Atelier Gaine Plasma - Marseille
06-11-2024

« IMPACT OF ION-NEUTRAL COLLISIONS IN FLUID MODELS OF PLASMA SHEATH »

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Summary

I. Context and motivation

II. A simple fluid model of a DC discharge

- Code framework
- Plasma fluid model with cold ion assumption

III. Role of collisions in plasma sheath formation

- First 1D gas discharge simulation results and analysis
- Comparison with fluid model from the literature and PIC results

IV. Impact of ion temperature dynamics in semi-collisional sheath

- Ion thermal energy equation
- Modified ion mobility formula
- Comparison of fluid results with self-consistent ion temperature computation and PIC results
- Ion-neutral charge exchange collisions

V. Conclusion & perspectives

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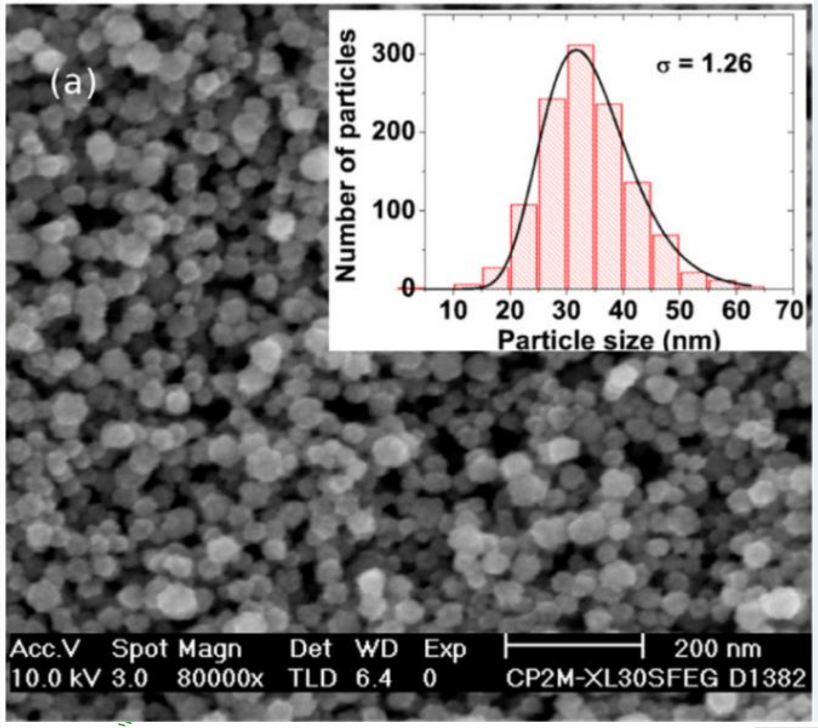
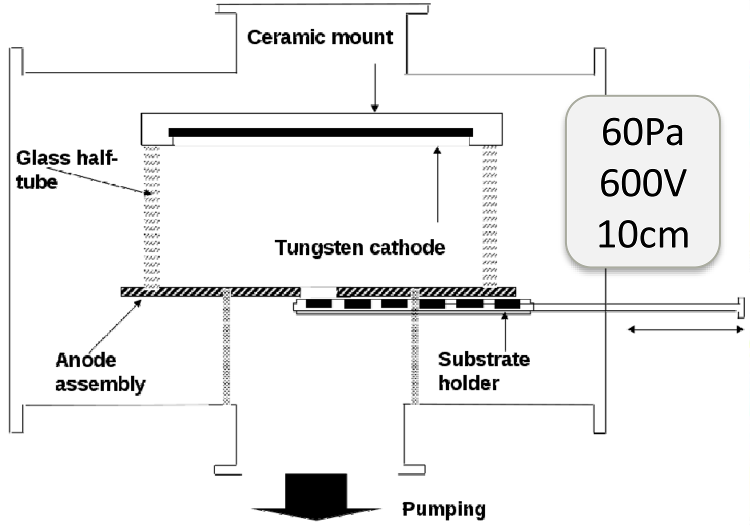
V. Conclusion & perspectives

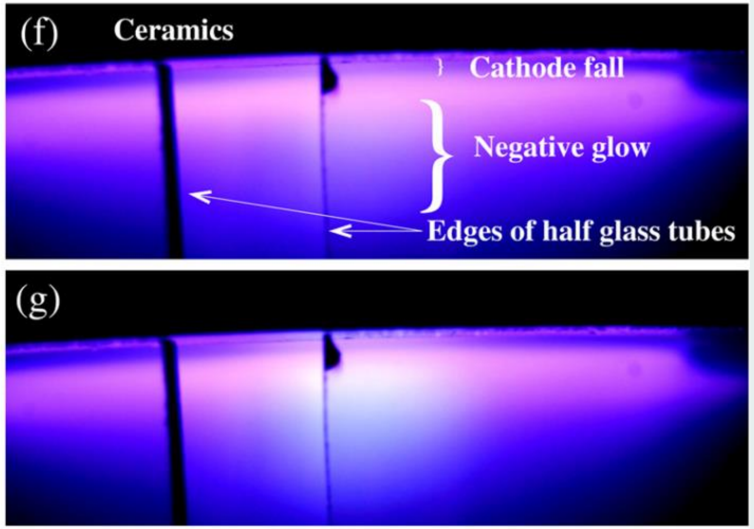
I. Context



- Direct-current glow discharge, moderate pressure range (10-100 Pa) can be used to grow nanoparticles [1]
- Cathode sputtering is generally the main source of matters for nanoparticle growth
- Acceleration of ions and production of fast neutral in the cathode sheath are essential to cathode sputtering



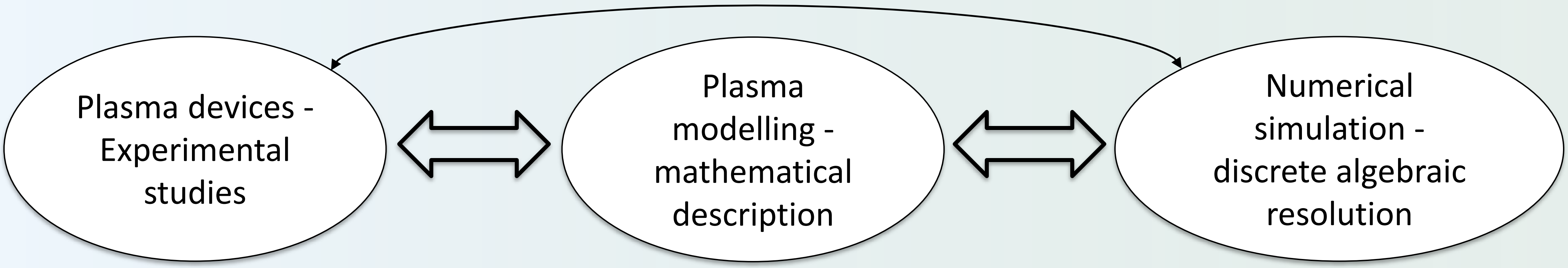
60Pa
600V
10cm



- Nanoparticle growth dynamics in DC glow discharge, including the cathode sheath ⇒ Development of a simulation code adapted to this regime.

