



## Research paper

## On the applicability of simplified state-to-state models of transport coefficients



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## ARTICLE INFO

## Article history:

Received 18 July 2017

In final form 19 August 2017

Available online 22 August 2017

## Keywords:

State-specific

Thermal conductivity

Bulk viscosity

## ABSTRACT

Thermal conductivity and bulk viscosity coefficients are studied in the state-to-state approximation to assess the importance of accounting for rovibrational coupling and increasing diameters of vibrationally excited molecules. Transport coefficients are computed in binary mixtures for a wide temperature range, and compared to those obtained for the rigid rotator model. It is shown that accounting for rovibrational coupling leads to a twofold decrease in the bulk viscosity coefficient and a 5–7% decrease in the thermal conductivity coefficient; accounting for variable diameters has no effect on the bulk viscosity, but leads to a larger decrease in the thermal conductivity.

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## 1. Introduction

Various approaches to modeling of strongly non-equilibrium flows exist, such as the one-temperature, multi-temperature, and state-to-state approximations. Of these, the state-to-state approximation, which assumes that characteristic times of vibrational energy transitions and chemical reactions are of the same order of magnitude as the gas-dynamic timescale, is the most detailed, since it can describe arbitrary vibrational energy distributions. For strongly non-equilibrium flows, the state-to-state description, while computationally expensive, provides the most accurate results and the best agreement with experimental data [1,2]. Due to significant increases in computational power, state-specific approaches have begun to receive more interest lately, including simulations which account not only for state-specific vibrational distributions, but also non-equilibrium rotational distributions [3–5], where the role of vibrational-rotational transitions may have a noticeable effect on the transport coefficients [6]. However, considering all the rovibrational states is very expensive from a computational point of view, and various energy binning approaches for the rovibrational levels have been proposed, both for CFD (Computational Fluid Dynamics) and DSMC (Direct Simulation Monte Carlo) simulation methods [7–10]. Despite this, the state-to-state simulations of viscous flows require the computation of state dependent transport coefficients obtained by solving large linear transport systems. While applying the state-to-state approx-

imation to inviscid 2-dimensional flows has been shown to be feasible, coupling the state-to-state approximation transport equations with the state-dependent transport coefficients computation can lead to an enormous increase in computational time. Given the growing interest in performing state-specific simulations of rarefied gas flows, it is of interest whether the rovibrational coupling significantly affects transport coefficients and whether simplified algorithms can be used to compute them, saving a large amount of computational effort.

Simplified state-to-state models for transport coefficients have been developed [11], which are based on two assumptions: (1) the molecular diameters are independent of the vibrational level, and (2) the molecules are rigid rotators, that is, their rotational energy is independent of the vibrational state. The influence of variable molecular diameters on the transport coefficients has been studied in [12,13] for gases with vibrational excitation and in [14,15] for electronically excited gases. It has been shown that accounting for the change in molecular diameter for vibrationally excited molecules has a small influence on the transport coefficients. For electronically excited gases, the influence of the variable diameter is more important [14,15]. However, up till now, no study of the importance of the second simplifying assumption (that the molecules are rigid rotators) has been performed.

The objectives of the present work are to compute thermal conductivity and bulk viscosity coefficients in the state-to-state approximation, taking into account the coupling between rotational and vibrational degrees of freedom and increasing of molecular diameter with vibrational energy, and to compare the results to those obtained in the frame of a commonly used simplified model of rigid rotator with fixed molecular size and constant

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specific heat. The calculations are performed for different mixture compositions in a wide temperature range (up to 40,000 K), so as to assess the role of the coupling under various conditions, including high-temperature conditions typical for high-velocity atmospheric re-entry problems [16,17]. The work is done within the framework of the modified Chapman-Enskog method [18], applicable for description of slip and continuum regimes, i.e., for Knudsen numbers in the range 0.0001–0.25, which corresponds to most atmospheric re-entry problems.

