NUMERICAL INVESTIGATION OF ION TRANSPORT IN THE MOMA ION MASS SPECTROMETER

Lubos Brieda
Particle In Cell Consulting LLC, Westlake Village, CA 91362, USA

Umeshkumar D. Patel, Andrej Grubisic, others *NASA Goddard Space Flight Center, Greenbelt MD 20770 USA*

The Mars Organic Molecule Analyzer (MOMA) is a miniature ion trap mass spectrometer designed for the upcoming ExoMars Rover mission[1]. The spectrometer uses laser desorption to ionize a Martian soil sample within an instrument internal clean zone maintained at ambient Martian pressure. A high-speed aperture valve transiently opens to allow ionized constituents, along with the ambient gas, to enter a vacuum cavity containing a linear ion trap mass spectrometer. The ambient clean zone and the vacuum cavity are connected via a few centimeter long aperture valve ion guide tube. In this paper, we present results from a recently completed numerical investigation of ion transport from the ion source across the ion guide. Specifically, we focus on collisional coupling between ions and the neutral molecules flowing into the vacuum cavity. The simulation domain contains the ambient region, and we consider the variation in ion conductance with ambient pressure. We also analyze the impact of a fixed potential bias applied to the aperture valve. Simulations are performed with a two-dimensional axisymmetric PIC / DSMC code Starfish[2]. Numerical results are compared to experimental data.

1. F. Goesmann, et. al., “The Mars Organic Molecule Analyzer (MOMA) Instrument: Characterization of Organic Material in Martian Sediments”, Astrobiology, Vol. 17, No 6-7, 2017

2. L. Brieda and M. Keidar, “Development of the Starfish Plasma Simulation Code and Update on Multiscale Modeling of Hall Thrusters”, 48th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, July 2012, pp. 1-30

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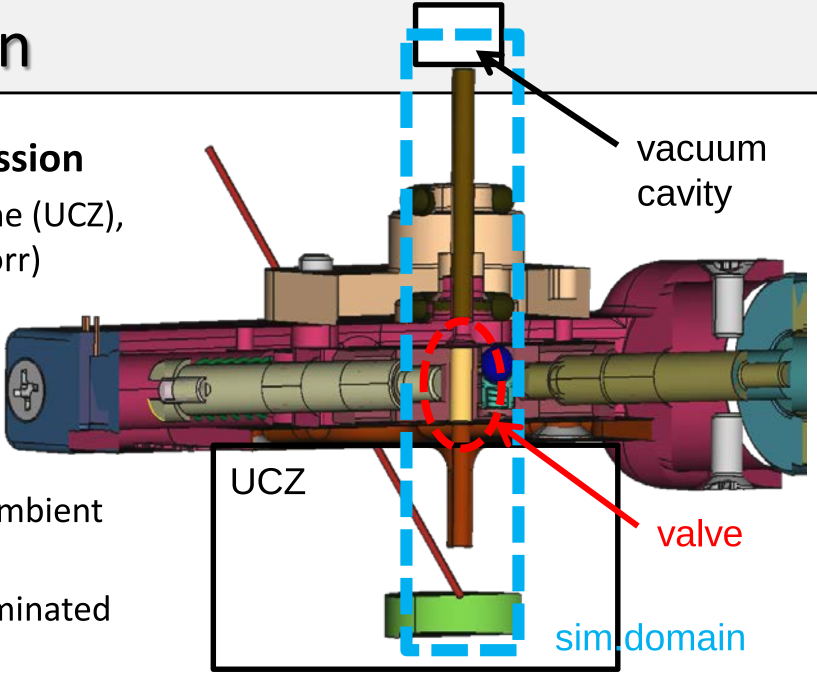
Lubos Brieda
Particle In Cell Consulting LLC, Westlake Village, CA, USA

Andrej Grubisic, Umeshkumar D. Patel
NASA Goddard Space Flight Center, Greenbelt, MD, USA