[1] Kishor, Couëdel and Aranas, Phys Plasmas 20, 043707 (2013)

I. Context


Plasma devices - Experimental studies

Plasma modelling - mathematical description

Numerical simulation - discrete algebraic resolution

- Numerical tools usually based on kinetic or fluid description

- Kinetic approach gives evolution of distribution functions in the phase-space.
  - Advantage: Description of physical mechanisms at play in the velocity space
  - Drawback: sometime difficult to interpret and time consuming

- Fluid approach is a reduction of the kinetic approach by integrating the velocity space
  - Advantage: access to more intuitive physical quantities and faster, lighter
  - Drawback: lose information from the velocity space, closure approximations
  - => Fluid models can be improved by adding appropriate physical ingredients
- Physics of DC discharge and the formation of plasma sheath in moderate pressure range (semi-collisional regime) using both approaches

I. Context

Ion-neutral elastic collisionality level and its impact to ion temperature [2]

$$\boxed{\alpha = \frac{\lambda_D}{\lambda_{\text{imfp}}} = \lambda_D n_{\text{gas}} \sigma_{\text{in}}}$$

Collisionless regime

- Low pressure plasma sheath
- Energy conservation of particles

Transitional regime

- Focus of this work
- Widening of distribution functions implies an increase of the thermal energy
- Non Maxwellian sheaths

Collision dominated regime

- Bulk plasma, high pressure discharges
- Heavy charged particles thermalized with the neutral background

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[2] Sheridan and Goree. Physics of Fluids B: Plasma Physics 3.10 (1991)

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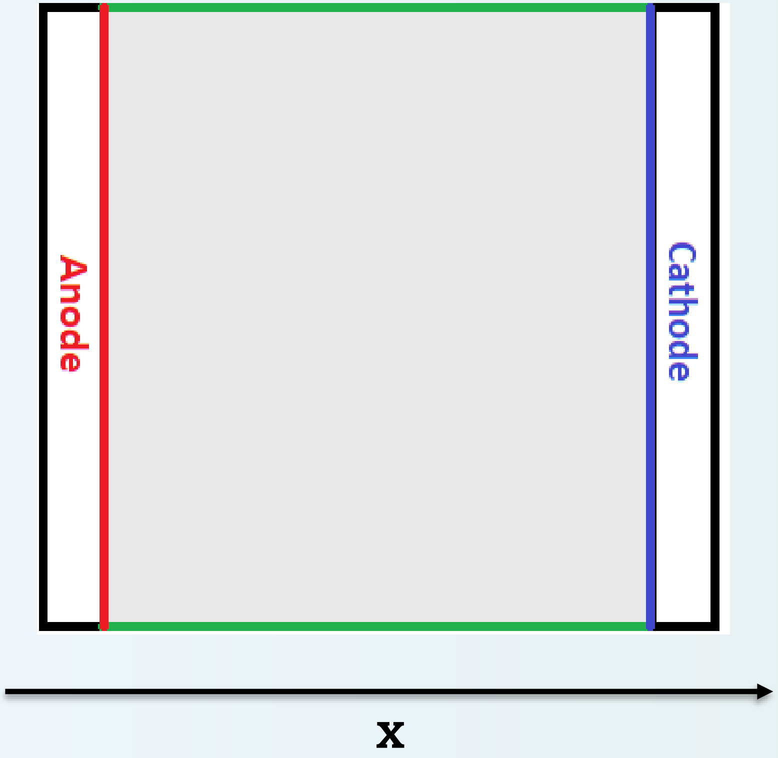
II. A simple fluid model of a DC discharge

Geometry and code Framework



- New plasma simulation code
- Fluid model in 1D discharge geometry
- DC discharge without magnetic field
- Electrons and one positive ion species considered in argon gas

- Fortran, MPI parallelization (future expansion to 2D/3D)
- Time resolution : explicit 4th order Runge-Kutta / 3rd order SSP Runge-Kutta
- Spatial discretization : 2^{nd} order centered Finite Difference scheme with shifted indices for vectors for numerical stability

II. A simple fluid model of a DC discharge

System of fluid equations – cold ion assumption

$n_e(t)$

$n_i(t)$

$$\frac{\partial n_s}{\partial t} + \nabla \cdot \vec{\Gamma}_s = S_s$$

$v_i(t)$

$$\frac{\partial \vec{v}_i}{\partial t} + (\vec{v}_i \cdot \nabla)\vec{v}_i + \frac{\nabla(n_i k_B T_i)}{n_i m_i} = \frac{e}{m_i}\vec{E} - (\nu_{in} + \nu_{iz}\frac{n_e}{n_i})\vec{v}_i$$

$\varepsilon_e(t)$

$$\frac{\partial(n_e \varepsilon_e)}{\partial t} + \nabla \cdot \vec{\Gamma}_{\varepsilon e} = -\vec{\Gamma}_e \cdot \vec{E} - \theta_e n_e$$

