On the accuracy of non-equilibrium transport coefficients calculation

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Abstract

The algorithms of non-equilibrium transport coefficients calculation in reacting gas mixtures are discussed. The influence of the molecular interaction potential on the transport properties is estimated in the various temperature ranges. © 2001 Published by Elsevier Science B.V.

1. Introduction

In the present paper some peculiarities of the transport coefficients calculation are discussed. The transport kinetic theory of polyatomic gases has been widely developed since the famous work of Eucken [1]. A great amount of papers and monographs are devoted to the mathematical study of dissipative properties in pure gases and gas mixtures. Transport processes under assumption of local thermal equilibrium are investigated in Refs. [2–9], transport coefficients in chemical equilibrium are given in Refs. [10–12]. Essentially non-equilibrium transport properties are considered in Refs. [9,12–17]. In these studies the efficient algorithms for the transport coefficients calculation are proposed, thermal conductivity, viscosity and multi-component diffusion coefficients are calculated with a high accuracy. However, up to now, in the numerical codes simulating various Navier–Stokes problems the quite trivial models of transport properties are usually introduced, this can give a noticeable error in the predicted values of heat fluxes. In gas mixtures the simplified expressions for the transport coefficients like Wilke and Mason–Saxena approximations for viscosity and thermal conductivity, respectively, are often used. The pure species transport coefficients are usually deduced from the constant Prandtl, Lewis and Schmidt numbers using experimental data or semi-empirical formulas for the viscosity coefficient. And even when more accurate methods of

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transport coefficients evaluation are applied, the rather old data on the collision integrals and molecular interaction potentials may lead to a considerable accuracy loss.

In this paper we discuss briefly three basic parts in the procedure of non-equilibrium transport coefficients calculation, which affect considerably their accuracy: (1) the choice of appropriate kinetic approach; (2) algorithms of linear transport system solution; (3) models of molecular interaction. The main focus is on the influence of molecular interaction potential and its parameters on the transport properties. Different potentials are studied, and the practical recommendations on the choice of potential and parameters for various air species at various conditions are proposed.

2. Kinetic models and algorithms

The method of transport coefficients evaluation must be chosen in accordance to the specific flow conditions. The majority of the models of non-equilibrium transport properties is based on the quasi-stationary one-temperature or multi-temperature distributions over vibrational levels. These distributions are valid under conditions when the characteristic times of chemical reactions exceed essentially the mean time of vibrational relaxation or of the VV vibrational energy exchanges within different modes. The transport terms for a polyatomic gas mixture in the one-temperature approach are given in Refs. [7,9,14], this model is based on the local equilibrium Boltzmann distribution over internal energy. The multi-temperature models for a gas mixture with internal modes and chemical reactions based either on the Boltzmann distribution with vibrational temperature $T_v \neq T$ or on the Treanor distribution are elaborated in Refs. [13–15].

Under high temperature conditions the rates of vibrational energy transitions become comparable with the rates of chemical reactions. It leads to a strong vibrational–chemical coupling, and the simulation of non-equilibrium flows in the frame of quasi-stationary distributions is not longer valid. In this case the detailed state-to-state approach is required: the Navier–Stokes equations must be solved with the equations for vibrational level populations, and the transport terms depend on the non-equilibrium vibrational distributions. The state-to-state kinetic transport theory has been developed in Refs. [16,17].

The procedure for the transport coefficients calculation differs for the various approaches [14]. It occurs due to the two facts. First, the transport coefficients are determined by the different sets of macroscopic parameters: species concentrations and gas temperature in the one-temperature approach, species concentrations, gas temperature and vibrational temperatures of molecular species in the multi-temperature approach, and, finally, gas temperature, vibrational level populations and atomic concentrations in the state-to-state model. Second, the linearized integral operator which determines the bracket integrals depends on the cross sections of the most rapid processes, and these processes are not the same in three approaches considered [14].