Introduction



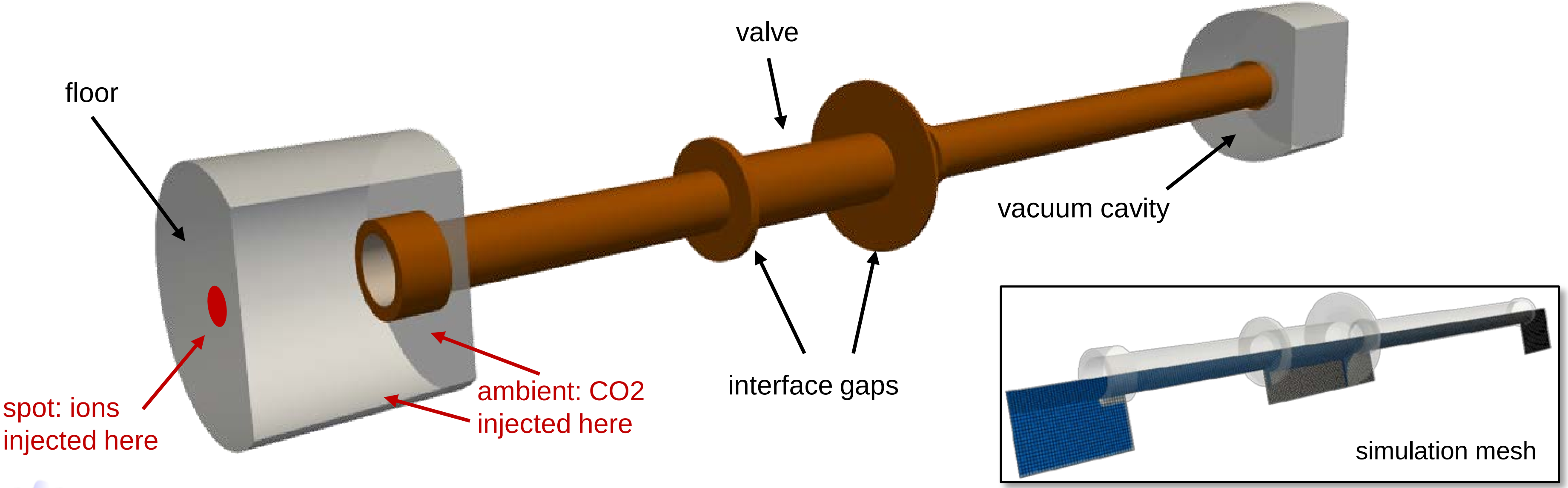
- **MOMA is an ion-spectrometer for the ExoMars Rover mission**
  - Collected Martian soil sample delivered into a UltraClean Zone (UCZ), maintained at ambient atmospheric pressure (~0.6 kPa/4.5 Torr)
  - UCZ separated from a vacuum cavity, housing a quadrupole mass spectrometer, by an aperture valve (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**

