A mixed Computational Fluid Dynamics and Direct Simulation Monte Carlo model of the intermediate pressure regions of a miniature ESI-MS

Edward J. Crichton, Rantej S. Kler, Richard W. Moseley

Microsaic Systems, Woking, United Kingdom

Overview
- Development of a Simion ion trajectory model incorporating results from both Navier Stokes based (NS) and Direct Simulation Monte Carlo (DSMC) solvers within openfoam.
- Experimental work to assess models validity.
- Comparison of the results from a commercial instrument (4500 MIDA) and new development prototype.

Introduction
The recent development of miniaturized electrospray mass spectrometers (ESI-MS) has led to efforts to maintain high sensitivity whilst minimizing footprint. Due to the experimental difficulties accessing these small and complex spaces, computational studies have increasingly become a useful complement to empirical study. During development of a new, lower pressure ion optic a review of the coupling between the interface and analytical chambers within our ESI-MS products (Microsaic MIDA®) was undertaken. Computational models of the outflow from new prototype and standard optics were undertaken to assess whether the local flow properties in the ionguide has been maintained with a simple scaling of components. Rough analysis of global Knudsen numbers imply transition from continuum flow within the setup resulting in the breakdown of the Navier-Stokes (NS) approach.

NS Breakdown
A number of different criteria for determining the applicability of NS to rarefied sonic flows have been suggested in the literature. Such as the gradient local length (GLL) based on a local Knudsen number for a flow property Q [1]:

$$Kn_{GLL} = \frac{\lambda_m}{Q} \frac{\partial Q}{\partial x} > 0.05$$

Or the validity of assumption underlying the derivation of the NS equations themselves [1]:

$$B = \frac{2}{3} \frac{(u_i^2 + v_i^2 + w_i^2)}{u_i^2} > 0.2$$

Programmable python filters in Paraview were developed to allow calculation of these parameters as fields over the domain. Contour plots of these criteria are shown in figure 2a) along with the more traditional Knudsen number ($Kn = \lambda / L$ where L is the tube diameter). All surfaces in the domain had Knudsen numbers > 0.05 so were to be assumed to be NS-slip.

1. Use this location as inlet for a 3D DSMC simulation 1/4 of the of the ionguide region.
3. Run trajectories in parallel via early access mode - incorporating simion HES collision model [6] with cross-sections taken from [7].

Results
Figure 3 compares experimental data with model output for adjusting the tube and lens at fixed ionguide voltage (1V). As all values below 1V are a retarding field transmission must incorporate viscous forces. Experimentally with approximately 1.3 the inflow there is negligible transmission below 1V and all 3 species behave identically.

Method
Work station: Linux 24 core intel 3GHz Xeon.

1. Compute 2D wedge with slip continuum physics of the inlet/tube lens (figure 2A).
- RhoCentralFoam(2): Laminar - Compressible - Parallel.
- Diffuse smoluchowskiJumpT, maxwellSlipU walls
- Empirically estimated mass flow rate inlet.
- waveTransmissive outlet.
2. Export a contour with breakdown parameter B > 0.2 in post processing.
3. Convert contour to stl file and use in meshing inlet in 2D DSMC wedge (dsmcFoamPlus 1.0).
4. Identify within the tube lens where gradient of $U$ and $T \sim 0$ in the axial direction.
5. Use this location as an inlet for a 3D DSMC simulation 1/4 of the ionguide region.
7. Run trajectories in parallel via early access mode - incorporating simion HES collision model [6] with cross-sections taken from [7].

Conclusions
- A reliable model of the ion trajectories within the slip to transition region of a MEMS based mass spectrometer has been developed.
- Previously reported [8] operating regime based on local properties has been confirmed in the model of the 4500 MIDA®.
- Similar local effects have been observed in the new case and are substantive enough to provide collisional cooling of ions at energies relevant to ‘in source’ CID.

References