Below a simple example is given. A comparison of the results obtained on the basis of state-to-state, multi-temperature and one-temperature models is shown in Fig. 1. The algorithms developed in Refs. [14,16] are applied to the (N_2, N) mixture flow behind a shock wave. The initial conditions are: $T_0 = 293$ K, $p_0 = 100$ Pa, $M_0 = 15$. In Fig. 1(a) the binary diffusion coefficient D_{N_2N} is presented as a function of the distance x from the shock, and in Fig. 1(b) one can see the total heat flux behind the shock. It is seen that the value of diffusion coefficient varies within 50% for different models, this variation is connected with the behavior of macroscopic parameters in the relaxation zone. Similar results are obtained for the remaining transport coefficients. The absolute value of the total heat flux, as it can be expected, decreases approaching the equilibrium, where all three approaches converge. On the contrary, in the beginning of the relaxation zone an essential discrepancy between the heat fluxes calculated using different models is observed. The one-temperature and two-temperature approaches give considerably lower values of the heat flux just behind the shock front.

It is evident that a comparison with experimental data is necessary for the validation of dif-
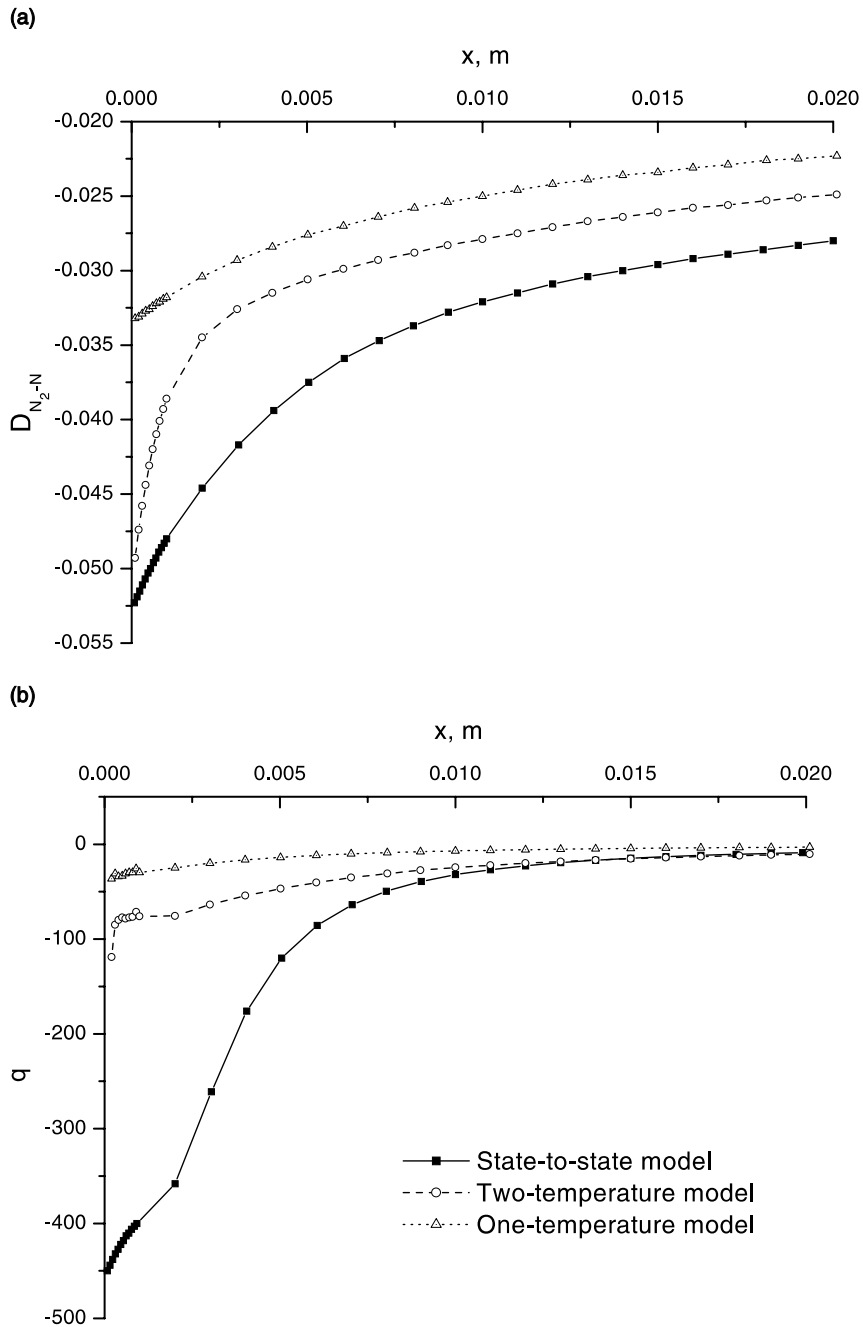
(a)