## 2. State-to-state approximation

The state-to-state model, valid when the rates of vibrational and chemical relaxation are of the same order as the rate of change of macroscopic flow variables, gives the following set of transport equations [18]:

$$\frac{dn_i}{dt} + n_{ci} \nabla \cdot \mathbf{v} + \nabla \cdot (n_{ci} \mathbf{V}_{ci}) = R_{ci}, \quad i = 0, \dots, L_c, \quad c = 1, \dots, L, \quad (1)$$

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla \cdot \mathbf{P}, \quad (2)$$

$$\rho \frac{dU}{dt} = -\nabla \cdot \mathbf{q} - \mathbf{P} : \nabla \mathbf{v}, \quad (3)$$

where  $n_{ci}$  is the number density of molecules of species  $c$  at vibrational level  $i$ ,  $\mathbf{v}$  is the flow velocity,  $\mathbf{V}_{ci}$  is the diffusion velocity of molecules of species  $c$  at vibrational level  $i$ ,  $R_{ci}$  is the relaxation term describing the change in the number density of species  $c$  with vibrational state  $i$  due to vibrational energy transitions and chemical reactions,  $\mathbf{P}$  is the pressure tensor,  $U$  is the specific total energy,  $\mathbf{q}$  is the heat flux.  $L_c$  is the number of vibrational levels of molecular species  $c$ ,  $L$  is the number of species in the mixture.

The specific total energy is given by the following expression:

$$\rho U = \frac{3nkT}{2} + \sum_{ci} \langle \varepsilon^{ci} \rangle_{rot} n_{ci} + \sum_{ci} \varepsilon_i^c n_{ci} + \sum_c \varepsilon_c n_c. \quad (4)$$

Here  $\rho$  is the density of the mixture,  $n$  is the number density of the mixture,  $k$  is the Boltzmann constant,  $T$  is the gas temperature,  $\langle \varepsilon^{ci} \rangle_{rot}$  is the average rotational energy of molecule of species  $c$  at vibrational level  $i$ ,  $\varepsilon_i^c$  is the vibrational energy of level  $i$  of molecular species  $c$ ,  $\varepsilon_c$  is the formation energy of species  $c$ ,  $n_c$  is the number density of species  $c$ . The average rotational energy is defined as

$$\langle \varepsilon^{ci} \rangle_{rot} = \frac{1}{\sigma} \frac{1}{Z_{rot}^{ci}} \sum_j s_j^{ci} \varepsilon_j^{ci} \exp\left(-\frac{\varepsilon_j^{ci}}{kT}\right), \quad (5)$$

where  $\varepsilon_j^{ci}$  is the rotational energy of level  $j$  of molecular species  $c$  at vibrational level  $i$ ,  $s_j^{ci} = 2j + 1$  is the degeneracy of rotational state  $j$ ,  $\sigma$  is a symmetry factor, equal to 1 for heteronuclear and 2 for homonuclear molecules, correspondingly, and  $Z_{rot}^{ci}$  is the rotational partition function:

$$Z_{rot}^{ci} = \frac{1}{\sigma} \sum_j s_j^{ci} \exp\left(-\frac{\varepsilon_j^{ci}}{kT}\right). \quad (6)$$

In the present work, we use the following expressions for the vibrational and rotational energies [19,20]:

$$\frac{\varepsilon_i^c}{hc} = \omega_e^c \left(i + \frac{1}{2}\right) - \omega_e^c x_e^c \left(i + \frac{1}{2}\right)^2 + \omega_e^c y_e^c \left(i + \frac{1}{2}\right)^3 + \omega_e^c z_e^c \left(i + \frac{1}{2}\right)^4, \quad (7)$$

$$\frac{\varepsilon_j^{ci}}{hc} = \left(B_e^c - \alpha_e^c \left(i + \frac{1}{2}\right)\right) j(j+1), \quad (8)$$

