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Molecular models for simulation of rarefied gas flows using direct simulation Monte Carlo method

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Abstract

The direct simulation Monte Carlo (DSMC) method is a technique for the numerical simulation of the rarefied gas flows by employing simulated molecules in simulated physical spaces. In the procedures involved in DSMC, the accuracy of the simulation of intermolecular collisions depends on the collision model adopted in the collision routine. The simplest molecular model is the hard-sphere model. In order to improve the accuracy of the simulations, more and more refined collision models were introduced for the use in DSMC. Thus, the variable hard-sphere, the variable soft-sphere, the generalised hard-sphere, the generalised soft-sphere and the variable sphere models were put forward by various researchers. And, all these models have met with varying degrees of success. Meanwhile, the Borgnakke–Larsen model, statistical inelastic cross-section models for both continuous and discrete internal energy and the dynamic molecular collision model were proposed for the treatment of polyatomic molecules in which transfer of energy among translational, rotational and vibrational degrees of freedom is possible. This paper gives a brief introduction to the intermolecular potentials based on which the molecular models have been constructed. Then the various models are introduced in the chronological sequence; finally concluding with a brief summary of the progress that has been made so far in this area.

Keywords: Interaction potentials; Molecular collision models; Particle simulation; Rarefied gas; Transition regime

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