(b)

Fig. 1. Binary diffusion coefficient, D_{N_2N} (m²/s) (a), and total heat flux, q (kW/m²) (b) calculated using different approaches as functions of x.

ferent models. Unfortunately, the experimental data on the heat transfer in the considered flow are not available. Nevertheless, it can be pointed out that only state-to-state description gives an adequate shape of vibrational distributions in strongly non-equilibrium conditions. For instance,

in papers [18–20] the experimentally measured vibrational distributions in optically pumped CO and other diatomic gases are compared with the state-to-state and quasi-stationary distributions. An excellent correlation between the state-to-state and measured distributions is observed, whereas all quasi-stationary models give a very poor agreement. This fact is a good reason to believe that the results of state-to-state simulation of the heat transfer in essentially non-equilibrium conditions will be much more accurate compared to the results obtained by means of quasi-stationary one-temperature or multi-temperature models.

Although an essential difference in the transport coefficients computation in various approaches exists, qualitatively the main algorithm remains the same. Thus, in all cases transport coefficients are found as solutions of similar linear algebraic systems derived from orthogonal polynomial expansions of the perturbed distribution functions [6,7,9,14]. The coefficients of the algebraic systems are the bracket integrals determined by the linearized integral operator of the most frequent processes. Applying some assumptions described in details in Refs. [7,9,14,16], the bracket integrals can be reduced to the combinations of collision integrals (see Refs. [3,4,9] for the definition).

At this step the procedure of transport coefficients calculation can be developed in two directions: the first one consists in analysis of linear transport systems and derivation of the approximate mixture-averaged formulas. These formulas are based on some additional assumptions and therefore their accuracy is not always high. On the other hand, mixture-averaged formulas express transport coefficients of a mixture in terms of pure species transport coefficients and thus permit to reduce the computational cost. Such approximations have been introduced by Wilke [21] and Mason and Saxena [22] for the viscosity and thermal conductivity coefficients, respectively, and more recently in Refs. [9,23,24] for all transport coefficients. For binary mixtures at low temperatures the approximate results given by Wilke and Mason–Saxena formulas correlate well with experimental data, but for complex mixtures and high temperature conditions their accuracy should

be further validated (see Ref. [9] for a detailed discussion).

More precise algorithms of transport coefficients calculation require solution of transport linear systems. The most evident way is the direct solution of algebraic systems by the Cramer's rule which allows one to express the transport coefficients explicitly as ratios of determinants. This algorithm is used in Refs. [2–4,7] for mixtures in thermal and chemical equilibrium and in Refs. [14,16] for various non-equilibrium conditions. In particular, in papers [15,17] the transport coefficients have been computed in the generalized multi-temperature and state-to-state approaches for shock heated gas mixtures. Nevertheless, solving the linear systems by the Cramer method is extremely computationally expensive. Another direct method using the Gaussian elimination is considered, for instance, in Ref. [24]. This method is noticeably less time consumable but still not satisfactory as a majority of direct methods. Recently the mathematical properties of transport linear systems have been studied carefully in Ref. [9] and new efficient iterative algorithms have been proposed. This technique provides very fast and accurate evaluation of transport properties.

