Colin Breslin

CHE 4291

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Gases in Microchannels and Nanochannels Summary

**Models used** –

molecular dynamics (MD)

monte Carlo (MC)

(They used both – MD-MC)

**Assumptions they made** –

Hard-sphere interactions btwn particles

Walls in simulation are modeled to be thermal walls

Once system reaches equilibrium, the flux of particles from one domain becomes constant

**Limitations encountered** –

Microchannel

The Knudsen number from the Navier-Stokes equations needs to equal 0.1 for gases, if greater than 0.1 Boltzmann Eqtns

(Kn=λ/L): λ- mean free path of the molecules; L- physical length of the system

Simulation at molecular level not nano

Coupling MC and MD

Size – 10 to 20 times the molecular diameter

Wall Effects

Using the DSMC, a particles real physical size is required for particles near the walls

MD-MC

The systems particle domains can be imported from MD to MC but not vice versa

**Software/Code used** –

Source [27] – K. Esselink and P. A. J. Hilbers, J. Comput. Phys. **106**, 108 (1993).

MC Simulator – FORTRAN77

MD Simulator - c

Interface written in PYTHON

**Chemistry formulas used for thermodynamics** –

Lennard-Jones potential

Microchannel-

MD

Navier-Stokes equations

Boltzmann eqtns

MC

Enskog eqtn

Equation numbers

1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15

**Anything of notable interest** –

MD used near boundaries for accuracy

MD too time consuming for dense gas in microchannel (use MC)

MC used for bulk (low computational cost)

The MD and MC can run simultaneously

If macroscopic properties are copied instead of single particles, MC to MD can work

Hybrid Simulator Components

MD component for MD simulations

MC component for MC simulations

Interface component between the MD and MC components leading to coupling

Two MD domain near walls, and one MC domain in middle

Most efficient is MD 10% and MC 90% of domain

MD-MC method is more efficient than pure MD or pure MC