

Hybrid Continuum and Molecular Modeling of Nano-scale Filter Flows

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Abstract

A novel hybrid method combining the continuum approach based boundary singularity method (BSM) and the molecular approach based direct simulation Monte Carlo (DSMC) is developed and then used to study viscous fibrous filtration flows in the transition flow regime, $Kn > 0.25$. First, the flow about a single fiber confined between two parallel walls is used to test the proposed hybrid method. The DSMC is applied to an annular region enclosing the cylinder and the BSM is employed to the entire flow domain. The parameters used in the DSMC and the coupling procedure, such as the number of simulated particles, the cell size and the size of the coupling zone are determined by inspecting the pressure drop obtained.

It is observed that in the partial-slip flow regime the results obtained by the hybrid BSM-DSMC method match the ones from the BSM combined with the heuristic partial-slip boundary conditions. For higher Knudsen numbers, the difference in pressure drop and velocity is significant.

The developed hybrid method is then parallelized by using MPI and extended for multi-fiber filtration flows. The multi-fiber filter flows considered are in the partial-slip and transition regimes. For $Kn \leq 0.25$, the difference in pressure drop between the BSM and hybrid method appears to be less than 10%. For $Kn = 0.75$, the difference in pressure drop approaches 20%. The computed velocity near fibers changes even more significantly with the increase of the Knudsen number, which confirms the need of molecular methods in numerical evaluation of the flow in filters.

Applications of the proposed numerical methodology include multi-particle interactions in particle capture mechanisms in filtration, signaling and sensing, to name a few applications. The proposed combined continuum and molecular methodology can incorporate surface chemical reactions and the electromagnetic forces in the DSMC procedure for Knudsen layer.