The Tang-Toennies potentials for the Boltzmann collision integrals

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Abstract. The Tang-Toennies model of interatomic potentials described realistically both attractive and repulsive parts are adopted for collision integrals in direct methods of solving the Boltzmann equation. The direct approach for solving the Boltzmann equation in framework of the UFS scheme is used. Collision integrals with the Tang-Toennies potential are evaluated. The shock wave structure is considered. A case of argon is studied and compared with known experiment.

Keywords: The Boltzmann equation, the Tang-Toennies interatomic potential, shock wave structure.
PACS: 51.10+y, 05.20Dd

INTRODUCTION

The problem of the correct description of processes in a rarefied gas at high temperatures is important. It is known that the Lennard-Jones potential is adequate for description of transport coefficients for temperatures up to 1000 K. For greater values of temperatures it is desirable to consider the other types of interatomic potentials. On the other hand, it has been noted in [1] that a shock wave structure for Mach numbers M>5 is not described adequately by the Maitland-Smith potential (that is caused by inaccuracy in the shape of this potential for high collision energies, corresponding to temperatures greater 2000 K).

The first features of the model by Toennies, based on a more fundamental basis in comparison with empirical models such as the Lennard-Jones potential, has been reported in RGD Symposium in 1974 [2], but through many years after some efforts the potential has the simple form with coefficients obtained in theoretical and experimental considerations. Therefore we intend to use the so-called Tang-Toennies (TT) model [3,4].

It is known that there are recent attempts to construct improved empirical potentials which gave better description of transport properties at high temperatures than the Lennard-Jones (12,6) potential, see, e.g. [5], where the potential with a more soft repulsive part, namely, (8, 6) is considered. On the other hand, the model potential of the VHS type are popular , especially in DSMC approaches. Such simple models are very important when studying complex problems of rarefied gas dynamics. Nevertheless, from our point of view, it is desirable to investigate more physical adequate models, constructed (in general parts) on the principles of quantum mechanics.

The direct method of solving the Boltzmann equation which developed in course of many years (see, e.g. [6]) is used now in a new approach combined some previous scheme, this method [7] applies in particular adaptive mesh refinement. Some known potential such as the Lennard-Jones one is implemented. This solver is used now to introduce the Tang-Toennies potential and to test it at first for simple problems.

The problem of a shock wave structure is studied.

THE TANG-TOENNIES POTENTIAL

Since its introduction predictions of the shapes of van der Waals potentials based on this model have been confirmed for many systems by detailed comparisons with the best available experimental data. In the TT model, the short-range repulsive Born-Mayer potential is added to the long-range attractive potential, which is given by the damped dispersion series

$$V(R) = V_{rep} + V_{att} = Ae^{-bR} - \sum_{n=3}^{N} f_{2n}(bR)\frac{C_{2n}}{R^{2n}},$$

where C_{2n} are the dispersion coefficients. The Born-Mayer range parameter b is the only parameter in the damping functions $f_{2n}(bR)$, for which, as a rule, the following formula to compute the damping functions is used

$$f_{2n}(r) = 1 - e^{-br}\sum_{\mathrm{m}=0}^{2n}\frac{(br)^m}{m!}.$$

They can be also expressed in terms of the incomplete gamma function

$$f_{2n}(r) = 1 - \frac{\Gamma(2n+1, r)}{2n!}.$$

It is often sufficient to take three dispersion coefficients, namely *N=5*. The comparisons in [4] demonstrated that the approximation with *N=5* is an adequate representation of the accurate potential in the van der Waals region. Thus, the simple variant of the TT model requires only five parameters. In addition to the first three leading dispersion coefficients, which are generally well known from theory, two more parameters describing the repulsive potential are required. These Born-Mayer parameters A and b are known from experimentally determined values of the well minimum R_m and the well depth ε. Studies of with many systems indicates that the Born-Mayer repulsive potential is usually a very good approximation. Nevertheless, as mentioned in [4] the Born-Mayer repulsive potential is, of course, only an approximation (in principle the repulsive potential can be obtained a priori from theory, such as from a self-consistent field (SCF) calculation with an additional exchange dispersion correction).

