Numerical Investigation of Ion Transport in the MOMA Ion Mass Spectrometer

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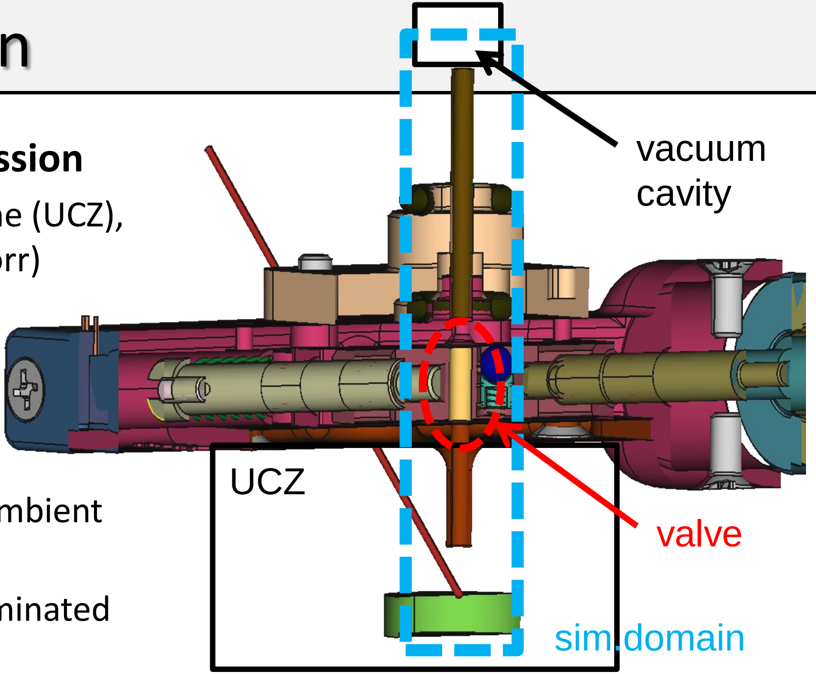
Lubos Brieda

Particle In Cell Consulting LLC, Westlake Village, CA, USA

Andrej Grubisic and Umeshkumar D. Patel

NASA Goddard Space Flight Center, Greenbelt, MD, USA

Introduction



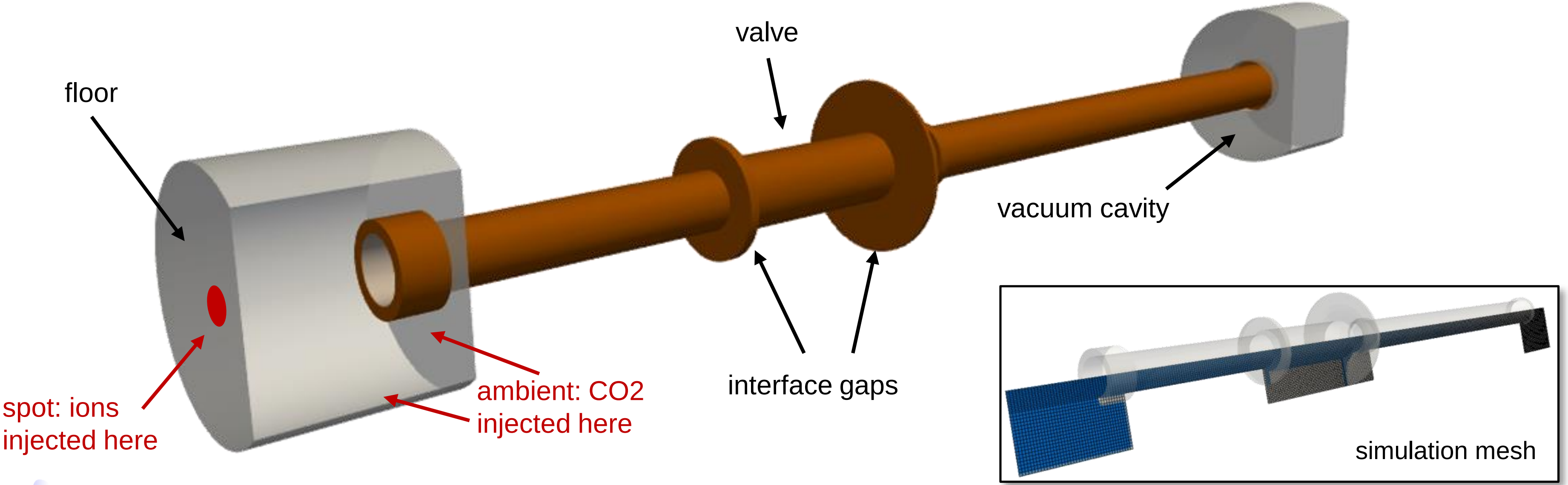
- **MOMA is an ion-spectrometer for the ExoMars Rover mission**
  - Collected Martian soil sample delivered into a UltraClean Zone (UCZ), maintained at ambient atmospheric pressure (~0.6 kPa/4.5 Torr)
  - UCZ separated from a vacuum cavity, housing a quadrupole mass spectrometer, by an aperture valve (APV) assembly
  - The main feature of the APV is a 3 cm long / 1.3 mm ID sectioned ion guide tube
  - A sliding mechanism aligns the middle section, allowing the ambient CO_2 to flow into the vacuum cavity
  - After a short interval to establish steady flow, the sample illuminated with several laser beam pulses
  - The desorbed ions become entrained in the CO_2 flow and are transported to the mass spectrometer