- Electron drift-diffusion flux

$$\vec{\Gamma}_e^0 = -\mu_e n_e \vec{E} - \nabla(D_e n_e)$$

- Poisson’s equation

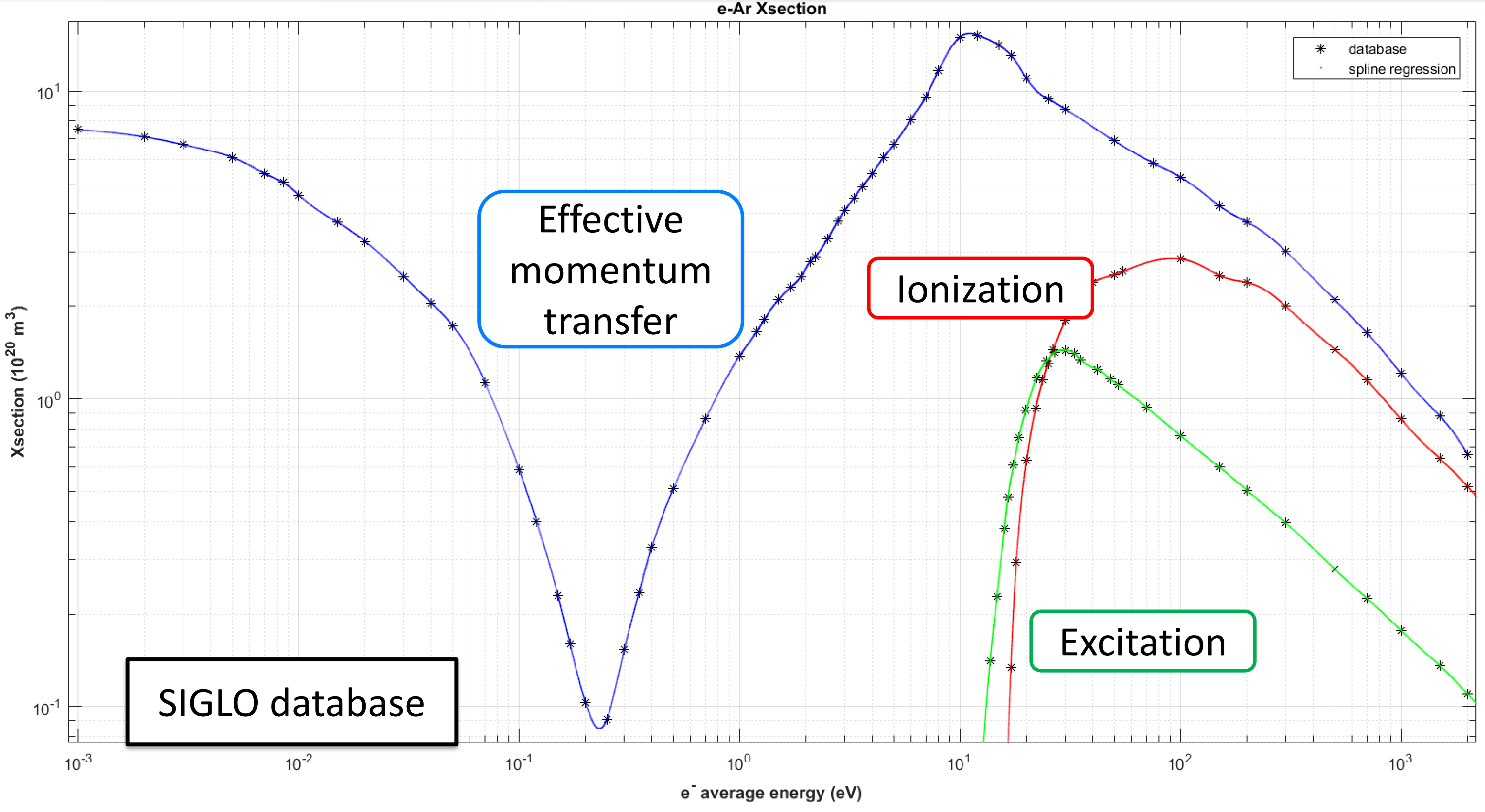
$$\Delta V = -\frac{e}{\varepsilon_0}(n_i - n_e)$$

- Fluid equations are moments of the Boltzmann-Vlasov equation
- Ion energy equation not solved, assuming cold ions at 300K all along the simulation
  - Thermalization due to collisions in the bulk plasma (weak electric field)
  - Collisionless sheath
- Poisson equation for sheath potential resolution (no magnetic field)

Bittencourt. Fundamentals of Plasma Physics. 3rd ed. Springer New York (2004)

Hagelaar, *“Modelling methods for low-temperature plasmas”*, Université Toulouse III Paul Sabatier (2008)

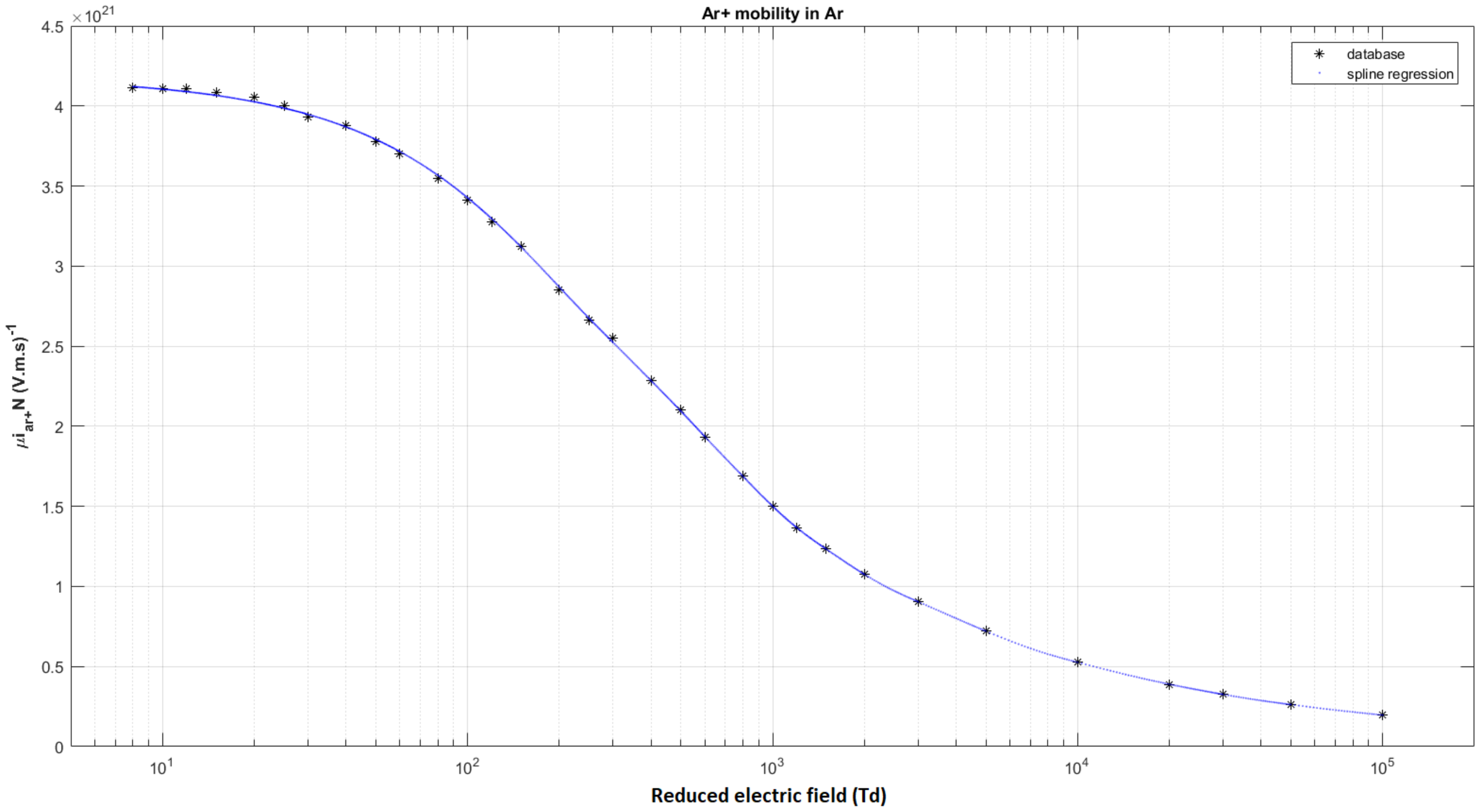
II. A simple fluid model of a DC discharge