Whereas the method described in Ref. [9] gives rather good results for the one-temperature and multi-temperature models, the calculation of state-to-state transport coefficients remains very slow because of the great amount of linear algebraic equations solved at each step of numerical simulation. In order to deduce the thermal conductivity and viscosity coefficients one must solve systems of $3N_v + 2L_{at}$ and N_{tot} equations respectively (N_{tot} is the total number of chemical and vibrational species: $N_{tot} = L_{at} + N_v$, L_{at} is the number of atomic species, $N_v = \sum_{c=1}^{L_{mol}} L_c$ is the total number of vibrational states, L_{mol} is the number of molecular species, L_c is the total number of vibrational energy levels in molecular species c). Besides that there are $N_{tot}(N_{tot} + 1)/2$ independent diffusion coefficient, each of them is found from the system of N_{tot} equations. It is obvious that such a scheme cannot be used in numerical simulations. In the recent paper [25] a simplified procedure of the state-to-state transport coefficients calculation is proposed. It permits to reduce essentially the

number of transport coefficients and algebraic equations, and at the same time, to maintain the advantages of the state-to-state transport theory. In particular, using these scheme, the thermal conductivity and viscosity coefficients are computed from the systems of $3L_{mol} + 2L_{at}$ and $L = L_{mol} + L_{at}$ equations; the number of independent diffusion coefficients is diminished to $N_v + L_{mol} + L(L+1)/2$, each coefficient is found from the system of only $L + 1$ equations. Such a simplification allows one to implement the state-to-state transport theory to the computational fluid dynamics and therefore to get more accurate results compared to the ones given by one-temperature and multi-temperature approaches.

3. Interaction potential and transport coefficients

Another important source of error in the evaluation of transport terms is the old data on the molecular interaction potentials for the computation of collision integrals. Indeed, for the exact solution of the transport linear systems as well as for the use of approximate mixture-averaged expressions, one needs the collision integrals. Since the work of Hirschfelder et al. [3] a large amount of collision integral calculations has been performed for different potential models: Lennard-Jones, Buckingham, Morse, Stockmayer, repulsive ones, etc. One can find the tables of collision integrals in Refs. [3,4,26], the approximate interpolating expressions are also given by many authors (see, for instance, Refs. [27–29]). Nevertheless, these data require an additional justification. The specific potential models are valid only in a limited temperature range, and the potential parameters should be chosen carefully in accordance with the experimental results.

Let us consider first the equilibrium transport properties of air species. We start the discussion from the transport coefficients of NO molecule which is less investigated than the remaining air components. The influence of the potential on the transport properties of N_2 and O_2 have been studied, for instance, in Refs. [16,30,31]. In the present study the shear viscosity η and heat conductivity coefficient λ of pure NO have been cal-

culated on the basis of the following models for the elastic collision integrals: the Lennard-Jones potential with the parameters σ (collision diameter) and ϵ/k (potential well depth) reported in Refs. [23,32]. The values of the parameters can be taken also from Refs. [3,33]. However, it is shown in Refs. [16,30] that using the data of Hirschfelder [3] leads to a significant underestimation of the transport coefficients at high temperatures. On the other hand, the data from Ref. [33] give results close to the ones obtained with the parameters taken from Ref. [23], that is why we limit our consideration by only two parameter sets. Two other models used for calculations are the repulsive potential with the parameters given by Ref. [34], and also approximate formulas for the collision integrals proposed in Ref. [29]. The results are compared with the experimental data [35–37], with the Blottner approximation for the viscosity coefficient [38], and with the reference data of American Society of Mechanical Engineers for the heat conductivity coefficient [39].

Figs. 2 and 3 plot the shear viscosity and heat conductivity coefficients calculated in the different temperature intervals ($200 < T < 1500$ K and $1500 < T < 10\,000$ K respectively). It is seen that the repulsive potential gives an essential deviation from the experimental data in the low temperature range ($T < 500$ K) where the main role in the interaction between particles belongs to the attraction forces. On the contrary, for the temperatures $200 < T < 1000$ K the Lennard-Jones potential fits very well the experimental results. The accuracy lies within 2% for the parameters from Ref. [32] (a mean error is about 0.8%), and within 5% for the parameters reported in Ref. [23]. The Blottner approximate formula [38] underestimates the viscosity coefficient up to 5–7%, and the Capitelli approximation [29] leads to a slight overestimation of η (about 3–4%). Finally, for the low temperature ($T < \epsilon/k$) the Lennard-Jones potential with the parameters from Ref. [32] is recommended for the shear viscosity computation.