Objective

- Ground testing at NASA Goddard indicated dependence of ion signal on: 1) the ambient pressure and 2) the APV applied voltage
- **Numerical investigation thus desired to obtain insight into ion dynamics**

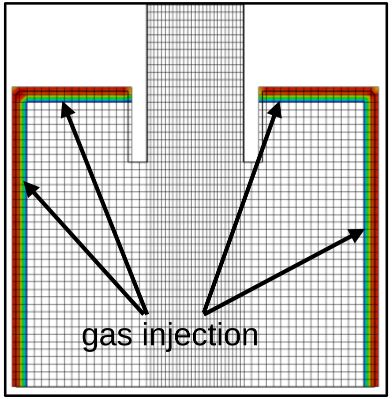
Simulation Approach

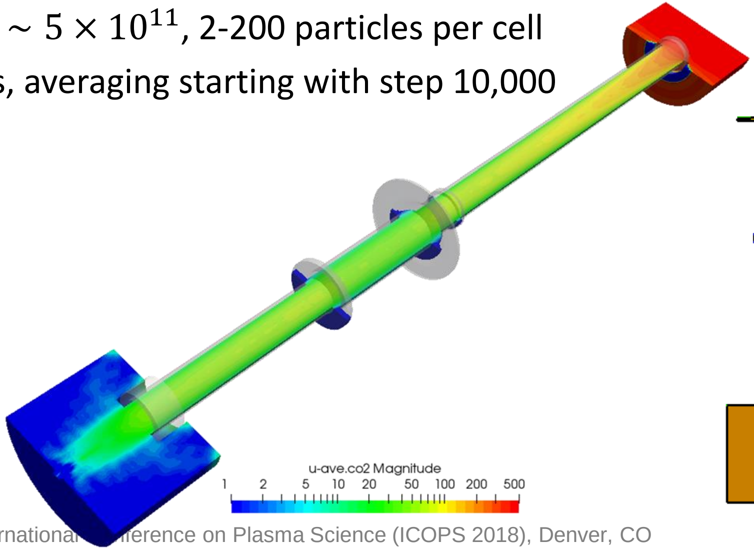
- The simulation needs to consider both plasma and gas dynamics
- Due to low operating pressure, ions and neutrals treated with a kinetic approach: Particle in Cell (PIC-MCC) for plasma and Direct Simulation Monte Carlo (DSMC) for gas
- Geometry exhibits axial symmetry, a 2D axisymmetric code used to reduce computational time
- Two phases: 1) DSMC simulation to establish steady-state CO_2 flow and 2) ion transport with "frozen" ambient gas
- Using a 2D, open-source Java code Starfish: *Brieda, L. and Keidar, M., "Development of the Starfish code...", 48th AIAA JPC, 2012*