RESULTS OF COMPUTATIONS FOR A SHOCK WAVE

This TT potential is implemented into the collision integral in the framework of the direct solution of the Boltzmann equation (see, e.g. [6]). For evaluating the collision integrals the quasi-Monte Carlo method with the Korobov sequences is used. The collision integrals are considered in the symmetric form of 8-fold integrals. The conservative correction for an arbitrary regular mesh in velocity space applied to the collision integral is used. The approach with a physical adequate model of atom-atom interactions is the general way of description of rarefied gas which is adopted in the UFS solver [7]. Application of e.g. the Lennard-Jones model is restricted by a range of some parameters. So we used this model for computation of the shock wave structure at not very high values of Mach numbers. The comparisons with experimental evidence were made at Mach numbers M=1.59 (Helium, temperature) and M=3.8 (Argon, density) demonstrated a good agreement of results, see [7].

Parameters of the Tang-Toennies potential are taken from [4]. The parameters for argon which are used in computations for this potential are as follows: R_m =7.1, ε x10^4 =4.54 (all values are in atomic units) denote the well minimum and the well depth respectively. Two parameters in the Born-Mayer potential are expressed through these well parameters, namely *A*=748.3, *b*=2.031 (in atomic units). The used dispersion coefficients are

$$C_6 = 64.30,\ C_8 = 1623,\ \ C_{10} = 49060.$$

All values are also in atomic units.

The problem of a shock wave structure is studied. The computations for shock wave structure were performed for Mach numbers M=2, 3, 4, 5, 7, 9. The inverse width of a shock is shown in Fig.1. Our results are shown by crosses. Other results are related to that given in [1]. It is known that, e.g. the Maitland-Smith potential is not very good for Mach numbers M>5 as it can be seen from Fig. 1. One can see that the inverse shock wave width is correctly described by the Tang-Toennies collisions up to Mach number M=9. For this value the inverse width is greater than the width according to the Alsmeyer experiment.

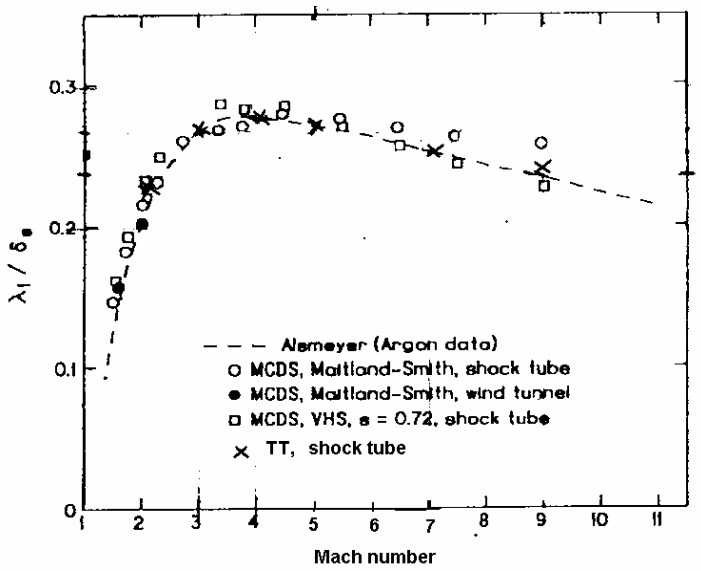

FIGURE 1. Dependence of inverse shock wave width on Mach number.

In Fig. 2 a comparison of the density profiles between a solution by the Boltzmann equation for the Tang-Toennies potential and the experimental data by Alsmeyer is presented, one can see a good agreement of results.

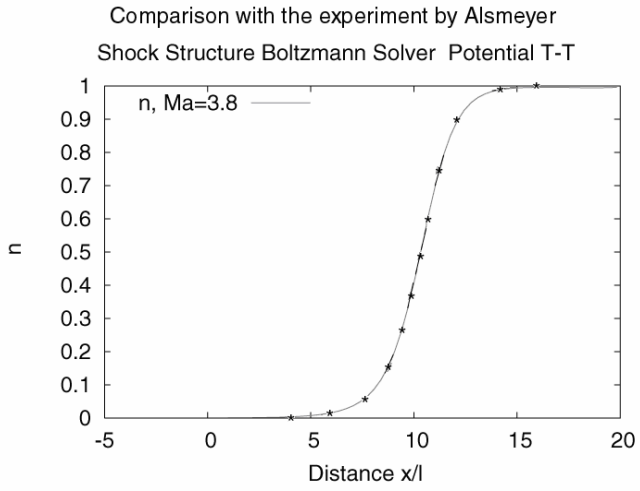

FIGURE 2. Comparison of densities by the experiment (a solid line) and by computations (stars) for M=3.8.

