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Eucken correction in high-temperature gases with electronic excitation

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In the present paper, thermal conductivity coefficient of high-temperature molecular and atomic gases with excited electronic states is studied using both the kinetic theory algorithm developed by authors earlier and the well known simple expression for the thermal conductivity coefficient proposed by Eucken and generalized by Hirschfelder. The influence of large collision diameters of excited states on the thermal conductivity is discussed. The limit of validity of the Eucken correction is evaluated on the basis of the kinetic theory calculations; an improved model suitable for air species under high-temperature conditions is proposed. © 2014 AIP Publishing LLC.
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I. INTRODUCTION

Transport properties in gases with internal degrees of freedom were extensively discussed in the literature during the last century. A simple model proposed in 1913 by Eucken¹ was based on the mean free path considerations. Although it does not have enough of a theoretical justification, it works rather well in many cases of practical interest and is still widely used in computational fluid dynamics (CFD). Later, rigorous kinetic theory algorithms for the calculation of transport coefficients were developed based on quantum mechanical,² classical,³ and quasi-classical⁴ approaches for weakly non-equilibrium gases. A major effort was put in by Mason and Monchick^{5,6} to develop transport algorithms for polyatomic gas mixtures and polar gases (see also Refs. 7–10). Efficient numerical algorithms needed for calculation of transport properties in complex mixtures were developed by Ern and Giovangigli.¹¹ Generalizations of the Eucken formula based on the kinetic theory were proposed in Refs. 12 and 13 for thermal equilibrium gases. Eucken approximation for local equilibrium ionized gases is widely discussed in the recent monograph.¹⁴

Starting in the 1960s, interest in the transport properties of strongly non-equilibrium gas flows has increased. For vibrationally non-equilibrium flows, thermal conductivity coefficients were derived in Refs. 15 and 16 for the harmonic oscillator model. Departures from the Boltzmann distributions typical for real gas flows of anharmonic oscillators are considered in Ref. 17. In the latter paper, a generalization of the Eucken factor is proposed for the case of complex Treanor-Gordiets vibrational distribution function.

Most of all above mentioned modifications of the Eucken correction treat only molecular species with excited rotational and vibrational degrees of freedom and neglect electronic excitation. The exception is the pioneering work by Hirschfelder¹² where he shows that metastable states cannot be described on the basis of the Eucken formula since they possess anomalously large collision diameters. However, no systematic evaluation of the contribution of electronic

states to the transport coefficients was done until the early 2000s. Recently, for high temperature flows it was shown that electronic excitation may play a significant role in the heat transfer.^{14,18–22} Taking into account electronic degrees of freedom results in the considerable increase of internal heat conductivity in molecular species as well as in the appearance of additional heat conductivity coefficient associated with electronic excitation in atomic species. Algorithms for the calculation of transport coefficients in gases with excited electronic states are developed in Refs. 14, 18, and 20. The computation costs of these algorithms can be rather high depending on the number of states considered; this prevents taking into account electronic excitation in hypersonic flow simulations. To address issues related to the computational costs, validation of the simple Eucken-like model accounting for the electronic states would be rather useful.

The objective of this study is to verify the validity of the Eucken and Hirschfelder expressions in high-temperature gases with electronic excitation. The paper is organized as follows. In Sec. II, we describe the theoretical model and its possible simplifications. In Sec. III, validation of the models is performed. At low temperatures, we check the accuracy of proposed formulas on the basis of available experimental data. Then we estimate the effect of atomic excited states with large diameters on the collision integrals specifying the thermal conductivity coefficients. After that we calculate the Eucken factors on the basis of the kinetic theory algorithms. Comparing the results of exact and approximate calculations, we assess the Eucken and Hirschfelder formulas for N₂, O₂ molecular species with rotational, vibrational, and electronic excitation as well as for N, O electronically excited atomic species.

II. THERMAL CONDUCTIVITY COEFFICIENTS: THEORETICAL MODELS

A. Kinetic theory approach

We consider molecular gases with excited rotational, vibrational, and electronic degrees of freedom and atomic species with excited electronic states under conditions of

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weak thermal non-equilibrium and strong chemical non-equilibrium. According to the cut-off criterion for atomic partition functions,²³ we take into account 170 and 204 excited electronic states for N and O atoms, respectively. For molecular species, we consider 5 and 7 electronic states in N₂ and O₂. Note that separation of different internal modes in molecules is not possible in the considered case because ro-vibrational and electronic levels are strongly coupled. Since electrons have no internal structure, and the same assumption is commonly applied to ionized atoms¹⁴ we do not consider them in the present study.