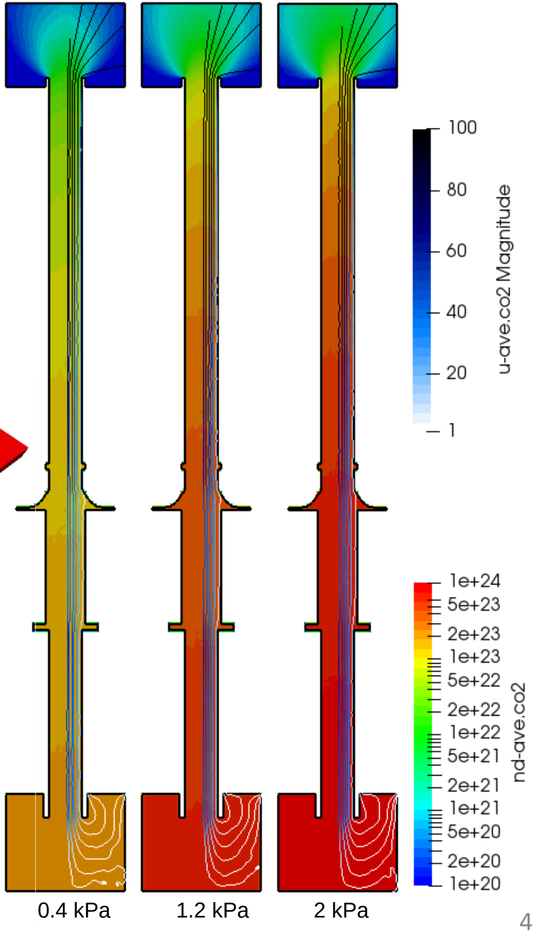


Gas Flow Results

- The first phase considered only the CO_2 flow
- CO_2 molecules injected into the simulation along the "ambient" zone boundaries utilizing a constant pressure source
  - Generates particles when partial pressure $P_i = n_i k T_i$ less than specified P_0
  - Initial velocities sampled from a half-Maxwellian along boundary normal
  - Considered $P_0 \in [3,6,9,12,15,18]$ Torr (0.4 to 2.4 kPa)
- The Variable Hard Sphere (VHS) model of Bird used for collision dynamics
  - Simulation-to-real particle ratio $\sim 5 \times 10^{11}$, 2-200 particles per cell
  - 100,000 $\Delta t = 10^{-8}$ s time steps, averaging starting with step 10,000

