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MODELING POLYATOMIC GAS FLOWS BY CLASSICAL TRAJECTORY DIRECT SIMULATION MONTE CARLO

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KEY WORDS

Rarefied gas dynamics, molecular collisions, transport properties

ABSTRACT

Modeling binary molecular collisions is an essential step in any rarefied gas flow study. When the working gas consists of monatomic species, atomic scattering can be described by simple analytical expressions [1] leading to accurate and relatively inexpensive Direct Simulation Monte Carlo (DSMC) implementations [2]. On the contrary, *realistic* treatment of collisions involving polyatomic species is not amenable to the simple theory sufficient to cope with atomic collisions. In the years, the difficulty has been tackled by introducing artificial mechanical models (rough or loaded spheres, rigid ovaloids) or stochastic phenomenological models designed to be used within DSMC simulations. The latter approach, mainly based on the ubiquitous Borgnakke-Larsen model [3], has proved quite viable and successful, since the very same model structure can be adapted to various gases by specifying the total collision cross section through the shear viscosity coefficient, the number and nature of internal degrees of freedom (rotational and/or vibrational) as well as the parameters(s) tuning the coupling between translational and internal degrees of freedom.

The progress of computational quantum chemistry methods is producing an increasing number of Potential Energy Surfaces (PES), accurately describing the interaction of molecular species with different levels of sophistication [4]. Given the proper PES, binary collisions between molecules can be numerically computed, taking care of the internal structure, by classical or semi-classical trajectory method. In 1997, Koura combined the deterministic calculation of binary molecular encounters with DSMC [5] to simulate molecular nitrogen flows. The technique, named CT-DSMC, resulted to be a successful one, but computationally too demanding. However, the method is very well suited for parallel computing and the availability of a variety of massively parallel architecture makes the technique interesting to investigate non-equilibrium polyatomic gas flows [6,7]. Recently, the authors applied CT-DSMC [7] to assess the accuracy of a PES for molecular oxygen [4], showing that experimental values of transport properties could be well reproduced. In the work described here we complete the investigation by studying the sensitivity of transport properties to variation of PES parameters within the error band suggested in Ref. [4]. Results suggest (see Figure 1) that volume viscosity, related to rotational relaxation rates is quite sensitive to variations of the anysotropic part of the PES. Furthermore the (non trivial) applicability of CT-DSMC to non-linear molecules, like water, will be discussed.
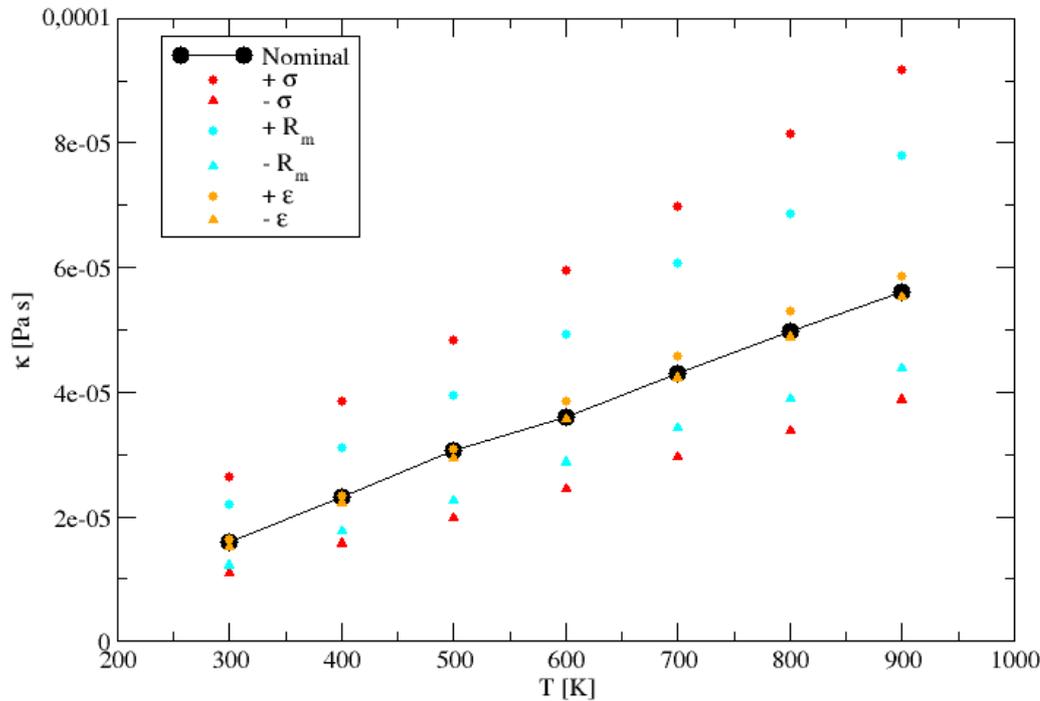
Figure 1: Response of computed volume viscosity k(T) to variation of Potential Energy Surface. *Black circles*: nominal PES [4]. *Yellow symbols:* variation of the potential well of isotropic contribution. *Cyan symbols:* variation of the potential minimum of the isotropic contribution. *Red symbols*: all PES parameters are given a variation of one standard deviation, as specified in Ref. [4].

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