We follow the kinetic theory algorithm for the calculation of transport coefficients developed in Ref. 20 for single-component electronically excited gases and extended later for non-equilibrium mixtures of neutral and ionized gases.²⁴ The model is based on the modification of the Chapman–Enskog method for flows with rapid and slow collisional processes.²⁵ For the present case, the zero-order distribution function is the combination of local equilibrium Maxwell and Boltzmann distributions over velocity and internal energy whereas chemical composition is found from the equations of strongly non-equilibrium chemical kinetics.

Using the rigorous Chapman–Enskog procedure, we obtain the first-order distribution function in terms of gradients of the macroscopic flow variables: temperature T , velocity \mathbf{v} , and species c number densities n_c . The partial thermal conductivity coefficient λ including contributions of translational λ_{tr} and internal λ_{int} degrees of freedom can be expressed in terms of the function \mathbf{A} which is associated with the temperature gradient in the expression for the first-order distribution function,²⁰

$$\lambda = \frac{k}{3} [\mathbf{A}, \mathbf{A}] = \lambda_{\text{tr}} + \lambda_{\text{int}}, \quad (1)$$

k is the Boltzmann constant. The function \mathbf{A} is expanded into double series of orthogonal Sonine polynomials in reduced velocity and Waldmann–Trübenbacher polynomials in discrete values of electronic energy for atoms and total internal energy including rotational, vibrational, and electronic for molecules. Finally, the thermal conductivity coefficients are found as solutions of transport linear systems involving as

coefficients the bracket integrals over cross sections of rapid processes (elastic collisions and internal energy transitions). Slow chemical reactions do not contribute to thermal conductivity coefficients, contrarily to the case of chemically equilibrium plasma^{14,18,19,26} where reactive contribution to the thermal conductivity coefficient, λ_{react} , is often introduced to describe chemical reactions. It is worth noting that the concept of reactive thermal conductivity coefficient for equilibrium plasma is an approximation limited by the fact that in a viscous flow, species molar fractions depend not only on the temperature T and pressure p but also on the velocity divergence $\nabla \cdot \mathbf{v}$ (see Ref. 20). Therefore, reactive thermal conductivity can be introduced rigorously only in non-moving gases ($\mathbf{v} = 0$) or incompressible flows ($\nabla \cdot \mathbf{v} = 0$). In the present model, chemical reactions affect the heat transfer through multi-component diffusion and thermal diffusion coefficients rather than through reactive thermal conductivity.

At the next step, on the basis of the common kinetic theory assumptions^{5,8} the bracket integrals are expressed in terms of $\Omega_{cd}^{(l,r)}$ collision integrals and integrals depending on the internal energy variation in inelastic collisions, $\Delta\varepsilon$. The collision integrals are then calculated using the approximate formulas given in Ref. 27; as is shown in Ref. 20, for electronically excited gases these high-temperature data are more realistic compared to those provided in Ref. 28. Estimates for the terms containing $\Delta\varepsilon$ are given in Ref. 24.

B. Eucken and Hirschfelder formulae

Eucken¹ proposed to express thermal conductivity coefficients as follows:

$$\lambda_{\text{tr}} = c_{v,\text{tr}} f_{\text{tr}} \eta, \quad \lambda_{\text{int}} = c_{v,\text{int}} f_{\text{int}} \eta, \quad (2)$$

where η is the shear viscosity coefficient, $c_{v,\text{tr}}$, $c_{v,\text{int}}$ are the constant volume specific heats for translational and internal degrees of freedom, and the factors f_{tr} , f_{int} are