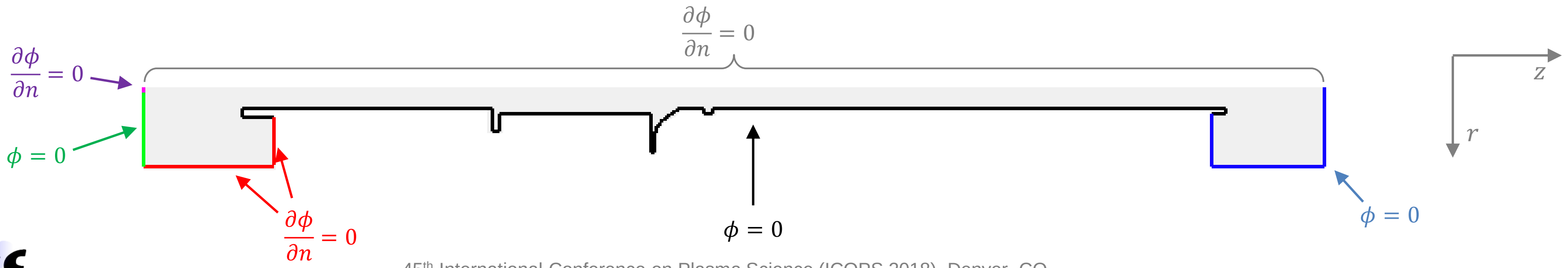






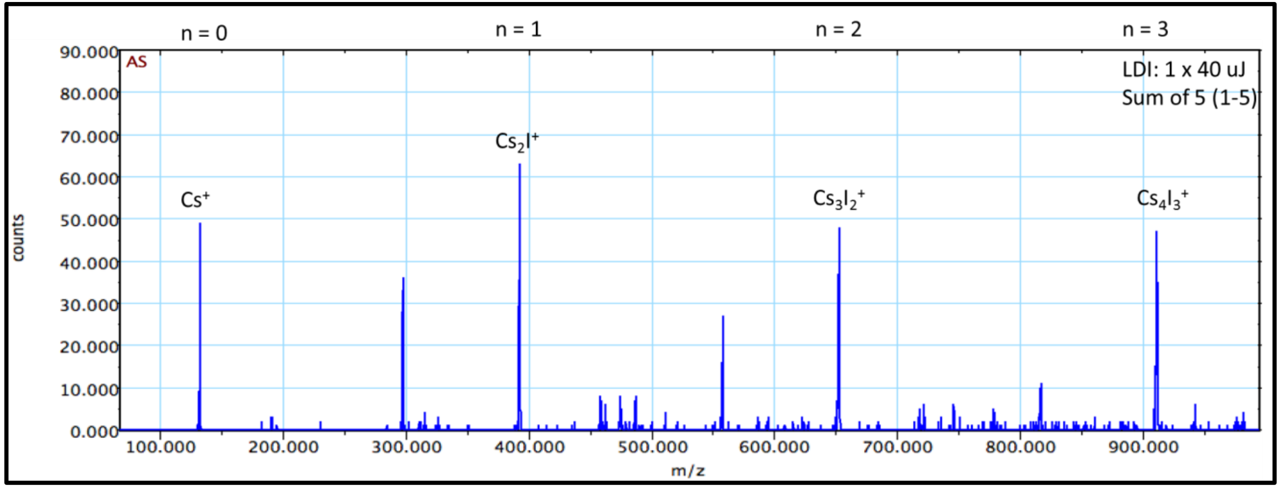
Plasma Numerical Model

- Ion mass transport simulations performed with the ES-PIC method
  - Just as in DSMC, ions represented by simulation particles
  - Particle positions integrated from $\frac{d\vec{x}}{dt} = \vec{v}$ and $\frac{d\vec{v}}{dt} = \frac{q}{m}\vec{E}$, where the electric field obtained from plasma potential $\vec{E} = -\nabla\phi$
  - Potential obtained from the Poisson's equation, $\epsilon_0 \nabla^2 \phi = e(n_i - n_e)$, the RHS is the charge density from particles
  - Ions impacting the valve are removed from the simulation (assumes surface neutralization)
  - 10 real-to-sim macroparticle weight, 40,000 $\Delta t = 5 \times 10^{-8}$ s time steps, averaging after step 10,000
- Ion-neutral coupling based on the MCC (Monte Carlo Collisions) algorithm
  - Ion density about 10 orders of magnitude smaller than the neutral density
  - DSMC applicable to species of comparable partial pressures, highly inefficient for trace species
  - MCC an alternate scheme in which a source particle collides with a target "cloud"
  - Momentum not conserved (since target material not affected) but negligible error given the massive ratio in species densities
  - Elastic collision performed by sampling a virtual target CO_2 particle from the steady-state stream velocity obtained in phase 1



Ion Source

- Below is the typical mass spectrum from the Martian soil stimulant
- The dominant species is Cs_2I^+, only this single species was included in this analysis

