

Abstract Submitted
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Hybrid Continuum and Molecular Modeling of Nano-scale Flows

ALEX POVITSKY, SHUNLIU ZHAO, Carleton University — A novel hybrid method combining the continuum approach based on boundary singularity method (BSM) and the molecular approach based on the direct simulation Monte Carlo (DSMC) is developed and then used to study viscous fibrous filtration flows in the transition flow regime, $Kn > 0.25$. The DSMC is applied to a Knudsen layer enclosing the fiber 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. Results are compared to the experiments measuring pressure drop and flowfield in filters. The optimal location of singularities outside of flow domain was determined and results are compared to those obtained by regularized Stokeslets. The developed hybrid method is parallelized by using MPI and extended to multi-fiber filtration flows. The multi-fiber filter flows considered are in the partial-slip and transition regimes. For $Kn \sim 1$, the computed velocity near fibers changes significantly that confirms the need of molecular methods in evaluation of the flow slip in transitional regime.

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