The same choice of the model can be suggested also for the calculation of heat conductivity in the low temperature interval (see Fig. 3(a)). However, for this coefficient the discrepancy between the experimental and calculated values is higher. The
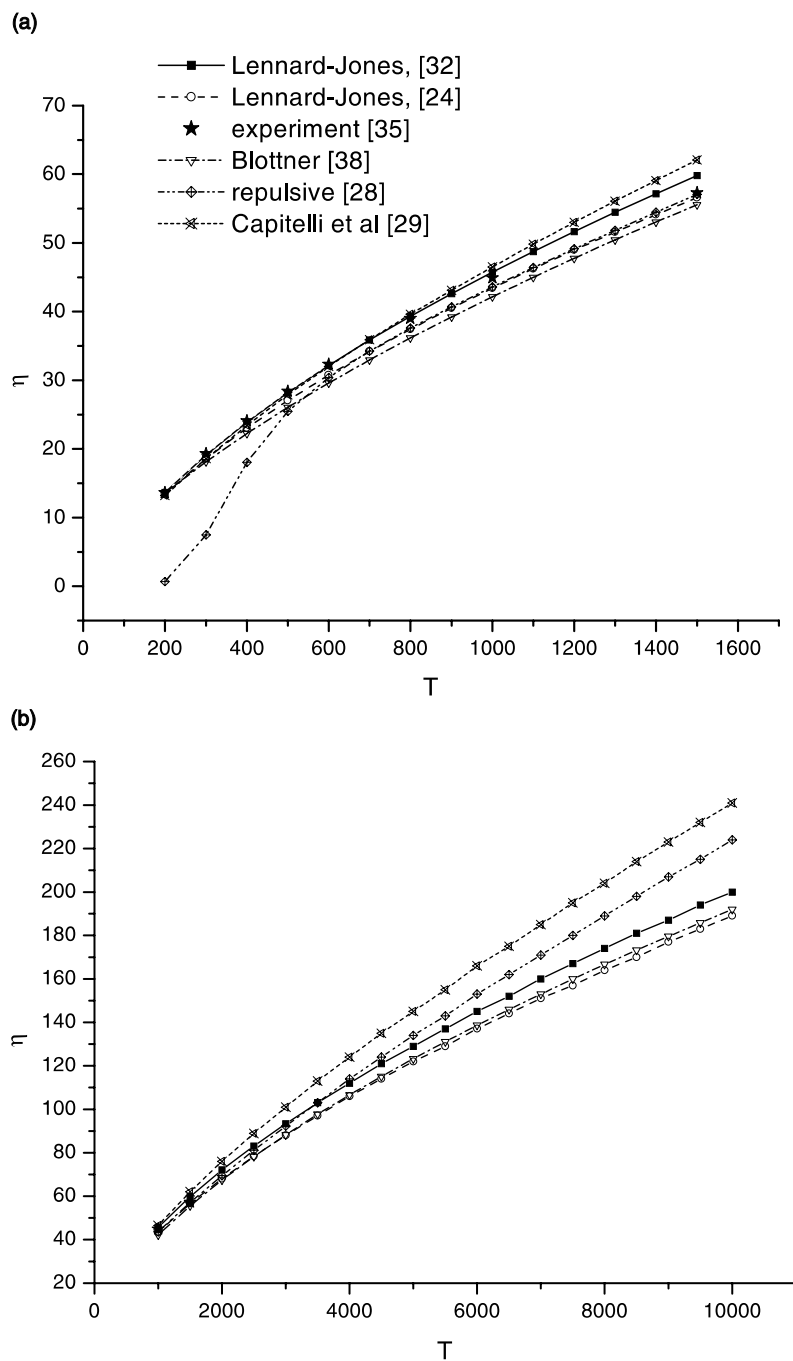
Fig. 2. Shear viscosity coefficient, η (10^{-6} Pa s) of NO at low temperatures (a) and at high temperatures (b).