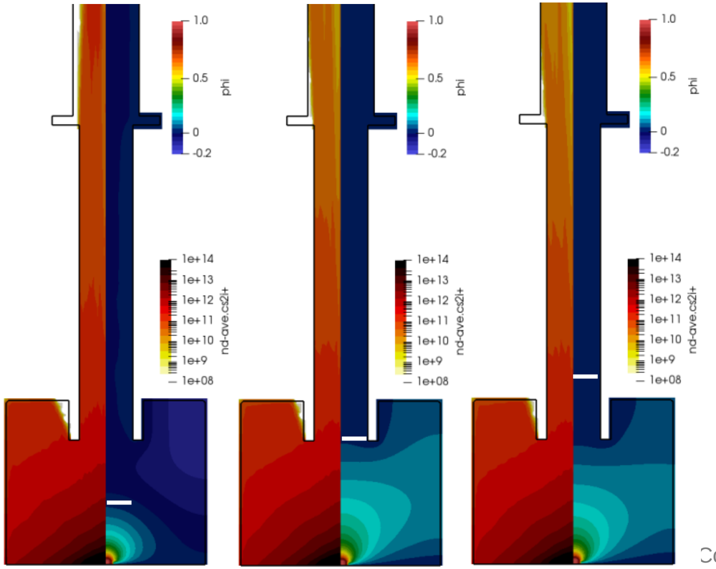


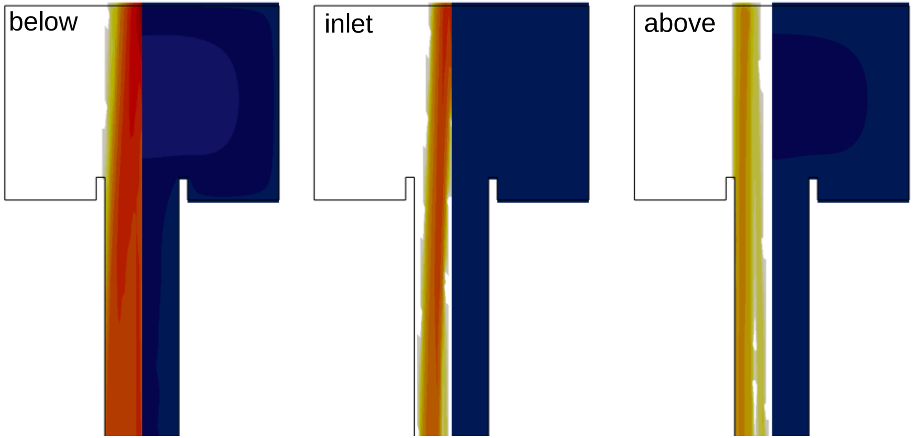
- GSFC measurements indicate approximately 10^9 ions (~0.1nC) generated per laser shot
  - Agrees well with a pit analysis at MPS, Goetz, et.al, "Characterization of mineral targets by laser desorption and ionization in preparation of the MOMA investigation onboard the EXOMARS-2018 rover" 47th Lunar and Planetary Sci. Conf, 2016
  - Laser shot lasts 10^{-9} s, typically deploy a pulse of 5 shots separated by 10 ms gap per valve opening
  - The time-averaged production rate then $\dot{N} = 10^{11}$ ions/s, or $\dot{m} = 6.52 \times 10^{-14}$ kg/s with Cs_2I^+ mass

The Trouble with Electrons

- The n_e term in the Poisson's equation is the electron density
- Not practical to simulate electrons as particles: requires tiny time steps, fine mesh, and a detailed treatment of boundaries to avoid instabilities
- Electrons typically modeled as fluid. If kT_e constant and no $\vec{B}$ field: $n_e = n_0 \exp\left(\frac{e(\phi - \phi_0)}{kT_e}\right)$
  - Difficulty in setting the reference values
  - Obtain different solution depending on where n_0 sampled

