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Flow of a monatomic rarefied gas over a circular cylinder: Calculations based on the *ab initio* potential method

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ABSTRACT

Two-dimensional flows of argon and helium over a circular cylinder are calculated by the Direct Simulation Monte Carlo (DSMC) method in the range of the free stream Mach number Ma_∞ from 0.5 to 10 in nearly free molecular, transitional, and nearly continuum flows. In DSMC simulations, inter-particle collisions are calculated with the *ab initio* (AI) potential method based on the interatomic interaction potentials established in quantum mechanical calculations. It is shown that the AI potential method enables computationally efficient simulations of multidimensional rarefied gas flows without introducing semi-empirical models of collision cross sections. The calculated values of the drag C_D and heat flux C_Q coefficients of the cylinder for Ar and He at the same values of Ma_∞, rarefaction parameter, and surface-to-free-stream temperature ratio are found to be different in less than 1%, ensuring small sensitivity of C_D and C_Q to the species of a monatomic gas. The simulation results obtained with the AI potential method are systematically compared with results obtained with the hard sphere (HS) molecular model. It is found that the choice of the HS diameter based on the condition of the identical viscosity of the real and HS gases at the free stream temperature ensures calculations of C_D and C_Q in sub- and supersonic flows at $Ma_\infty \leqslant 2$ with errors less than 3% and 6.5%, correspondingly. For hypersonic flows, this choice of the HS diameter is unsatisfactory and results in the errors up to 7% in C_D and 28% in C_Q. A semi-empirical rule that defines an optimum HS diameter in super- and hypersonic flows is suggested. With the use of this rule, the HS model is capable of predicting C_D and C_Q with errors less than 1% and 3%, correspondingly, and also provides a good accuracy in calculations of local flow parameters.

1. Introduction

The Direct Simulation Monte Carlo (DSMC) method [1] currently is the major numerical tool for computer modelling of rarefied gas flows. It is a particle-based simulation method, where a gas flow is represented by a set of simulated particles, which participate in binary collisions with each other and move freely between collisions. The core of the DSMC method is a procedure for stochastic sampling of binary collisions between simulated particles, which is derived in agreement with the collision term in the Boltzmann kinetic equation [2]. In order to apply this method for practical problems, one needs to use a molecular model that defines the collision frequency and post-collisional velocity of simulated molecules. Such a molecular model is usually formulated in terms of the collision cross sections [1]. For monatomic gases, the collision cross section can be deduced from the known potential curve, describing the interaction energy of a pair of molecules as a function of distance between them, e.g., [1,3]. At the same time, the collision cross sections traditionally used in DSMC simulations are formulated in the form of semi-empirical models, which are developed to fit experimental values of gas viscosity and other transport properties at a particular temperature. The hard sphere (HS) and variable hard sphere (VHS) models are among the most popular molecular models for DSMC simulations of non-reactive gas flows [1]. Since all such molecular models are approximative, the degree of their accuracy must be verified against models that accurately describe mechanics of inter-particle collisions.

Recently, a method enabling the use of arbitrary interatomic potentials for DSMC simulations of monatomic gas flows was developed in Ref. [4] and then applied to study a number of rarefied gas flows [5–7]. In this approach, the post-collisional velocities of simulated molecules are defined based on the preliminary tabulated dependence of the deflection angle [1] on the energy of colliding particles and geometric impact parameter [8]. This

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approach can be used for arbitrary potentials, including the semi-empirical Lennard-Jones potential and *ab initio* potentials established in quantum mechanical calculations, e.g., [9,10]. Hereinafter, this approach is termed the "*ab initio* (AI) potential method," since it is capable of calculating the post-collisional velocities from the first principles. A similar approach for calculations of binary collisions based on the Lennard-Jones potential was suggested in Ref. [11], where the dependence of the deflection angle on the energy and impact parameter is approximated by high-order polynomials. It is worth noting, however, that the representation of the deflection angle in the AI potential method [4] in the tabulated form enables faster sampling of post-collisional velocities and requires only a tiny fraction of computer memory used in typical DSMC simulations.

The goal of the present paper is threefold. First, we demonstrate that the AI potential method developed in Ref. [4] can be efficiently used for DSMC simulations of multidimensional rarefied gas flows over bodies in a broad range of flow conditions, from sub- to hypersonic velocities and from the nearly free molecular to nearly continuum flow regimes. For this purpose we performed systematic simulations of rarefied gas flows over a circular cylinder based on the AI potential method for argon and helium. Second, we compare the flows of argon and helium calculated based on the AI potential method in order establish how the local flow parameters in reduced units as well as the drag and heat flux coefficients of the cylinder in cross-flow depend on the gas species and free stream temperature. Finally, we compare the results obtained based on the AI potential method with results based on the simple and robust HS model in order to quantify the errors introduced by the application of the HS model in calculations of the drag and heat flux coefficients. We chose only the HS model for comparison with the AI potential method, because the HS model is known to be the simplest molecular model for kinetic simulations, it was used in multiple theoretical and numerical studies, and its predictions, in reduced units, do not depend on the gas species. The last property makes the HS model particularly attractive for multiple problems in aerothermodynamics.