[3] Pitchford and Boeuf, The SIGLO database (2014). URL http://www.lxcat.net.

II. A simple fluid model of a DC discharge

Experimental Ar+/Ar mobility database



Ellis76 [4],
Phelps91 [5]

$\vec{E}$/N, 300K

$$\nu_{in} = N\frac{e}{m_i \mu_i N}$$

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[4] Ellis, Rai, McDaniel, Mason and Viehland, Dat. and Nucl. Data Tables, 1976, 17: 177.

[5] Phelps, Journal of Physical and Chemical Reference Data, 1991, 20.3: 557-573.

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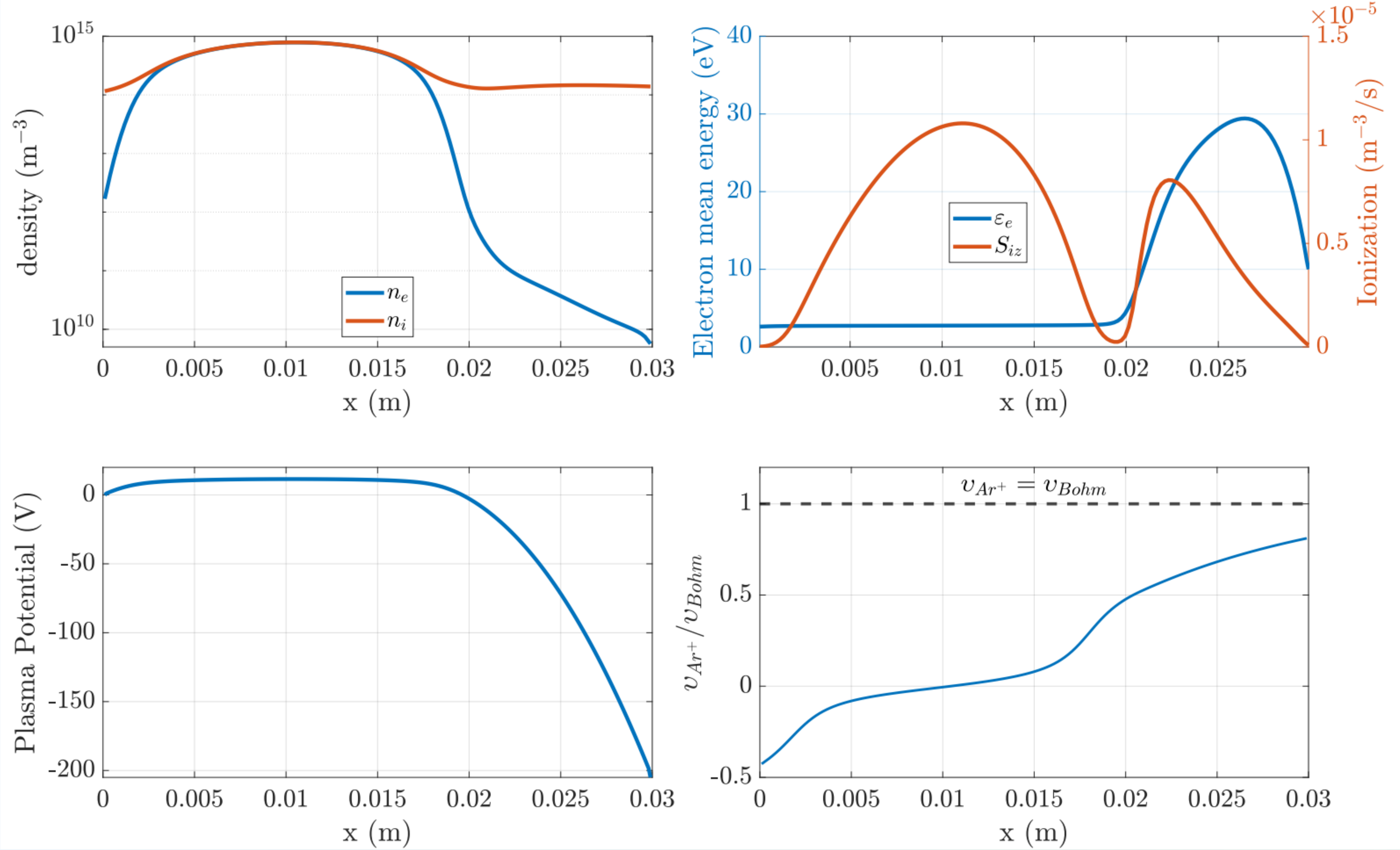
III. Validation of the model