$$f_{\text{tr}} = \frac{5}{2}, \quad f_{\text{int}} = 1. \quad (3)$$

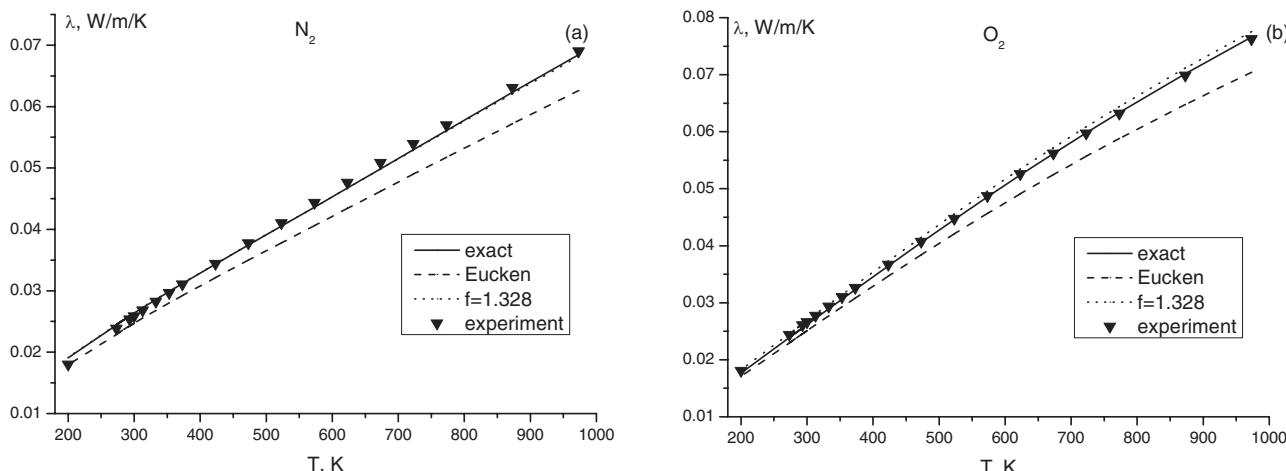


FIG. 1. Thermal conductivity coefficients as functions of T . (a) N₂ and (b) O₂.

TABLE I. The diameters of nitrogen and oxygen excited atoms.

Species	State, i	σ_i (Å)
N	$1S^2 2S^2 2P^3$	3.16
	$1S^2 2S^2 2P^2 3S$	8.74
	$1S^2 2S^2 2P^2 4S$	20.85
O	$1S^2 2S^2 2P^4$	2.69
	$1S^2 2S^2 2P^3 3S$	8.15
	$1S^2 2S^2 2P^3 4S$	20.84

Hirschfelder¹² improved this simple result using the kinetic theory reasoning. He showed that in a single-component gas,

$$f_{\text{int}} = \frac{\rho D}{\eta}, \quad (4)$$

ρ is the density, D is the self-diffusion coefficient. Moreover, estimating this factor on the basis of the Lennard-Jones and Buckingham interaction potentials, he found that for a wide variety of species, f_{int} is approximately constant,

$$f_{\text{int}} = 1.328. \quad (5)$$

Such a simple representation provides a surprisingly good accuracy for non-polar gases with excited rotational and vibrational modes at moderate temperatures. However, no assessment was done for high temperature air species with electronic excitation. In Sec. III, we present results of our calculations.

III. RESULTS AND DISCUSSION

We consider molecular and atomic nitrogen and oxygen with excited internal degrees of freedom in the temperature range 200–25 000 K. First we check the low-temperature conditions where experimental data on molecular thermal conductivity are available. For the assessment of our model, we choose high-fidelity correlations²⁹ for the thermal conductivity coefficients based on experimental measurements;^{30–32} the correlation accuracy is within 3%–5%. In Fig. 1, the thermal conductivity coefficients for molecular species are presented

as functions of temperature. The coefficients are calculated using the exact kinetic theory methods and simplified Eucken and Hirschfelder expressions. While a good agreement with experimental measurements is obtained for both exact formulation and Hirschfelder model (the discrepancy does not exceed 2%), the Eucken formula underestimates the thermal conductivity coefficients up to 7%–10%.

Let us discuss now the influence of the diameter of electronically excited atoms on the thermal conductivity in the temperature range where electronic excitation may play an important role. As is pointed out by Hirschfelder,¹² “the excited electronic species correspond to giant molecules much larger in size than the normal ground state molecules.” Therefore, he emphasizes that the Eucken approximation cannot be applied for those excited states. We estimated the contribution of several excited states to the collision integrals $\Omega^{(l,r)}$. The collision diameter σ (Å) was calculated using the approximate Slater formula:¹²

$$\sigma = n^*(2n^* + 1)/(Z - S)a_0 + 1.8\text{ Å}, \quad (6)$$

where a_0 is the radius of the first Bohr orbit, Z is the atomic number, S is the Slater screening constant, and n^* is the Slater effective principal quantum number for the outermost orbital. The diameters of several excited atomic states are given in Table I.