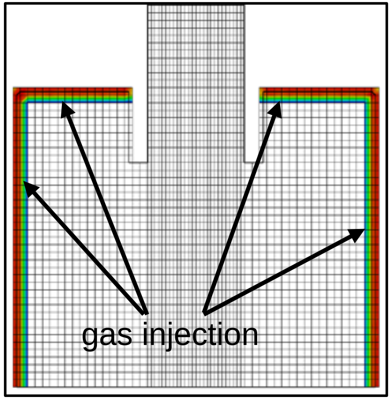
Simulation Approach

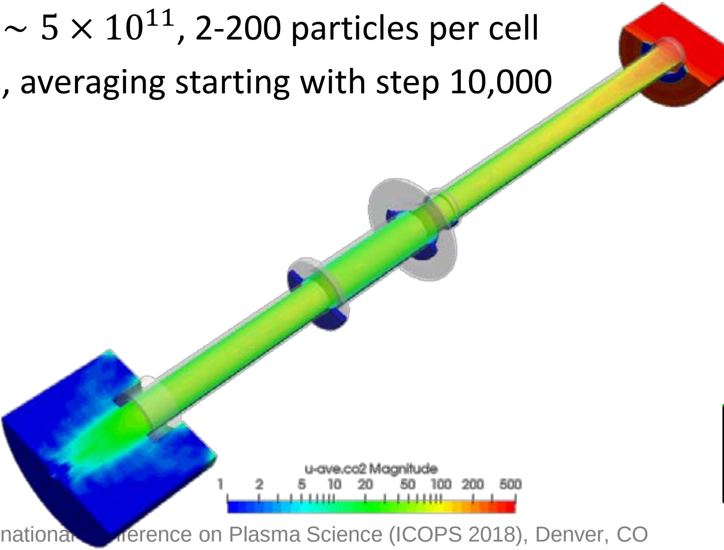
- The simulation needs to consider both plasma and gas dynamics
- Due to low operating pressure, ions and neutrals treated with a kinetic approach: Particle in Cell (PIC-MCC) for plasma and Direct Simulation Monte Carlo (DSMC) for gas
- Geometry exhibits axial symmetry, a 2D axisymmetric code used to 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*

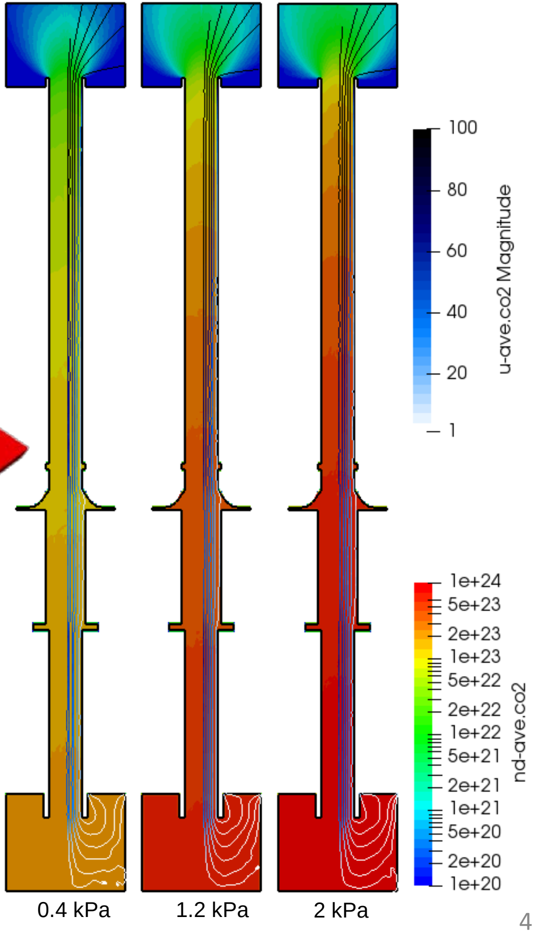


Gas Flow Results

- 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
- 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