- Test simulation parameters for the cold ion plasma fluid model

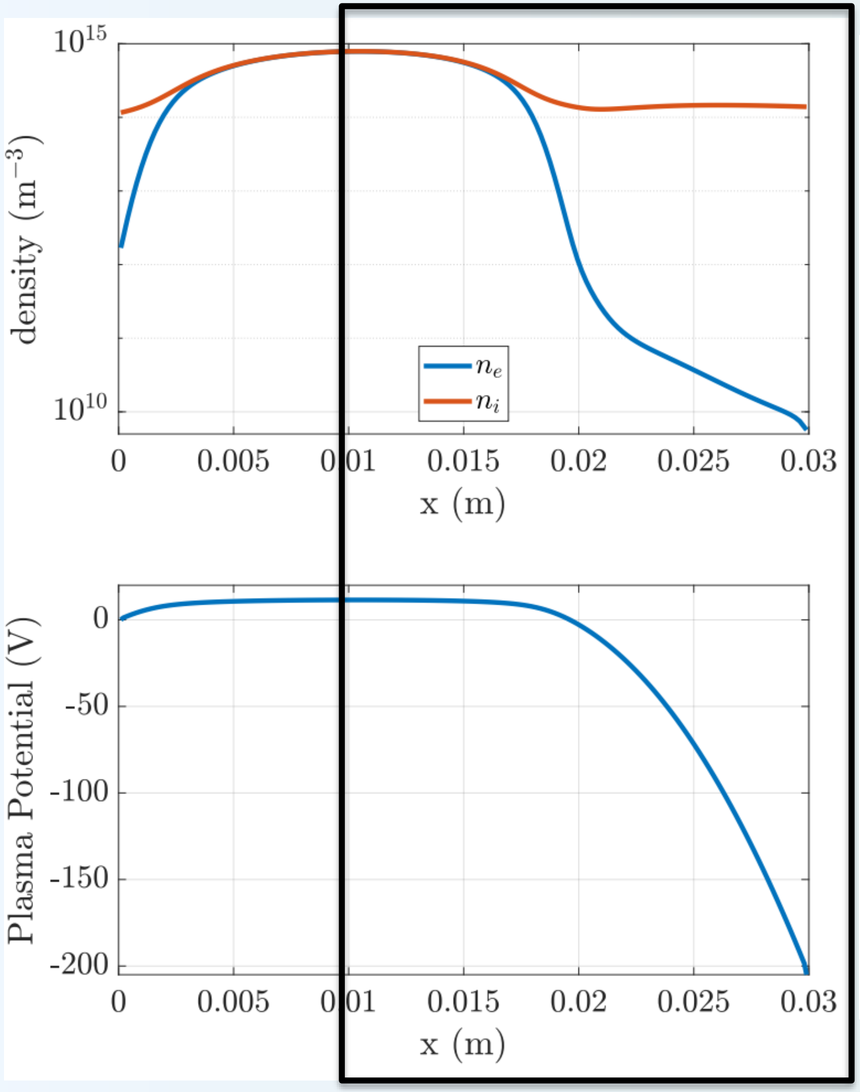
L	**Initial n_{plasma}**	**Initial ε_e**	**V_{bias}**	**P**	**T_{gaz}**	**γ**
3 cm	10^{13} m^{-3}	2 eV	-205 V	30 Pa	300 K	0.05

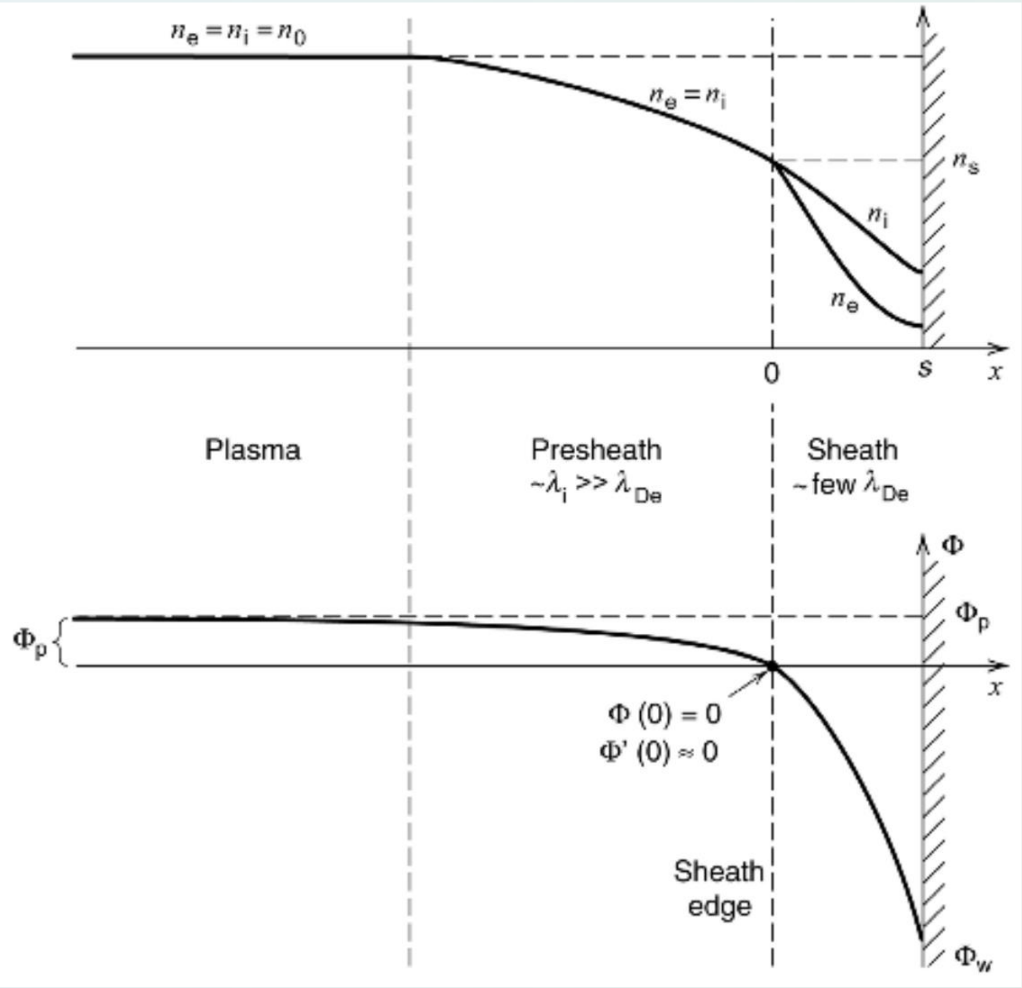
- 1D fluid discharge simulation including sheaths
- Background gas temperature fixed at 300K
- Ion temperature also fixed at 300K (cold ions)