In Fig. 3 density profiles for larger Mach numbers, namely, M=5 and M=7 according to the direct solution of the Boltzmann equation for the Tang-Toennies potential are given.

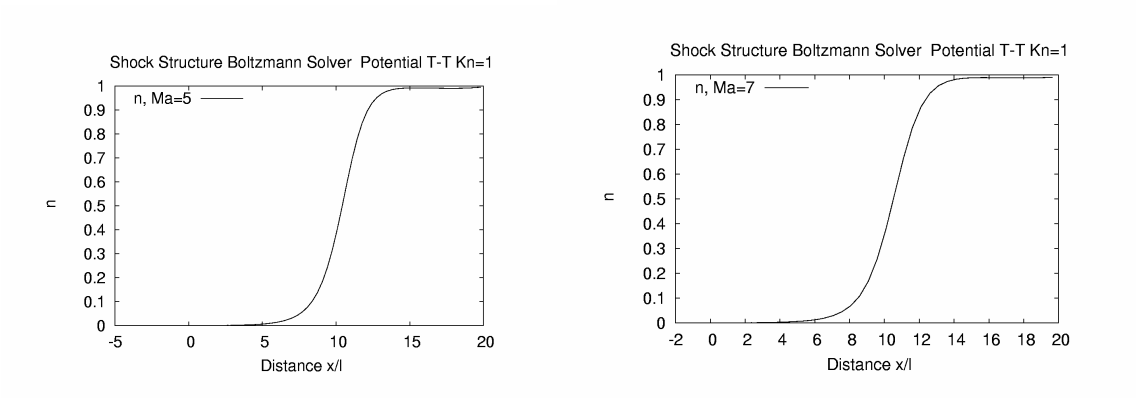

FIGURE 3. Densities for M=5 and M=7.

In Fig. 4-5, for these Mach numbers physically interesting values such as velocity, temperatures and heat flux are shown.

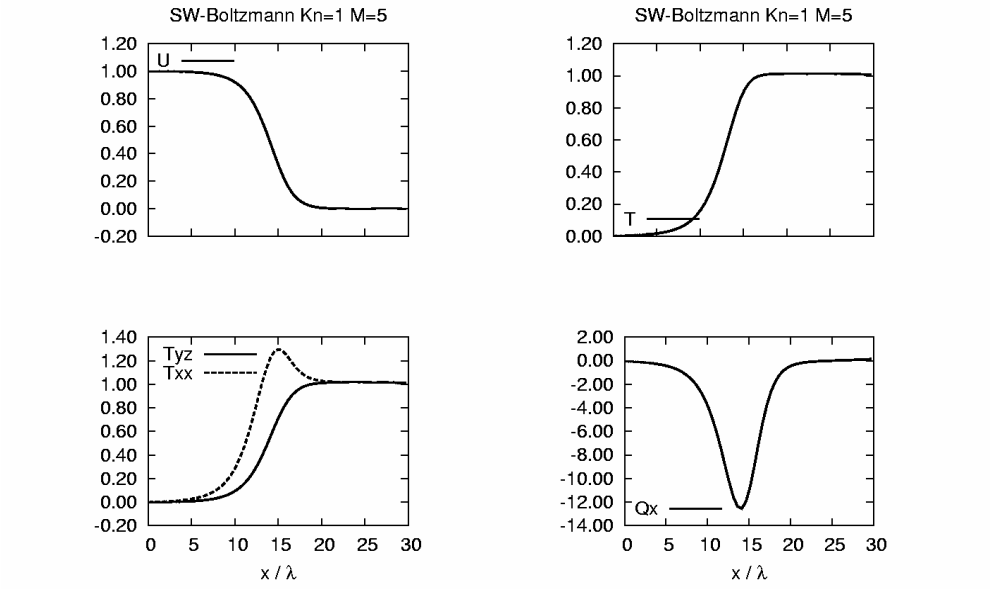

FIGURE 4. Velocity, temperature, longitudinal and transverse temperatures and heat flux at Mach number M=5.