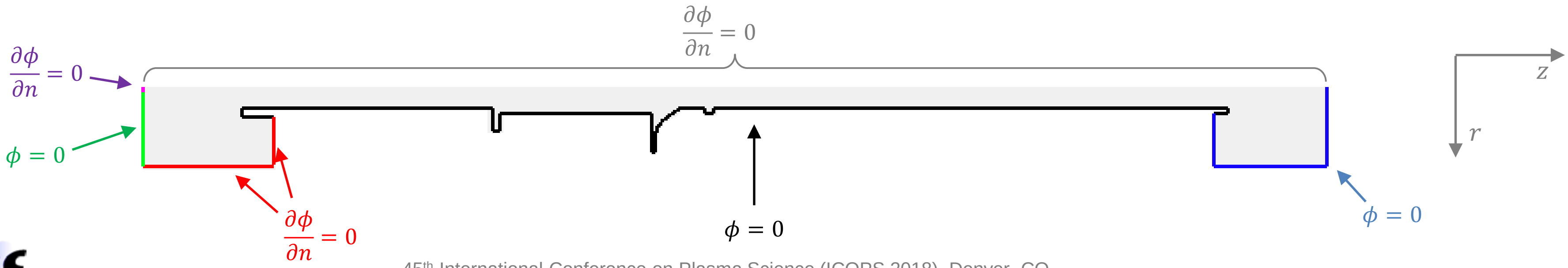






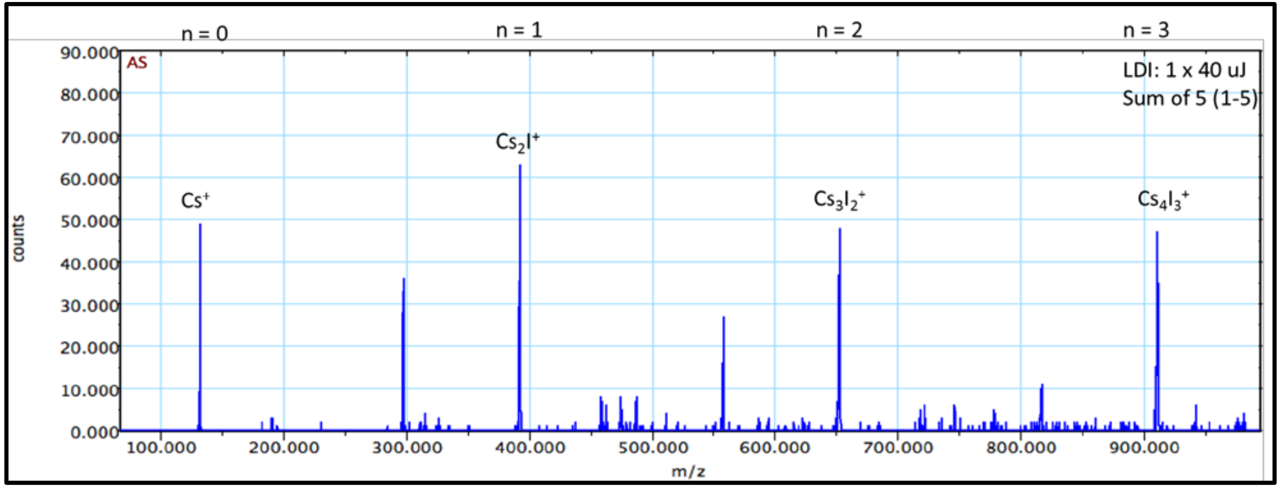
Plasma Numerical Model

- 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 15 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