The flow over a cylinder in the transitional flow regime is one of the major problems that are traditionally used for testing new numerical approaches and molecular models in the rarefied gas dynamics. This flow was a subject of multiple theoretical, e.g., [12–21], and experimental, e.g, [22,23], studies. The kinetic simulations of flow over a cylinder were performed using the DSMC method [12,14,16,18,20] and direct numerical solution of the Bhatnagar-Gross-Krook model kinetic equation [13,15,17,19,21].

Our main finding is that the local distributions of gas parameters in reduced units as well as the drag and heat flux coefficients of the cylinder are marginally affected by the monatomic gas species and dimensional free stream temperature in the whole range of flow conditions under consideration. We also found a simple rule that defines the HS molecular diameter and ensures small errors in calculations of the drag and heat flux coefficients based on the HS model.

The paper is organized as follows. In Section 2, a kinetic model of monatomic gas flow over a cylinder is described. The criteria of flow similarity are formulated in Section 3. The algebraic relationships for the cylinder drag and heat flux coefficients in the free molecular flow regime are presented in Section 4. The DSMC method, its numerical parameters, and validation of the computational code are discussed in Section 5. Then, in Sections 6–8, the results obtained for sub-, super-, and hypersonic flows based on the AI potential method and HS molecular model are described and compared with each other. The conclusions for all flow regimes under consideration are presented in Section 9. Finally, Appendix A contains data on comparison of the CPU times required for the DSMC collision sampling based on the HS model and AI potential method.

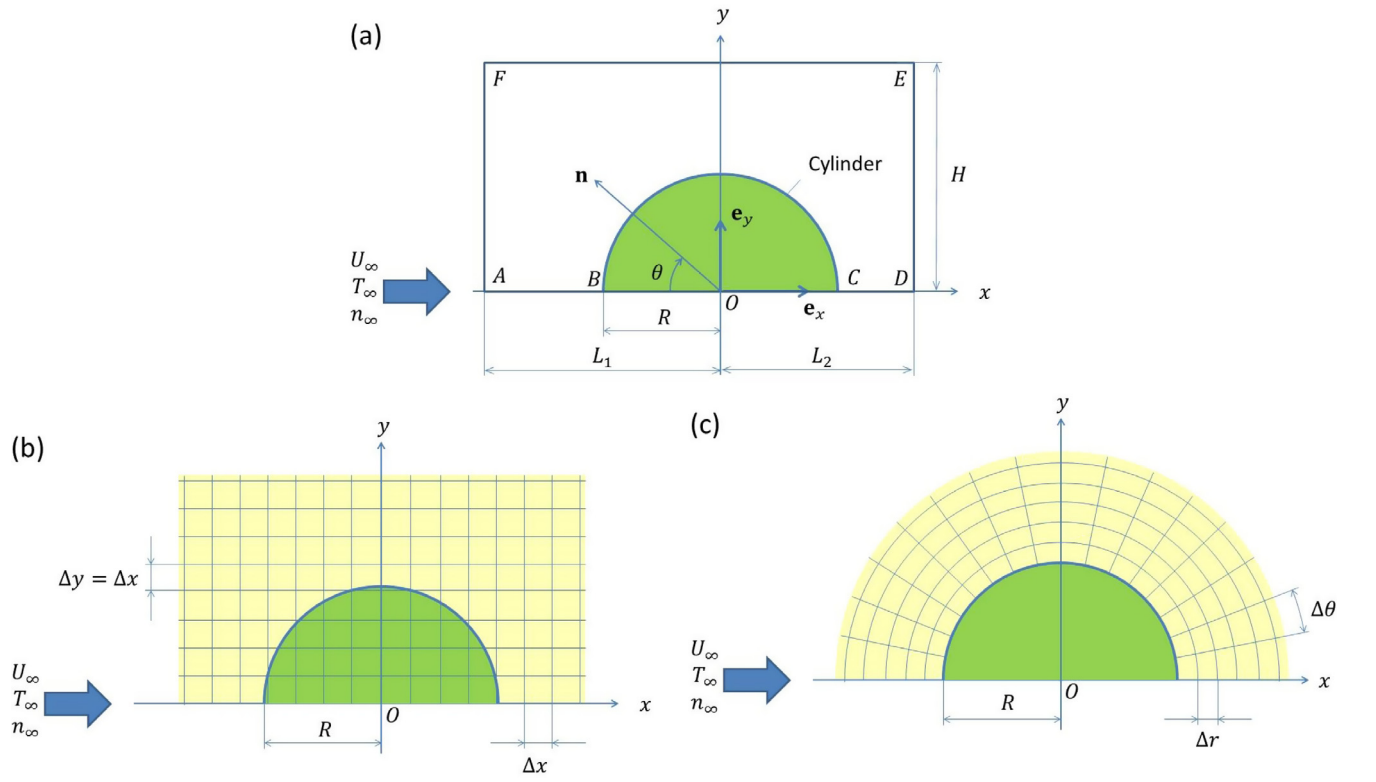

Fig. 1. Sketch of Cartesian coordinates *Oxy* and computational domain *ABCDEF* (a), as well as computational meshes used for collision sampling (b) and calculation of macroscopic gas parameters (c) in simulations of two-dimensional flow over a circular cylinder. The plane $y = 0$ is assumed to be the flow plane of symmetry.