Dynamic Simulation Tools for the Analysis and Optimization of Novel Collection, Filtration and Sample Preparation Systems

We have developed novel multiphysics simulation capabilities to address design and optimization needs in the general class of problems that involve the transport of air- and water- borne species and fluid (liquid and gas phases) through sieving media. This new capability is designed to characterize subsystem efficiencies, such as filter efficiency, based on the details of the microstructure, surface interactions, and environmental effects.

To accomplish this we developed new lattice-Boltzmann (LB) simulation tools that include detailed microstructure descriptions, relevant surface interactions, and temperature effects, and that will be able to handle both liquid and gas phase systems. Additionally, the new capability has been used to help design particle-focusing apparati, predict shear forces on adhered species, and evaluate the permeability of porous materials, all in support of LLNL programs.

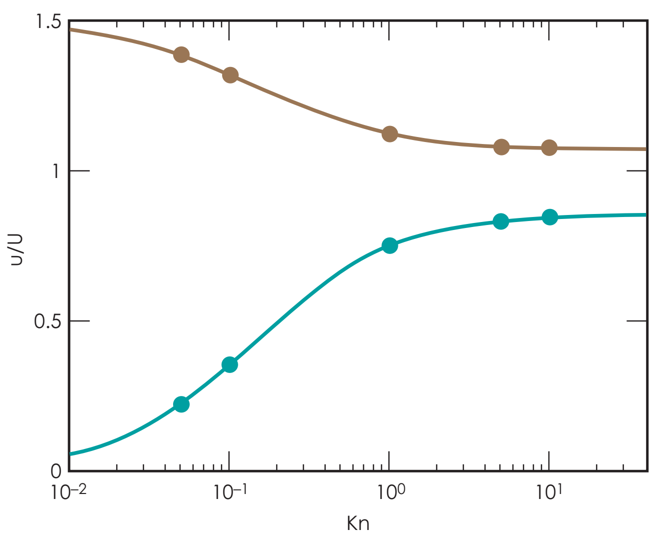

Figure 1. Dimensionless fluid slip velocity in channel flow, predicted using the new LB boundary condition (circles), compared with predictions from theory (lines), as a function of *Kn*.

Project Goals

The goal of this project was to equip scientists and engineers with the computational tools to analyze and optimize novel collection, filtration, and sample preparation systems. Specifically, our goal was to develop tools that describe macroscopic transport phenomena in filtration, sample preparation, and filtration (porous media) systems, based on the details of the micro- and nanostructure.

Relevance to LLNL Mission

This work directly impacts continuing and future LLNL efforts that involve filtration, collection, and sample preparation. This capability is directly applicable to characterization of transport in porous media and multi-component sample preparation for detection systems relevant to LLNL programs such as Weapons, Energy and Environment, Medical Technology, Chemical and Biological Counter-Proliferation, Genomes to Life, and Homeland Security. The capability has been demonstrated and used to meet customer needs in the areas of aerosol transport, adhesion and re-suspension, and fluid and chemical transport in porous media.

FY2005 Accomplishments and Results

In FY2005, our effort was focused on fluid and suspension transport for a useful spectrum of Knudsen numbers (*Kn*). To accomplish this, the particle dynamics capability was augmented to account for particle Reynolds-number effects in aerosol transport phenomena

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in the gas phase. This advancement enabled the study of bulk phase gas and particle dynamics. However, in such flow conditions, the fluid experiences increasing slip as *Kn* increases; therefore, to ensure accurate prediction of fluid and particle transport properties, the boundary condition at solid surfaces must account for a *Kn*-dependent slip condition. A major accomplishment was the development of a novel, *Kn*-dependent, boundary condition that enables accurate prediction of fluid slip velocities for a wide range of conditions (Fig. 1).

As shown in Fig. 1, our results exhibit nearly exact agreement with theory. Prior to this breakthrough, LB boundary conditions were accurate to $Kn < 1$. This result constitutes a significant improvement over the state of the art.

Our particle dynamics/tracking capability was further advanced to handle complex geometries. To demonstrate this new advancement, the capability was used to explore and optimize particle focusing (sample preparation/conditioning) for mass spectrometry, *i.e.*, particle transport and focusing in rarified gas conditions. Figure 2 shows the results from actual design simulations that were later used to support related DARPA research efforts.

In addition to developing new gas phase fluid and particle dynamics capabilities, the force prediction in external field(s) modules was augmented in the viscous suspension capability. This was accomplished through advancing the accuracy of the dielectrophoretic (DEP) force prediction by including higher order moments such as the quadrupole contribution to the DEP force. This new advancement was incorporated into the viscous fluid/suspension capability.

Related References

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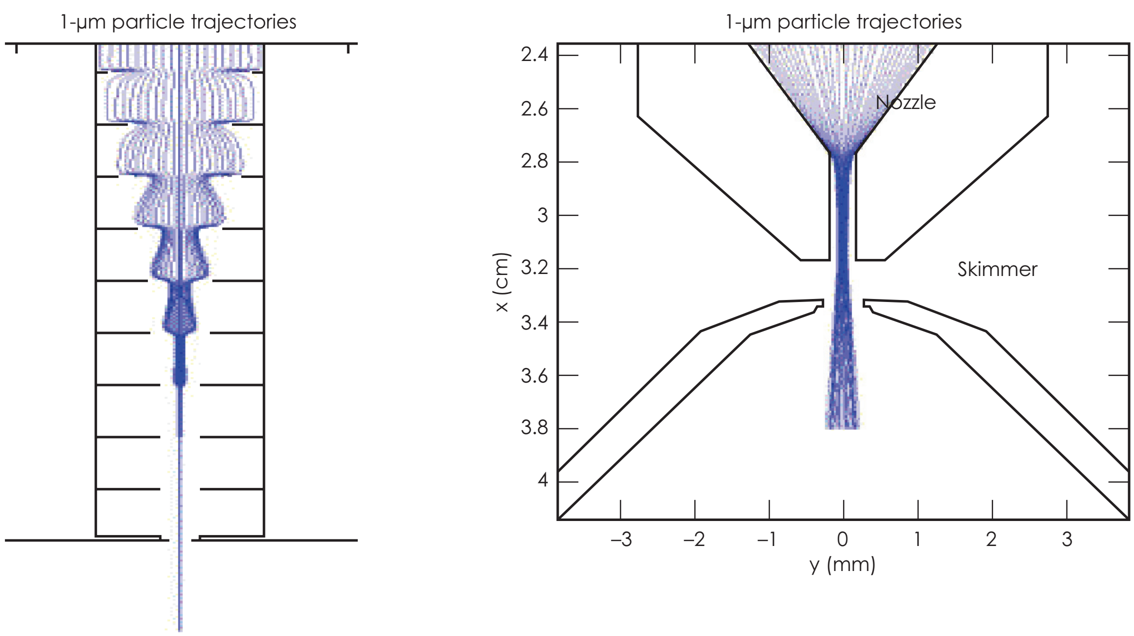

Figure 2. Particle trajectories in "inlet" design for mass spectrometry.