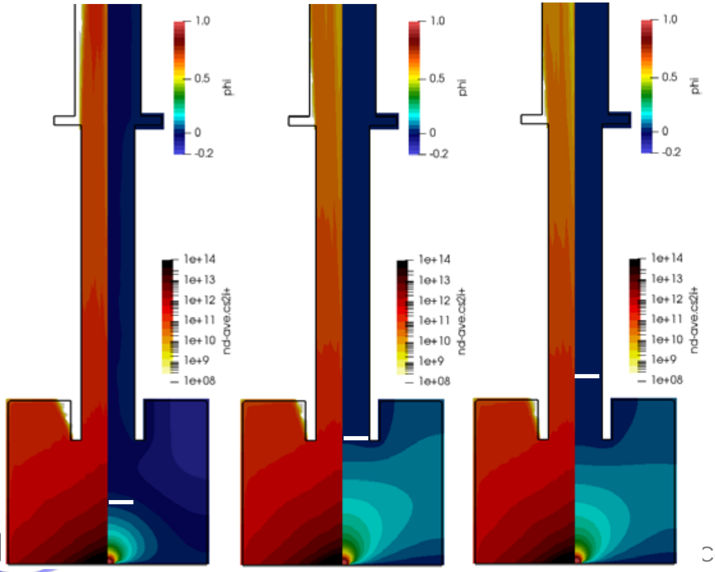


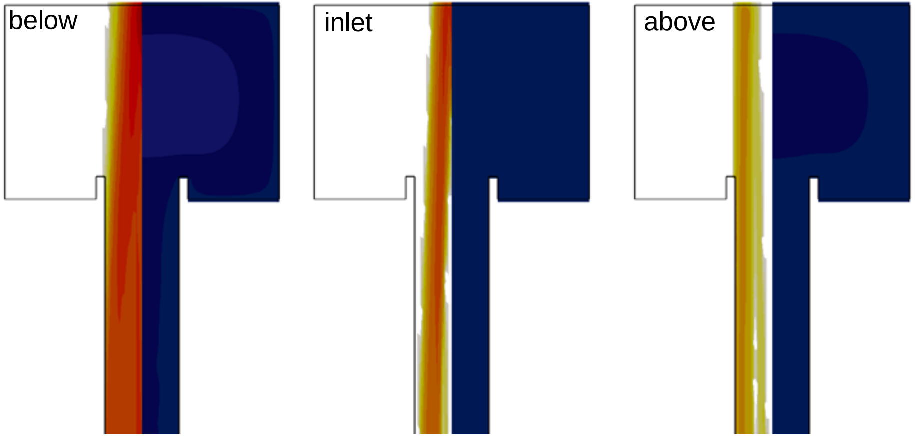
- GSFC measurements indicate approximately 10^9 ions (~0.1nC) generated per laser shot
  - Agrees well with a pit analysis at MPS, Goetz, et.al, "Characterization of mineral targets by laser desorption and ionization in preparation of the MOMA investigation onboard the EXOMARS-2018 rover" 47th Lunar 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

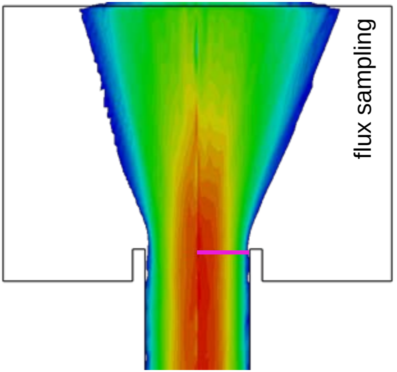
Simulations hence only suitable for obtaining qualitative trends



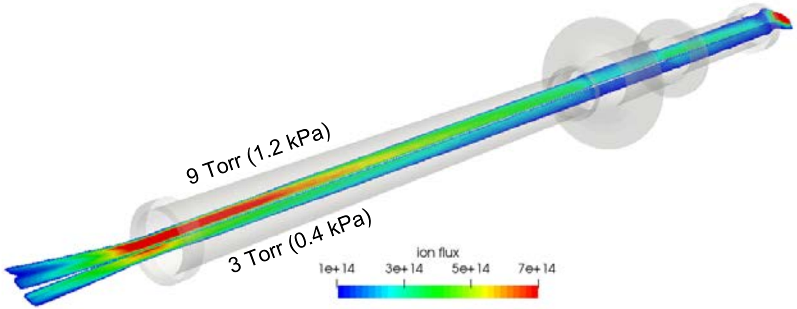


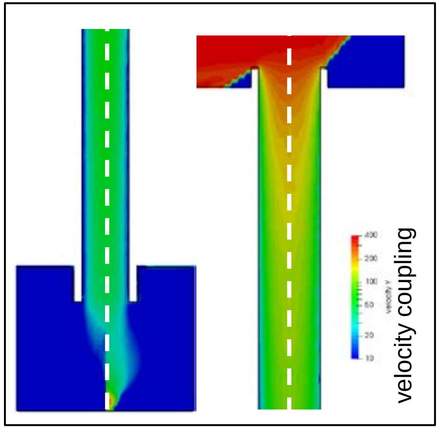
- The only difference between these cases is the n_0 sampling location (the white line), $\phi_0 = 0$ V, $kT_e = 1$ eV.
- Subsequent sims used the "inlet" configuration: sampling at guide inlet