We calculated the collision integrals $\Omega^{(1,1)}$, $\Omega^{(2,2)}$ using two approaches: in the first case, we take into account the variable collision diameter σ_i for the excited states $i = 1, 2, 3$ indicated in Table I; in the second case, we assume equal diameters for all internal states. Expressions for collision integrals include the term $\sum_{ij} \frac{1}{4}(\sigma_i + \sigma_j)^2 x_i x_j$, x_i is the molar fraction of the corresponding internal state; for the case of equal diameters we have $\sum_{ij} \sigma^2 x_i x_j = \sigma^2$.

The collision integrals were calculated neglecting successively the third excited state and both the second and the third excited states with varying diameters (the latter case corresponds to $\sigma = \sigma_1 = \text{const.}$) The relative error in the integral $\Omega^{(1,1)}$ is plotted in Fig. 2. Although the collision cross sections for the excited states are large, their influence on the collision integrals at $T < 20 000$ K is rather low and the error does not

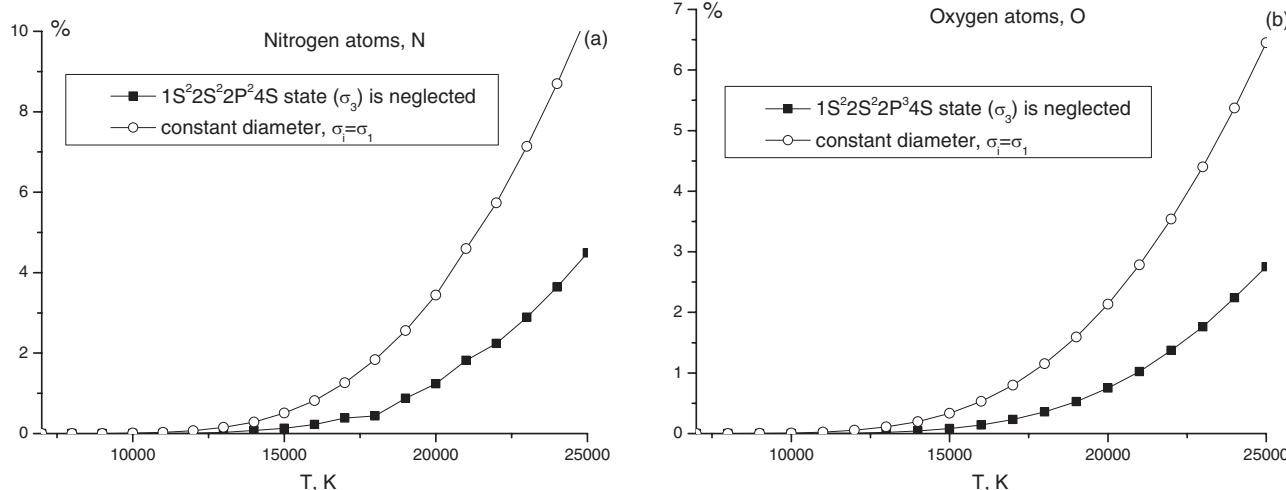
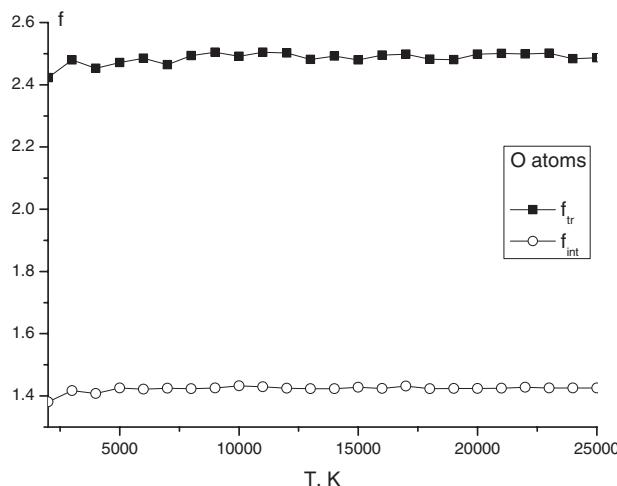


FIG. 2. Relative error (%) in collision integral $\Omega^{(1,1)}$ obtained neglecting excited states with variable diameters. (a) Nitrogen atoms and (b) Oxygen atoms.