<u>Simulations hence only suitable for obtaining qualitative trends</u>

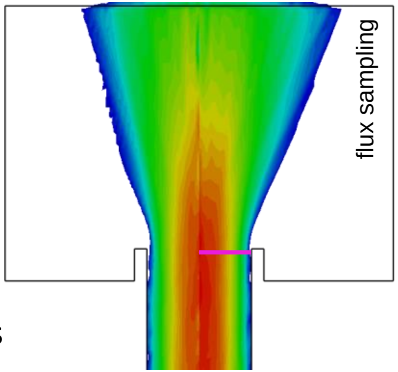


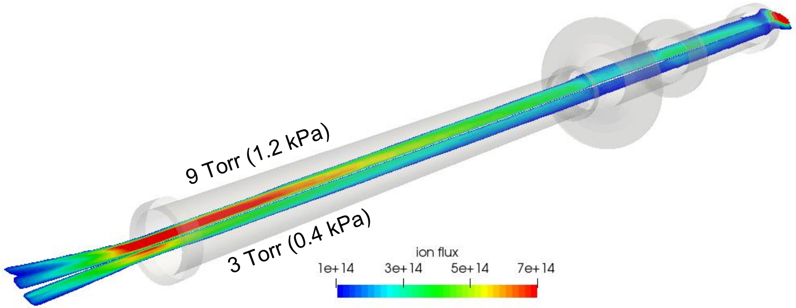


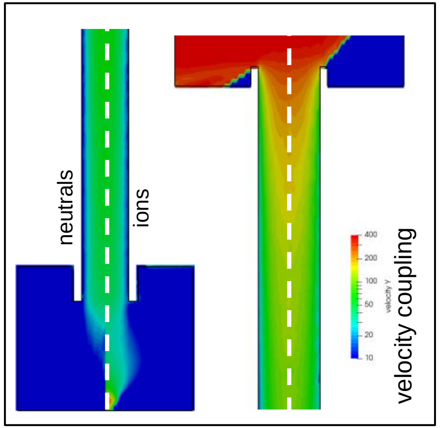
- The only difference between these cases is the n_0 sampling location (the white line), $\phi_0 = 0$ V, $kT_e = 1$ eV.
- Subsequent sims used the "inlet" configuration: sampling at guide inlet

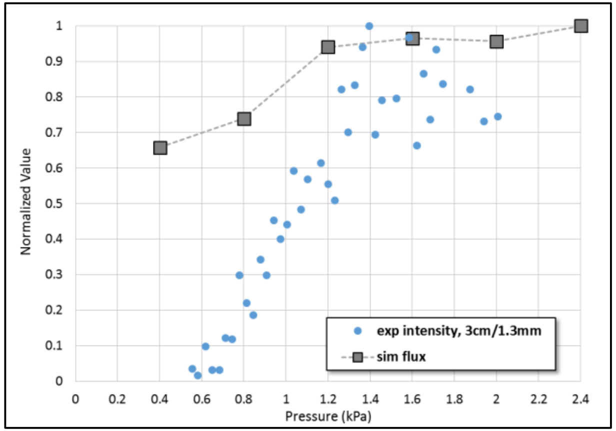
Pressure Dependence

- Simulations predict increasing ion signal with CO_2 pressure
  - Agrees with experimental data, signal rise less steep than observed
  - Strong impact of ambient gas temperature on simulated signal ($v_{drift} < v_{thermal}$), $CO_2 - CS_2I^+$ cross-section only estimated
- Strong coupling of ion and gas velocities observed
  - Drag the primary transport mechanism, initial ion velocity decays rapidly due to collisions
- **The simulation fails to capture the observed quenching of signal at $P \sim 2$ kPa**
  - Mechanism unclear, possible suspects include surface charging and mass spectrometer saturation



