Accounting for rotational non-equilibrium effects in subsonic DSMC boundary conditions

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Abstract

From study of the kinetic theory of dilute gases, it becomes clear that the sub-sonic, implicit boundary conditions which are commonly used in direct simulation Monte Carlo simulations of micro-scale channel flows do not take any form of rotational non-equilibrium into account. The consequences of not considering non-equilibration of the rotational mode are discussed and a few form of the boundary conditions which attempt to take this effect into account are proposed. It is shown that for a highly compressible test case involving these implicit boundaries in the literature that a degree of rotational non-equilibrium is present. The changes in the recovered macroscopic properties when the new boundary is applied in the same case include an improved rotational temperature distribution and a slightly lower velocity at the channel exit. A further test case exhibiting no rotational non-equilibrium was performed and it is shown that the macroscopic properties which are recovered are essentially the same for both boundaries. The results indicate that the newly proposed outlet boundary condition increases the range of applicability of these types of boundary conditions, without adding any significant computational expense.