III. First 1D gas discharge simulation results and analysis



III. First 1D gas discharge simulation results and analysis

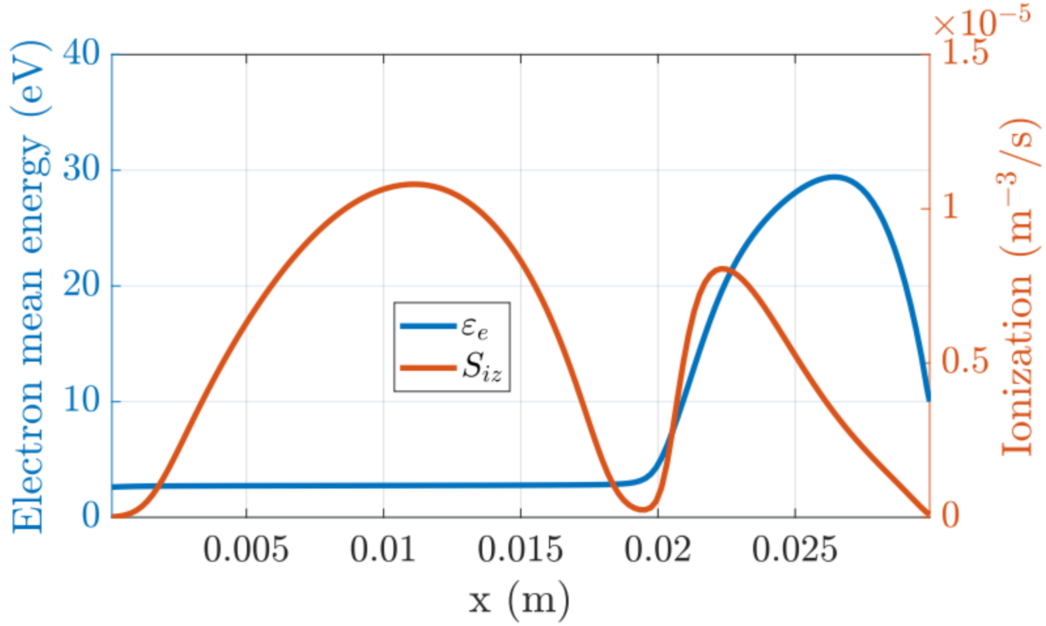


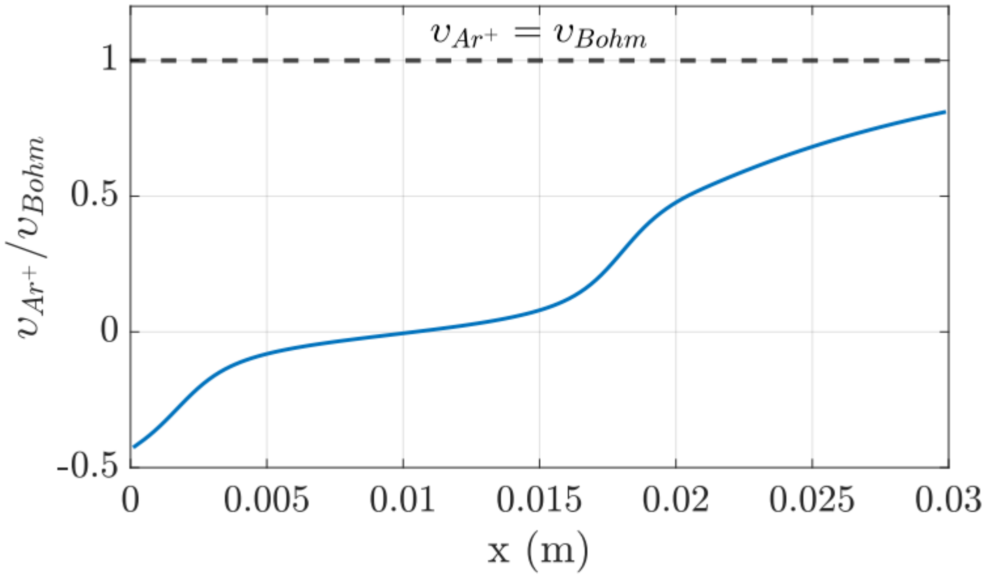


- Plasma potential profile show good agreement
- Disagreement with the collisionless theory in the cathode sheath

Lieberman and Lichtenberg. *Principles of Plasma Discharges and Materials Processing*. Ed. by John Wiley & Sons. John Wiley & Sons, Inc. (2005)

III. First 1D gas discharge simulation results and analysis





- Disagreement with the collisionless theory of cathode sheath
  - Ion density profile
  - Slow calculated ion exit velocity
  - Non negligible ionization source term inside the sheath
- -> Validation with fluid results from the literature and kinetic simulation results

III. Comparison with fluid model from the literature and PIC results

- Simulation parameters from SOMAFOAM and Deconinck's fluid models [8, 9]

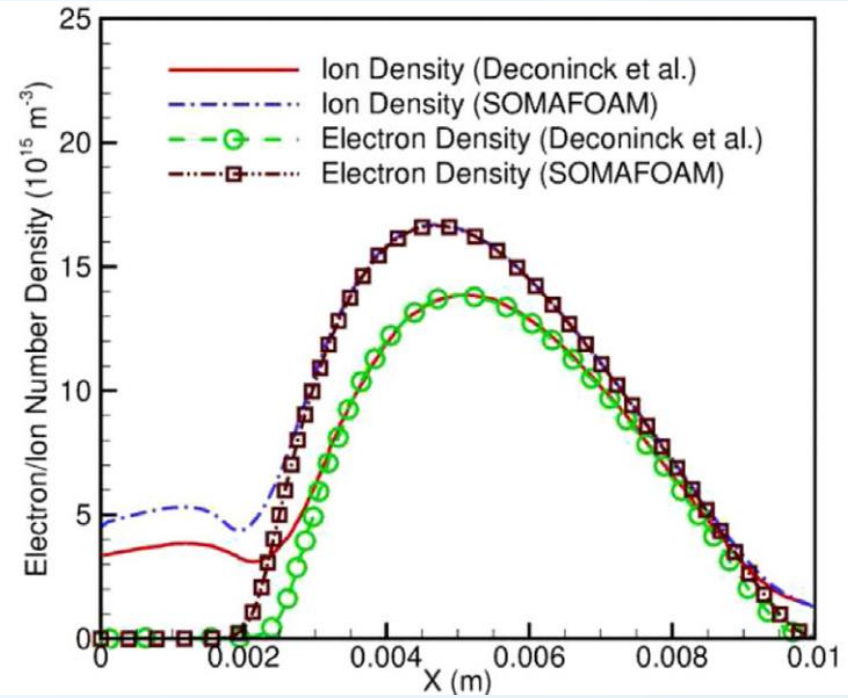
L	Initial n_{plasma}	Initial ε_e	V_{bias}	P	T_{gaz}	γ
1 cm	10^{14} m^{-3}	2 eV	250 V	130 Pa	300 K	0.05