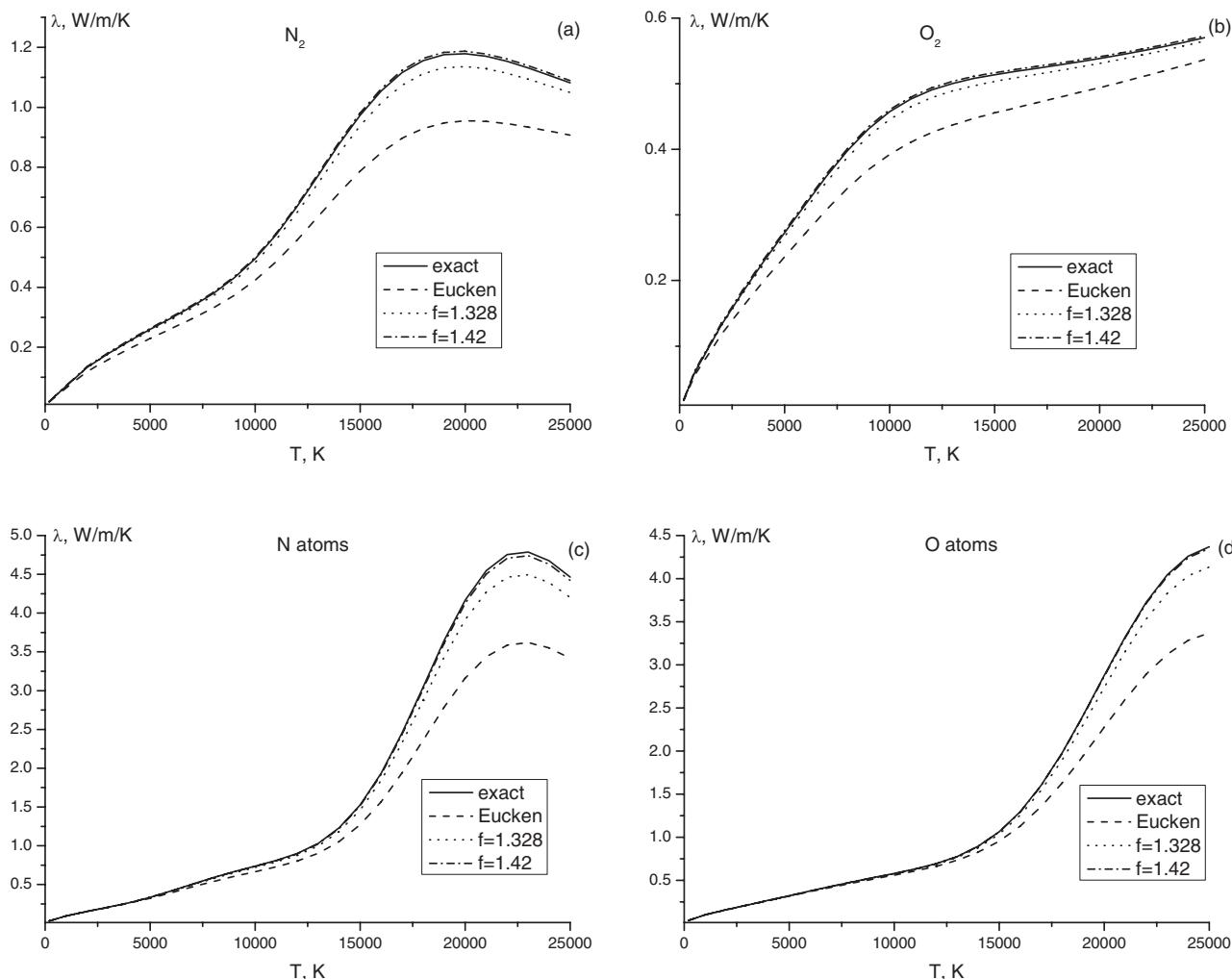
FIG. 3. Factors f_{tr} , f_{int} as functions of T . Atomic oxygen.

exceed 3.5% for N and 2.2% for O at $T = 20\,000$ K. The influence of the highly excited state ($i = 3$) is found to be less compared to that of states $i = 1, 2$. Similar results are obtained for other collision integrals and molecular species. For

$T > 20\,000$ K, the error increases sharply and exceeds 10% for nitrogen atoms at $T = 25\,000$ K. Therefore, the accuracy of results in the temperature range 20 000–25 000 K becomes worse, whereas for $T > 25\,000$ K the model with constant diameters is not applicable anymore.