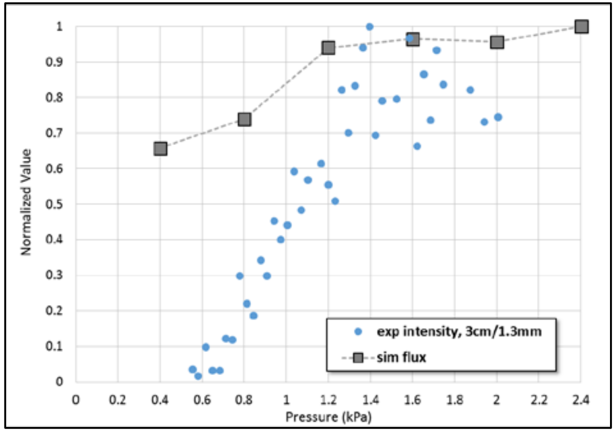
Pressure Dependence



- 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 $P\sim2$ kPa**
  - Mechanism unclear, possible suspects include surface charging and mass spectrometer saturation

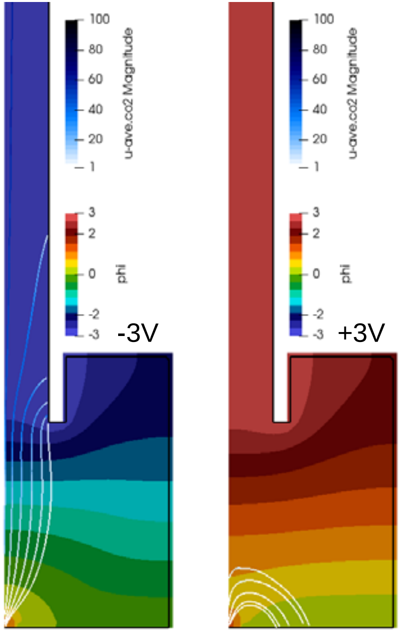


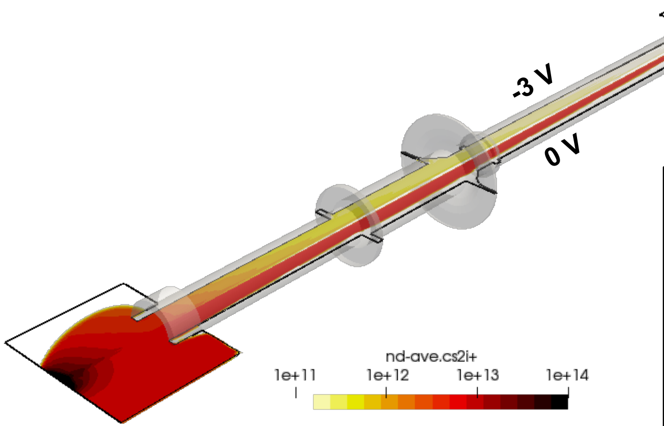


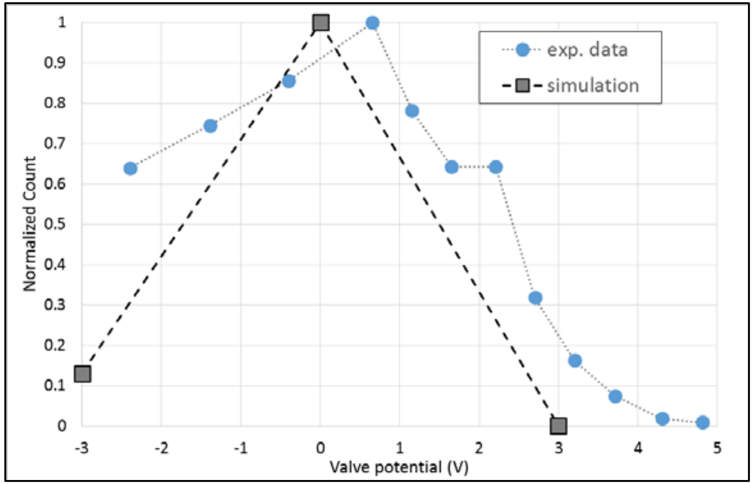


APV Bias Potential

- 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

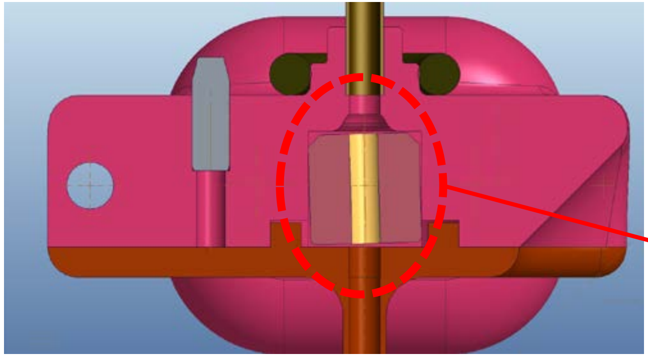


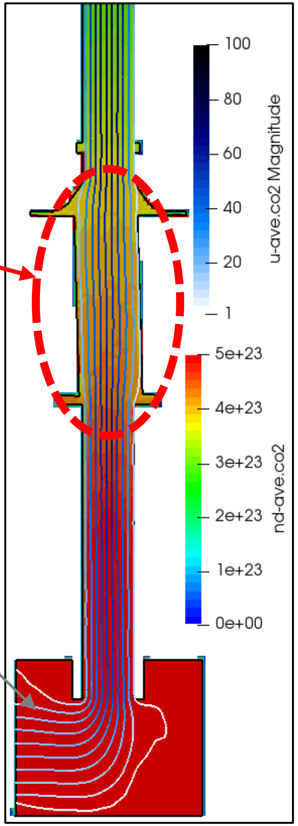