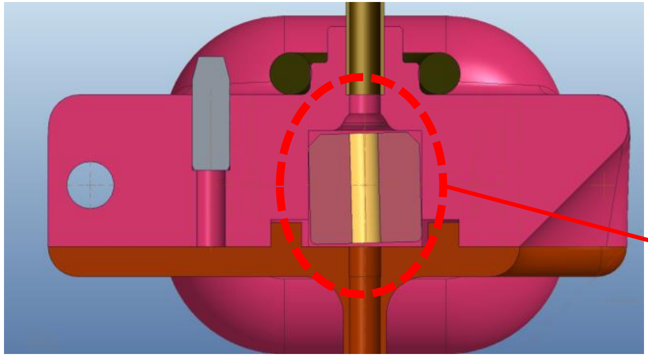


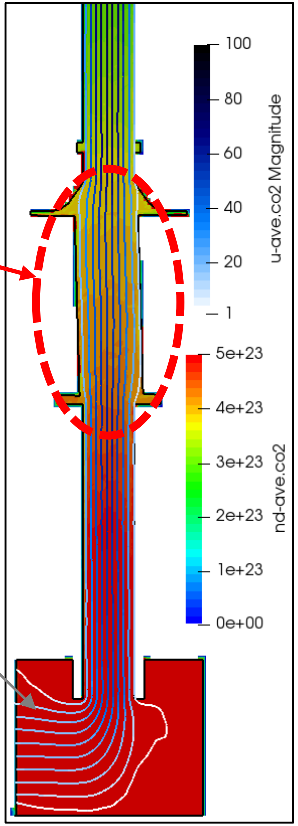




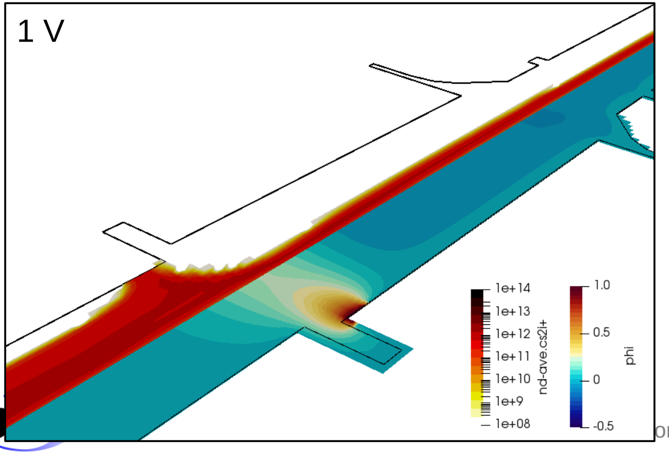
Additional Studies

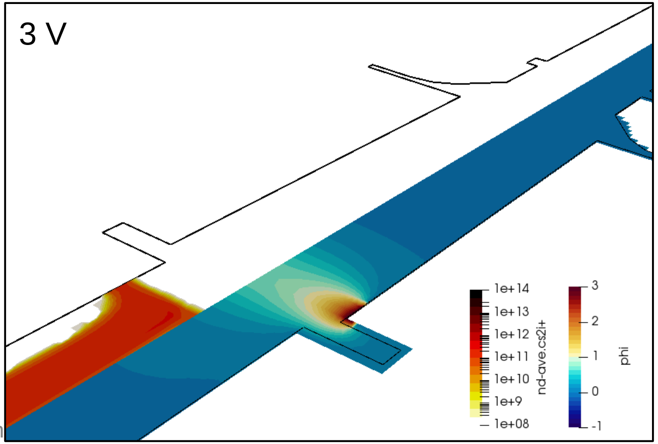
- Valve thru-hole not completely axial due to clearance between the upper and lower ion tube segments
  - Maximum rotation 1.6 degrees
  - No-longer axi-symmetric, simulated as a 2D XY slice
  - DSMC simulation does NOT indicate presence of vortices or similar flow feature that would limit ion flow
- Also interested in surface charging
  - Of interest is the lubricant used on the sliding mechanism
  - Small charge buildup (<=1V) sufficient to restrict the ion flow, complete blockage with 3 V
  - Self-consistent surface charging algorithm (not available) needed to estimate local surface charge





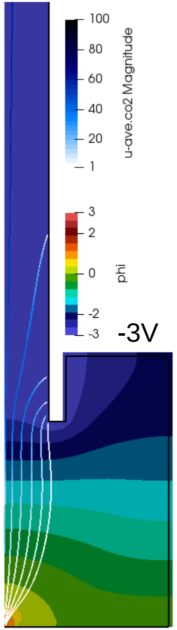
asymmetry in flow lines due to non-identical sizes of the ambient region to satisfy mesh-coupling limitations of the constant pressure source