Lennard-Jones potential with the parameters proposed by Ref. [32] gives a mean error about 3.5%, using the parameters from Ref. [23] enlarges the deviation up to 7–9%, the approximate ex-
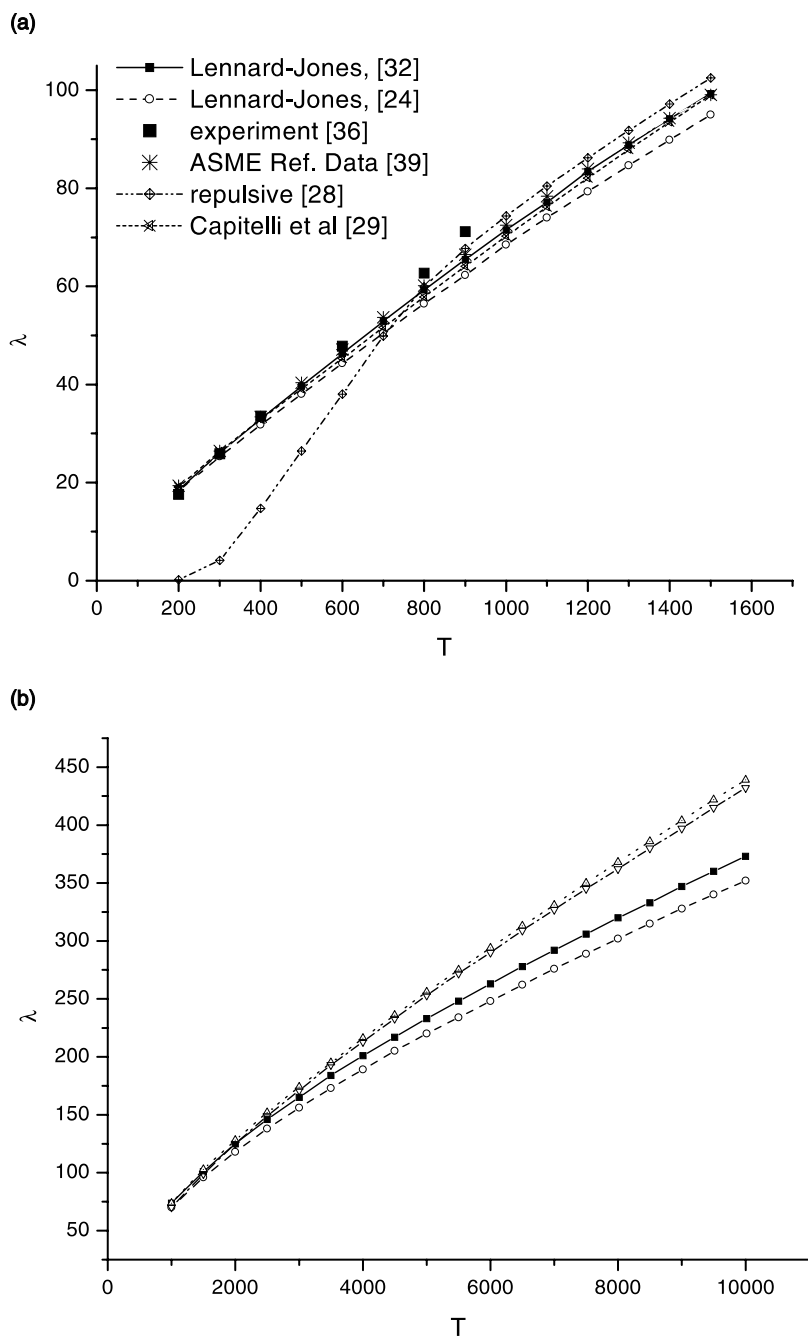
(a)

(b)

Fig. 3. Thermal conductivity coefficient, λ (10^{-3} W/m K) of NO at low temperatures (a) and at high temperatures (b).

pressions from Ref. [29] also lead to some under-estimation of λ (about 6%). One should mention here that for N_2 and O_2 molecules the best fit with experimental data at the low temperature range is achieved using the Lennard-Jones potential with parameters given in Ref. [23]. The recommended

Table 1
Parameters for the Lennard-Jones potential

Interaction	σ (Å)	ϵ/k (K)	Ref.
N$_2$–N$_2$	3.621	97.5	[23]
O$_2$–O$_2$	3.458	107.4	[23]
NO–NO	3.47	119	[32]
N–N	3.298	71.4	[23]
O–O	2.75	80	[23]

parameters of the Lennard-Jones potential for low temperature air species are summarized in Table 1. The parameters for the interaction between dissimilar species can be calculated using the rules described in Ref. [4].