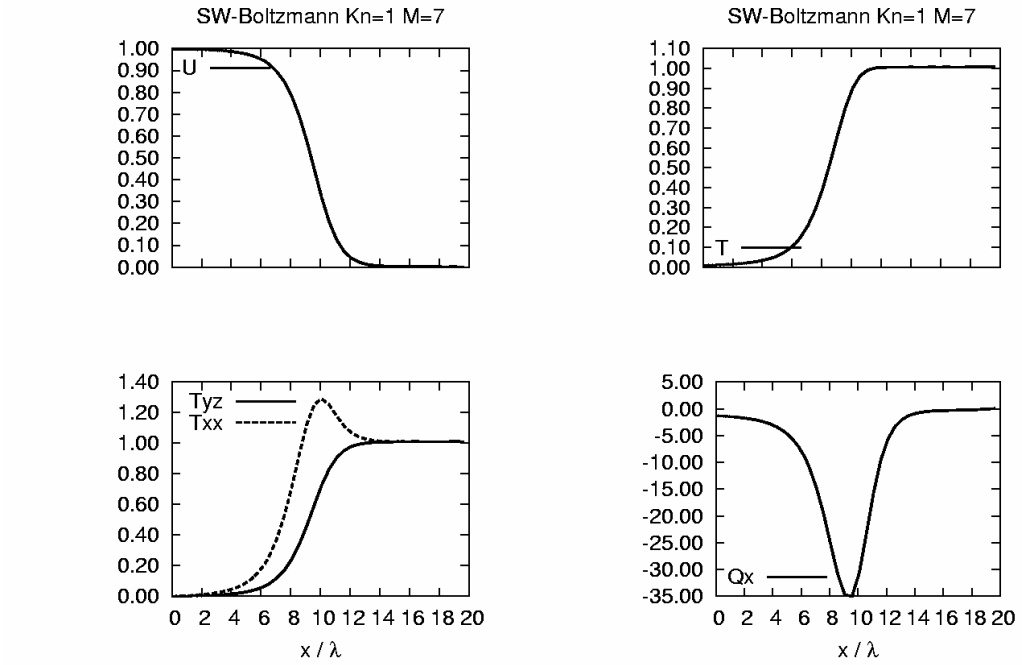

FIGURE 5. Velocity, temperature, longitudinal and transverse temperatures and heat flux at Mach number M=7.

CONCLUDING REMARKS

The first computations of the shock wave structure on the basis of the direct solving the Boltzmann equation with the Tang-Toennies potential provide encouraging results and one can expect to obtain in this way a model describing processes at high energies better than on the basis of the previous models (of course it needs to reproduce results by Muntz et al. for the Maitland-Smith potential by means of the direct solving the Boltzmann equation). Nevertheless, for large values of Mach numbers (M~10) the shock width is less than that according to experimental evidence. The other elaboration is proposed in [8] where for high temperature the Born-Mayer potential is used. Here the transport coefficients are determined by means of the Tang-Toennies potential by computing the binary collision integrals according to the Chapman-Enskog method. In this paper some modifications for the Tang-Toennis potential are proposed. The first one concerns changing the damping function, namely

$$f_{2n}(r) = 1 - e^{-zbr} \sum_{m=0}^{2n} \frac{(zbr)^m}{m!},$$

where the additional parameters z=1.385 yields a better description of the potential at high temperatures where repulsive effects are dominant.

Our first calculations with this correction confirm the tendency of the density profile to be less steep. In any case it is desirable to have the other improvements. The matching between the Tang-Toennies potential for relatively small temperatures and the Born-Mayer potential is proposed in [8]. It is possible that it is one of the methods to describe high temperature phenomena more realistically.

ACKNOWLEDGMENTS

This work is supported by the Project N15 of the Presidium of Russian Academy of Sciences and in part by the Russian Foundation for Basic Researches, Grant N 04-01-00347.

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