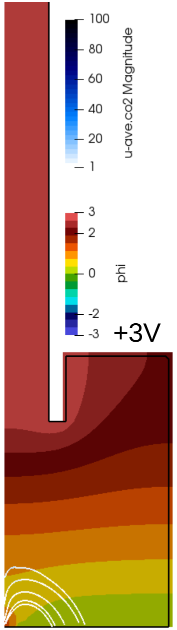


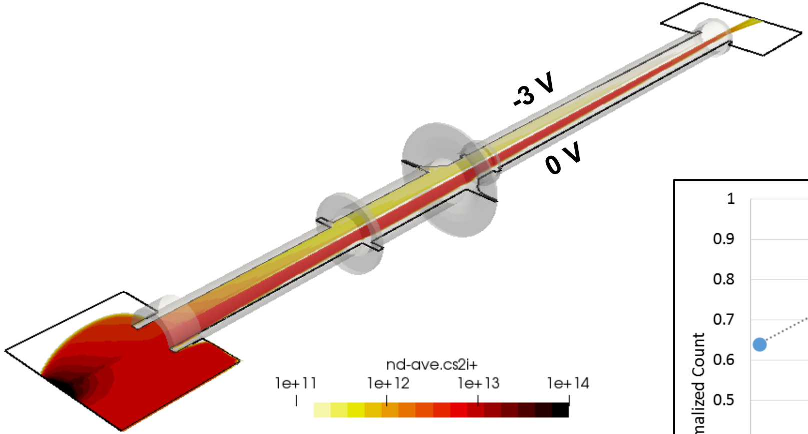


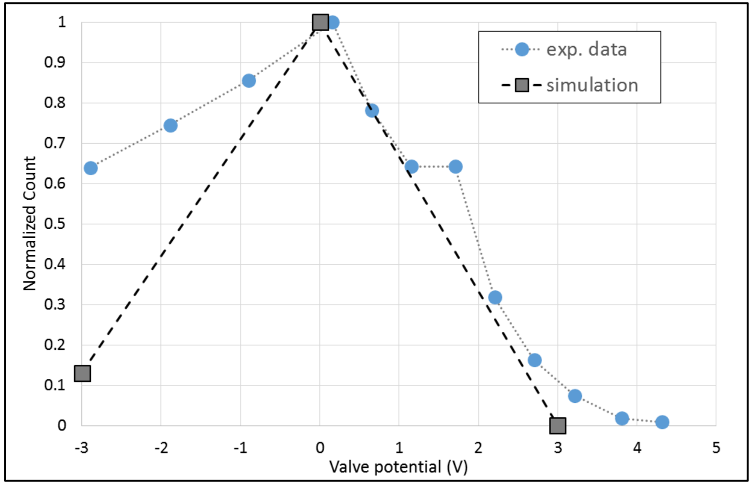
APV Bias Potential

- The APV voltage can be biased positive or negative
- Initially hypothesized that negative bias potential could increase ion signal, experimental and numerical results indicate not to be the case
  - Negative bias potential results in a “plasma lens” at the entrance diverting ions towards the wall
  - Positive bias repels ions from the inlet









Conclusion

- DSMC and PIC/MCC simulations performed to study the ion transport in MOMA ion mass spectrometer aperture valve
- Simulations recover most of the trends observed experimentally: ion signal increases with background pressure, and biasing the APV potential results in a signal decrease
- The simulation fails to recover a sudden drop in signal seen around 2 kPa
  - Considered sliding mechanism misalignment (no effect) and surface charging (possible effect but model not robust enough to determine likelihood)
  - Signal drop could also be arising from a charge saturation in the ion mass spectrometer
- Results obtained on a standard desktop workstation, would benefit from a supercomputer time to improve the resolution of the plasma sheath and the boundary layer
- The simulation code used in this study can be downloaded from **particleincell.com/starfish** or **github.com/particleincell/starfish-LE/**
- Contact: lubos.brieda@particleincell.com

Questions?