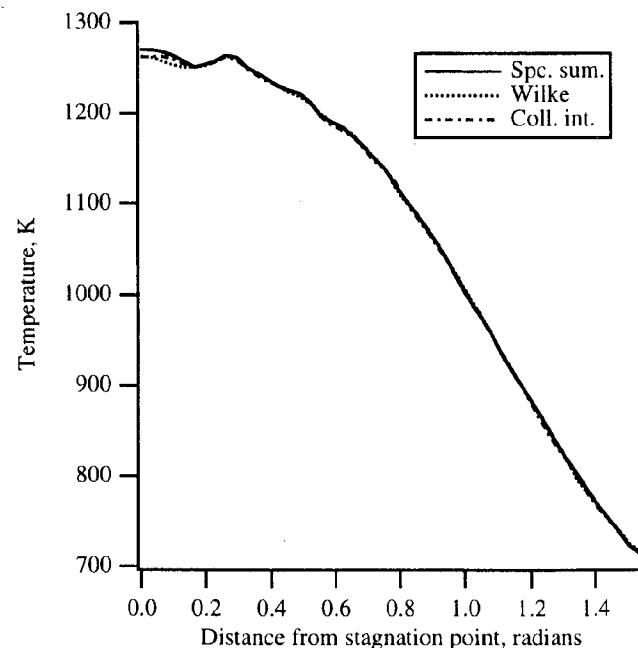


Fig. 8h. Radiative equilibrium surface temperatures, 50km.

Figure 8. Effect of mixture transport model on computed temperatures.

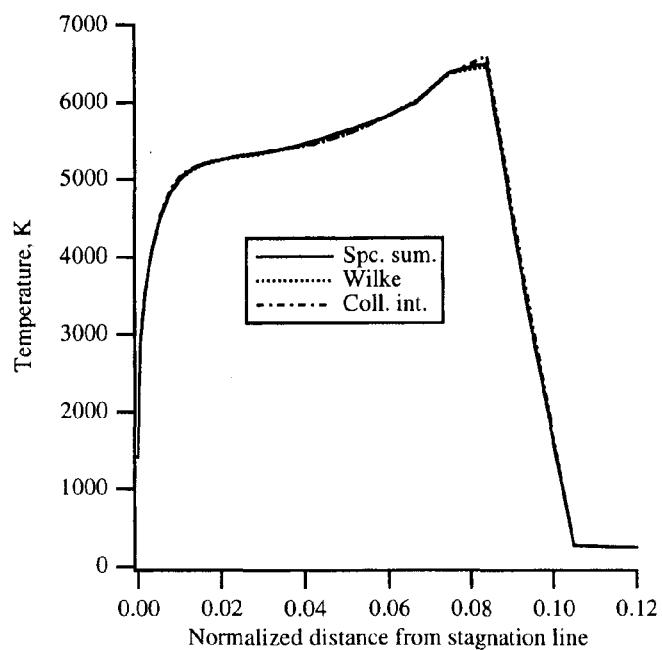


Fig. 9a. Stagnation line temperatures, 60 km

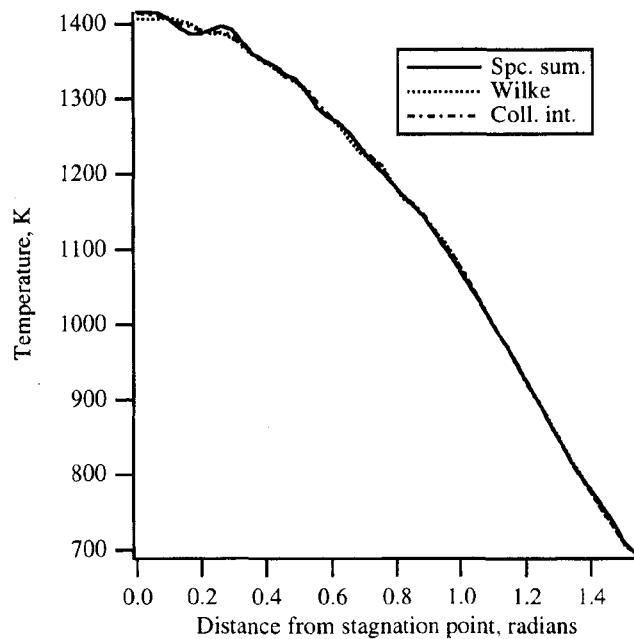


Fig. 9b. Radiative equilibrium surface temperatures, 60km.

Figure 9. Effect of mixture transport property model on computed temperatures, 11 species air.