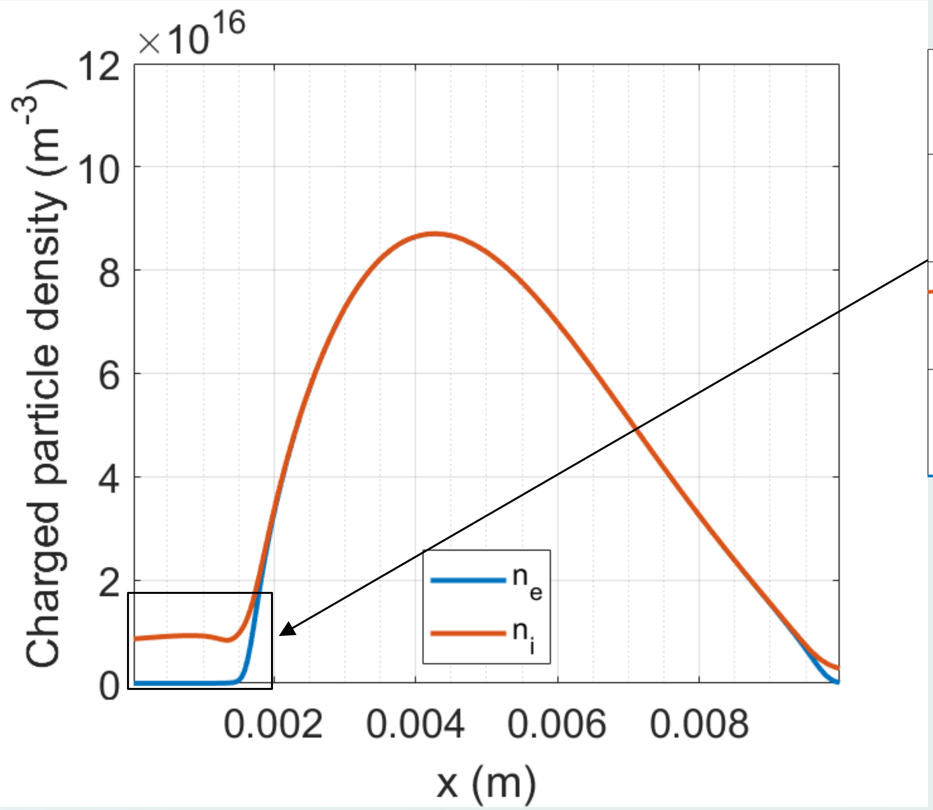
- 1D fluid discharge simulation including sheaths
- Background gas and ion temperature fixed at 300K
- Further validation with kinetic simulation

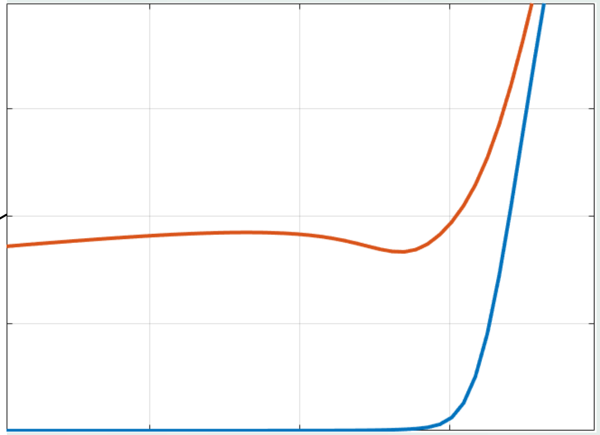
[8] Abhishek Kumar Verma, Computer Physics Communications, 263-107855 (2021)

[9] Deconinck, Mahadevan and Raja, Comput. Phys. 228 (12) (2009) 4435–4443.

III. Comparison with fluid model from the literature and PIC results







- Argon
- 1cm
- 250V DC
- 1Torr ≈ 130Pa

- Our code qualitatively recovers other published fluid simulation results
- Ion density hump in the cathode sheath also observed in fluid code results presented in the literature [8,9]
- Further validation of the code using a commercial PIC code VSIM from TechX [10]

[8] Abhishek Kumar Verma, Computer Physics Communications, 263-107855 (2021)
[9] Deconinck, Mahadevan and Raja, Comput. Phys. 228 (12) (2009) 4435–4443.
[10] Tech-X Vsim: Multiphysics simulation software for your complex problems. https://www.txcorp.com/vsim/

III. Comparison with fluid model from the literature and PIC results

- Simulation parameters used in the PIC code

L	Initial n_{plasma}	Initial ε_e	V_{bias}	P	T_{gaz}	γ
1 cm	10^{14} m^{-3}	2 eV	250 V	130 Pa	300 K	0.05

- Background neutral gas temperature fixed at 300K
- The treatment of collisions slightly differ in fluid codes and the PIC code