A moderate effect of huge excited state diameters on the transport coefficients of a local chemically equilibrium nitrogen plasma is reported also in Ref. 14. For a hydrogen plasma, the influence is much stronger,¹⁴ and applying the Eucken formula is questionable. It is worth mentioning that the role of atomic diameters can be more important in the state-to-state approach under significant departures from the Boltzmann distribution. However, the Eucken correction is not applicable for the state-to-state model since in this case, the transport of electronic energy is governed by diffusion and not by thermal conductivity processes.

In Fig. 3, typical behavior of atomic oxygen Eucken factors f_{tr} , f_{int} derived from the results of exact kinetic theory calculations using Eq. (1) is presented. It is seen that for $T > 5000$ K, they are nearly constant, with the average values $f_{tr} = 2.5$, $f_{int} = 1.42$. For other species, the average value of f_{int} is also very close to 1.42 and thus larger than that proposed by Hirschfelder.

FIG. 4. Thermal conductivity coefficients as functions of T . (a) N_2 , (b) O_2 , (c) N, and (d) O.

In Fig. 4, we compare the thermal conductivity coefficients calculated using the exact kinetic theory method, the Eucken formula (2) with $f_{\text{int}} = 1$, and the corrected Eucken formula with $f_{\text{int}} = 1.328$ and $f_{\text{int}} = 1.42$. One can notice that the original Eucken formula does not work for high temperatures; the discrepancy reaches 20%–25%. The Hirschfelder correction provides much better accuracy in the wide temperature range: for molecules, the error does not exceed 3.5% whereas for atoms, the maximum discrepancy of 5%–6% is attained for temperatures 20 000–25 000 K. Finally, the value $f_{\text{int}} = 1.42$ obtained in the present paper, provides an excellent agreement (with the error within 1%) in the temperature range 5000–25 000 K for molecules, and in the whole considered temperature range for atoms. Note that for molecules at $T < 3000$ K, $f_{\text{int}} = 1.328$ given by Hirschfelder provides better accuracy; for atoms at low temperatures, the difference cannot be distinguished because the contribution of electronically excited states to their thermal conductivity is negligible.

Based on the above analysis, we can recommend using Eq. (2) with

$$f_{\text{tr}} = \frac{5}{2}, \quad \begin{cases} f_{\text{int}} = 1.328, & T < 3000 \text{ K} \\ f_{\text{int}} = 1.42, & 3000 < T < 25\,000 \text{ K} \end{cases} \quad (7)$$

for the calculation of thermal conductivity coefficients in high-temperature nitrogen and oxygen flows with electronically excited species. The accuracy of this approach is rather good for $T < 20\,000$ K but becomes worse in the temperature range 20 000–25 000 K since the role of variable collision diameters becomes important.

It should be pointed out that in the present study, we calculate the internal specific heats by direct summation over all excited states which is a time consuming procedure. In computational fluid dynamics, it is more efficient to use polynomial fits provided in Ref. 23 for the internal specific heats.

IV. CONCLUSIONS

The validity of the Eucken and Hirschfelder approximate expressions for the thermal conductivity coefficient in high-temperature gases with electronic excitation is assessed. Thermal conductivity of electronically excited N₂, O₂, N, and O is calculated in the temperature range 200–25 000 K using both rigorous kinetic theory method and simplified formulae. For the kinetic model based on the Boltzmann distribution over internal energy, the effect of varying diameters of excited states is found to be weak up to 20 000 K. Validation of the simple Eucken formula with different factors f_{int} against experimental data and exact kinetic theory calculations is carried out. In the temperature range 3000–20 000 K, a good accuracy of the modified Eucken correction with $f_{\text{int}} = 1.42$ is shown. We recommend using this value for the high-temperature hypersonic air flow simulations. For molecular species at lower temperatures, the value proposed by Hirschfelder $f_{\text{int}} = 1.328$ is recommended.

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