where  $h$  is Planck's constant,  $c$  is the speed of light, and  $\omega_e^c, \omega_e^c x_e^c, \omega_e^c y_e^c, \omega_e^c z_e^c, B_e^c, \alpha_e^c$  are spectroscopic constants. The number of vibrational levels of molecular species  $c$  is determined from the condition that the vibrational energy must not exceed the dissociation energy of the species  $D_c$ :

$$\varepsilon_{L_c}^c < D_c \leq \varepsilon_{L_c+1}^c, \quad (9)$$

while the number of rotational levels  $L_{rot,ci}$  at each vibrational level  $i$  is determined in a similar manner, but taking into account the vibrational energy:

$$\varepsilon_{L_{rot,ci}}^{ci} < D_c - \varepsilon_i^c \leq \varepsilon_{L_{rot,ci}+1}^{ci}. \quad (10)$$

If we assume that  $\alpha_e^c = 0$  and that the number of rotational levels is independent of the vibrational level ( $L_{rot,ci} = L_{rot,c0} = L_{rot,c}$ ), the rotational degrees of freedom are independent of the vibrational degrees of freedom, and the molecule is a so-called "rigid rotator".

Constitutive equations for the diffusion velocities, stress tensor and heat flux in the first-order approximation of the the generalized Chapman-Enskog method are as follows [18]:

$$\mathbf{V}_{ci} = -\sum_{dk} D_{cidk} \mathbf{d}_{dk} - D_{T_{ci}} \nabla \ln T, \quad (11)$$

$$\mathbf{P} = (p - p_{rel}) \mathbf{I} - 2\eta \mathbf{S} - \zeta \nabla \cdot \mathbf{v} \mathbf{I}, \quad (12)$$

$$\mathbf{q} = -\lambda' \nabla T - p \sum_{ci} D_{T_{ci}} \mathbf{d}_{ci} + \sum_{ci} \left( \frac{5}{2} kT + \langle \varepsilon^{ci} \rangle_{rot} + \varepsilon_i^c + \varepsilon_c \right) n_{ci} \mathbf{V}_{ci}. \quad (13)$$

where  $D_{cidk}, D_{T_{ci}}$  are vibrational state-specific diffusion and thermal diffusion coefficients,  $p = nkT$  is the pressure,  $p_{rel}$  is the relaxation pressure,  $\eta$  is the shear viscosity coefficient,  $\zeta$  is the bulk viscosity coefficient,  $\lambda'$  is the partial thermal conductivity coefficient,  $\mathbf{I}$  is a unit tensor,  $\mathbf{S}$  is the rate-of-shear tensor, and  $\mathbf{d}_{dk}$  are diffusive driving forces.

Since in the present work we are interested in the effect of the coupling between rotational and vibrational degrees of freedom on the bulk viscosity coefficient  $\zeta$  and the thermal conductivity coefficient  $\lambda'$ , we shall forego the definitions of other transport coefficients, for more detail and methods of their calculation, the reader is referred to [18].

The generalized Chapman-Enskog method allows one to construct a numeric scheme for the calculation of the transport coefficients, by expanding the first-order correction to the distribution function in series of Sonine and Waldmann-Trübenbacher polynomials, and expressing the transport coefficients via the expansion coefficients.

The thermal conductivity coefficient  $\lambda'$ , which describes energy transfer due to elastic collisions and translational-rotational and rotational-rotational energy exchanges in the state-to-state approach, can be expressed in terms of these expansion coefficients  $a_{ci,10}, a_{ci,01}$  in the following way [21]:

$$\lambda' = \sum_{ci} \frac{5}{4} k \frac{n_{ci}}{n} a_{ci,10} + \sum_{ci} \frac{m_c}{2} \frac{n_{ci}}{n} c_{rot,ci} a_{ci,01}, \quad (14)$$

where  $m_c$  is the mass of molecular species  $c$ , and the specific heat of rotational degrees of freedom is defined as

$$c_{rot,ci} = \frac{\langle (\varepsilon^{ci})^2 \rangle_{rot} - \langle \varepsilon^{ci} \rangle_{rot}^2}{m_c k T^2}. \quad (15)$$

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