With temperature rising the estimation of the model accuracy becomes difficult because of the lack of experimental data, especially for the heat conductivity. It is known [29,31,34,40] that at high temperature the Lennard-Jones potential does not give satisfactory results, and it is necessary to take into account the repulsive forces. The best way to proceed is to choose the repulsive potential in the form proposed by Cubley and Mason [40]: $V = V_0 \exp(-\beta r)$, r is the distance between interacting particles, V_0, β are the potential parameters. These parameters for different chemical species interaction can be found in Refs. [29,34,40], the values used in the present paper are given in Table 2. In the paper [28] the interpolating formulas for the collision integrals computed on the basis of the

Table 2
Parameters for the repulsive potential

Interaction	V_0 (eV)	β (Å^{-1})	Ref.
N$_2$–N$_2$	415.7	2.573	[34]
N$_2$–O$_2$	2316	3.267	[34]
N$_2$–NO	52.38	1.761	[34]
N$_2$–N	184.9	2.614	[34]
N$_2$–O	860.4	3.331	[34]
O$_2$–O$_2$	1.485×10^4	3.964	[34]
O$_2$–NO	6373	3.644	[34]
O$_2$–N	905.7	3.32	[34]
O$_2$–O	4530	4.039	[34]
NO–NO	2678	3.303	[34]
NO–N	428.6	2.983	[34]
NO–O	2142	3.717	[34]
N–N	86.0	2.68	[40]
N–O	348.2	3.41	[40]
O–O	1410	4.14	[40]

repulsive potential are obtained, these formulas are applied for the calculations.

In order to validate our results we have computed the shear viscosity coefficient of five components partially dissociated air. In this case the experimental results up to 6000 K are available in Ref. [37]. In Fig. 4 the results obtained by means of the models [26–29], are compared with the experimental data and with the calculations on the basis of the Lennard-Jones potential. Using the models proposed by Refs. [28,29] leads to a good agreement with experimental data in the whole temperature range, while the Lennard-Jones potential and the model proposed in Ref. [27] underestimate significantly the viscosity coefficient. The model of Yun and Mason [26] also predicts the values of viscosity close to experiment, however, in the temperature interval $3000 < T < 6000$ K its accuracy is worse compared to the models Refs. [28,29]. At $6000 < T < 10\,000$ K the results of this models and repulsive models given by Refs. [28,29] converge.

In Figs. 2(b) and 3(b) the shear viscosity and heat conductivity coefficients of NO are presented for high-temperature. In both cases the Lennard-Jones potential with different parameters as well as the Blottner formula for the shear viscosity lead to lower values of transport coefficients compared to the models [28] and [29]. The repulsive potential [28] with parameters from [34] and the model of Capitelli [29] give approximately the same values of the heat conductivity. In the absence of experimental data on high temperature transport coefficients of NO and other separate air species it is difficult to decide which model gives the most reliable results. Nevertheless, one can expand the results obtained above for partially dissociated air to the case of pure species. It is shown that the Lennard-Jones potential underestimates significantly the high temperature air viscosity coefficient. One can suppose that the same effect takes place in pure gases. Finally, in high temperature interval $(T > \epsilon/k)$ we recommend the repulsive model [28] for practical use.