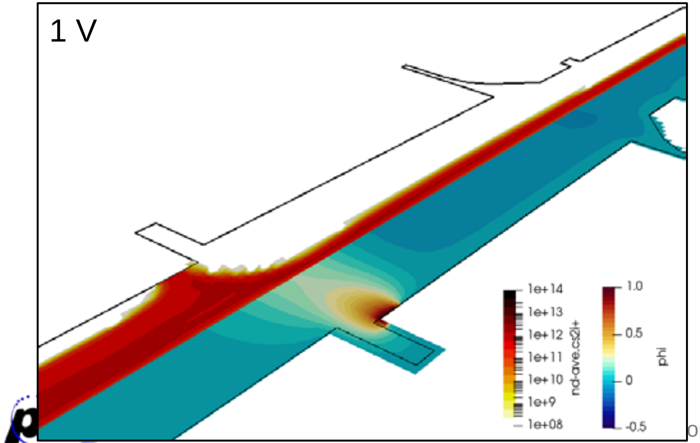
Additional Studies

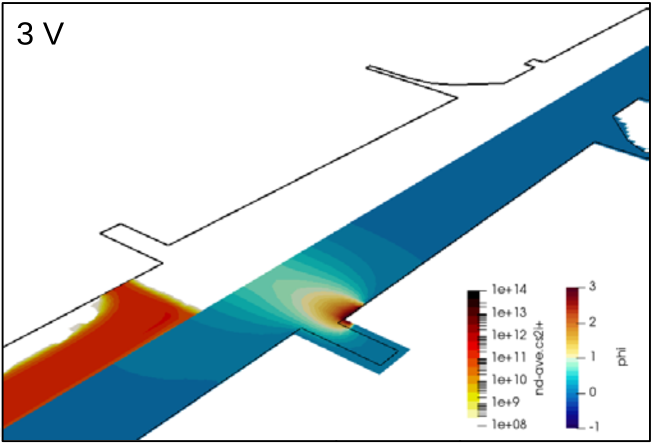
- Valve thru-hole not completely axial due to clearance between the upper and lower ion tube segments
  - Maximum rotation 1.6 degrees
  - No-longer axi-symmetric, simulated as a 2D XY slice
  - DSMC simulation does NOT indicate presence of vortices or similar flow feature that would inhibit ion flow
- 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





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?