The above discussion concerns the role of different potentials under chemically and thermal equilibrium conditions. In order to check the non-equilibrium case, the total energy flux behind
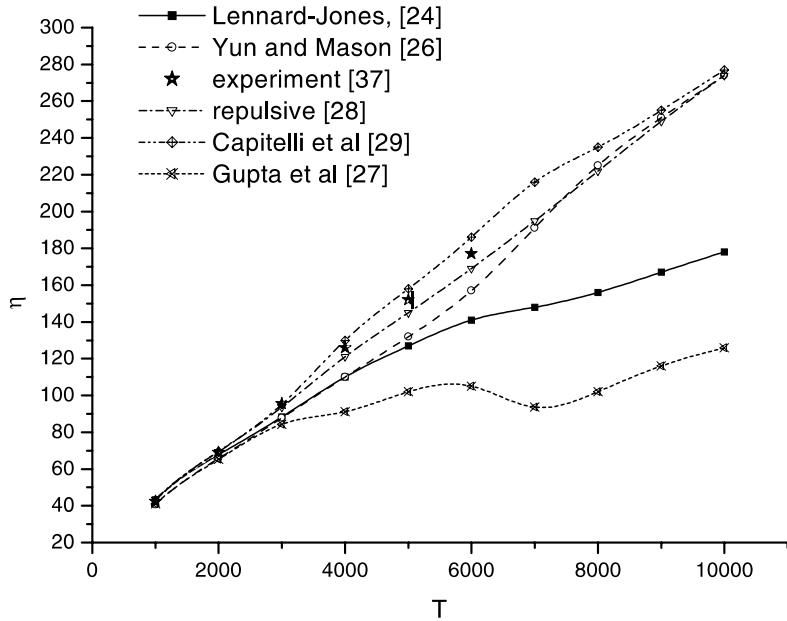
Fig. 4. Shear viscosity coefficient, η (10^{-6} Pa s) of partially dissociated air.

a shock wave has been computed using the Lennard-Jones potential and the repulsive potential (formulas of Ref. [28]) in the most detailed state-to-state approach. The flow conditions are given in the previous section. The comparison is shown in Fig. 5. A noticeable discrepancy is found between
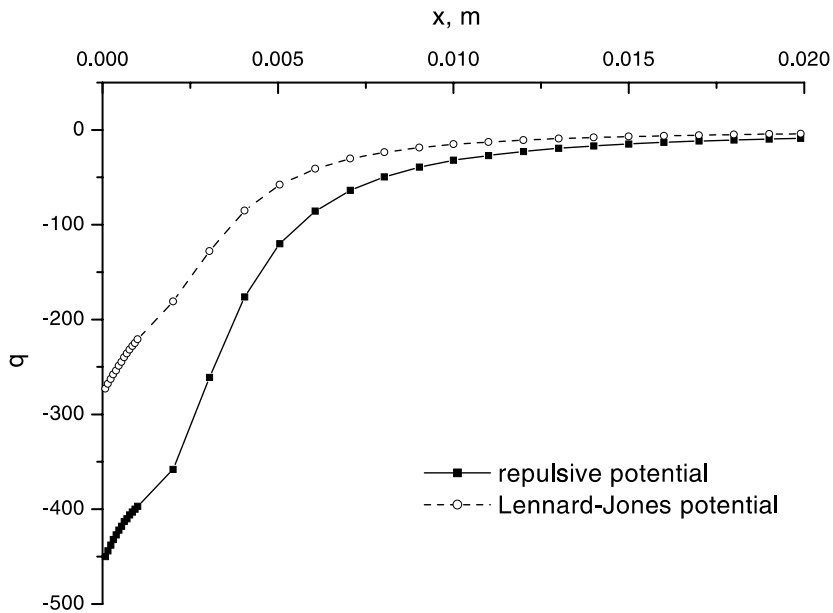

Fig. 5. Heat flux q, kW/m^2, as a function of x.

the two fluxes, the heat flux calculated using the Lennard-Jones potential is about twice less than the one computed with the repulsive potential. Therefore the proper choice of the interaction potential is very important for the correct evaluation of the heat transfer in reactive gas flows.

4. Conclusions

The transport properties in a non-equilibrium reacting gas mixture flow are considered on the basis of the kinetic theory. Three main factors influencing the accuracy of transport coefficients are discussed: the kinetic approach; the algorithm of linear transport systems solution; the model of molecular interaction. The state-to-state kinetic approach is expected to be more precise under strongly non-equilibrium conditions compared to quasi-stationary models. The algorithm proposed in Ref. [9] provides the most rapid and accurate solution of transport linear systems. The effect of the molecular interaction model on the transport coefficients and heat flux also is found to be important. The Lennard-Jones potential with parameters from Ref. [23] (for N_2 and O_2) and from [32] (for NO) gives the best accuracy for low temperatures ($T < \epsilon/k$), for higher temperature the repulsive potential from Ref. [28] with parameters given in Ref. [34] or the data from Ref. [29] are recommended.

Acknowledgements

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