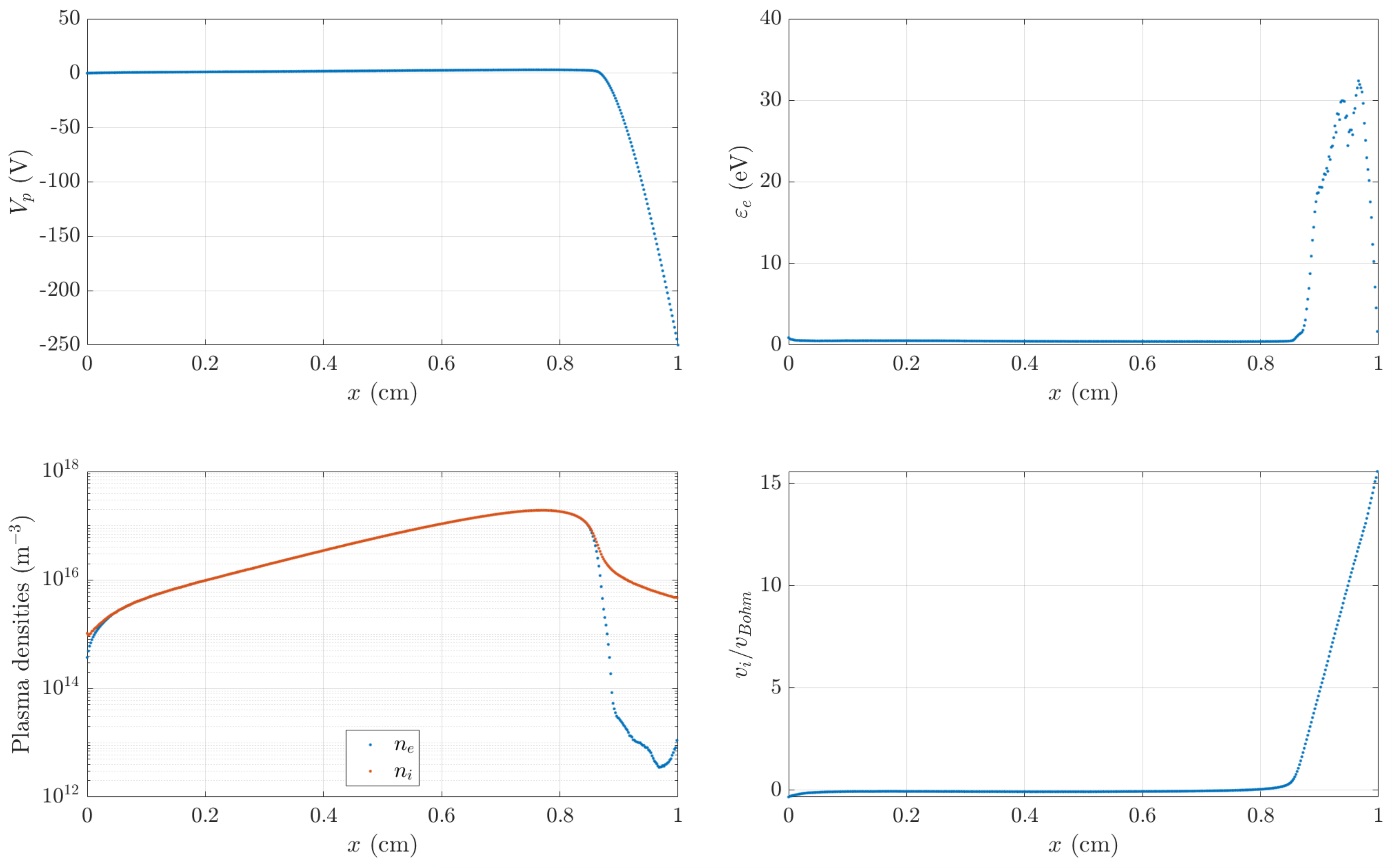
Fluid

- Siglo database, Maxwellian electrons
- E-n ionization, elastic collision
- i-n elastic collisions (derivation of fluid equations), but other collisions are partially taken into account (experimental database)

PIC

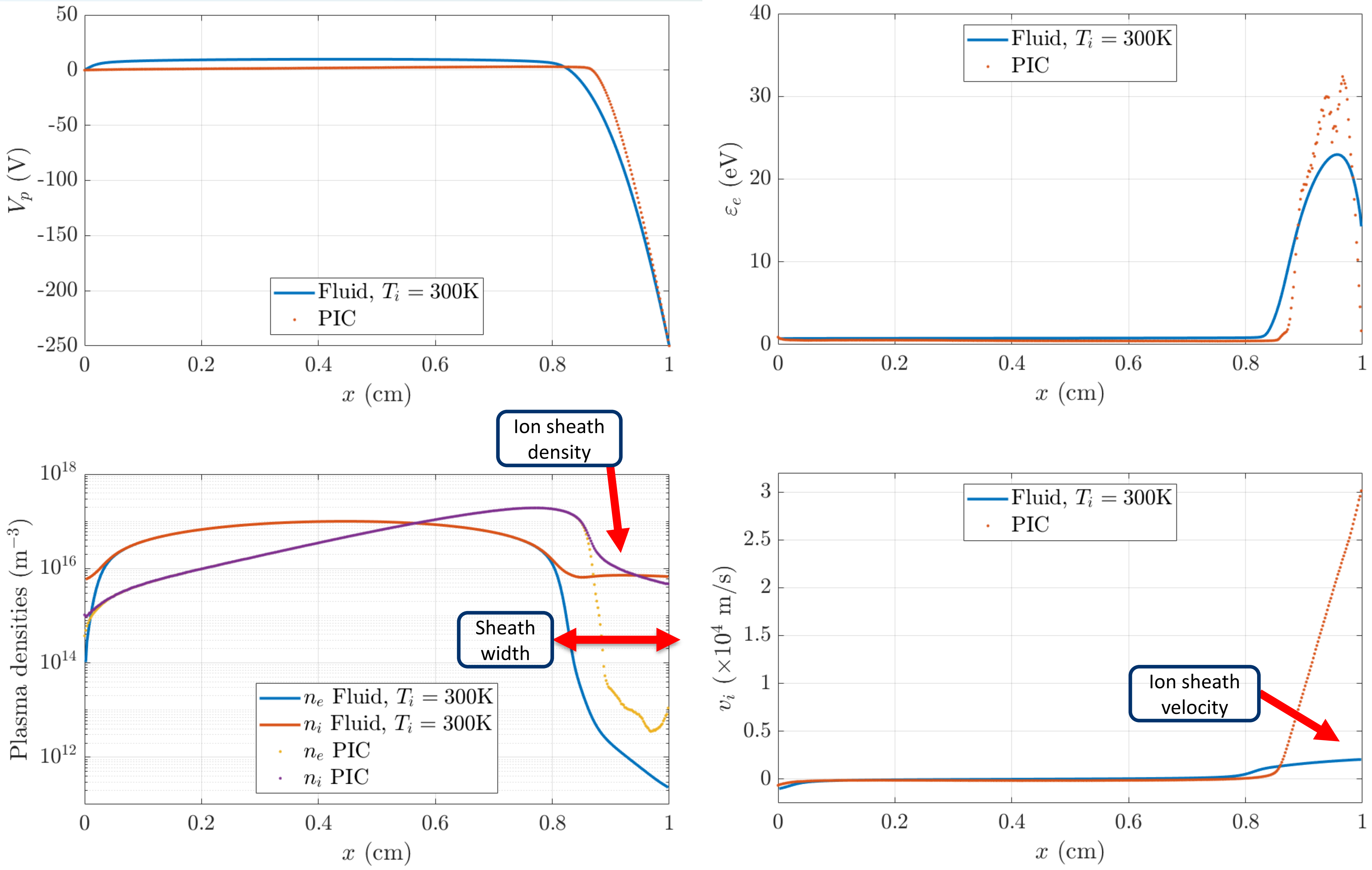
- Siglo database
- E-n ionization, elastic collision
- 2 cases presented
    - i-n elastic collisions only
    - i-n elastic and charge exchange collisions

III. Comparison with fluid model from the literature and PIC results



- PIC simulation result with only ion-neutral elastic collisions
- Disagreement with the fluid results in the cathode sheath
    - Ion density profile
    - ion exit velocity

III. Comparison with fluid model from the literature and PIC results

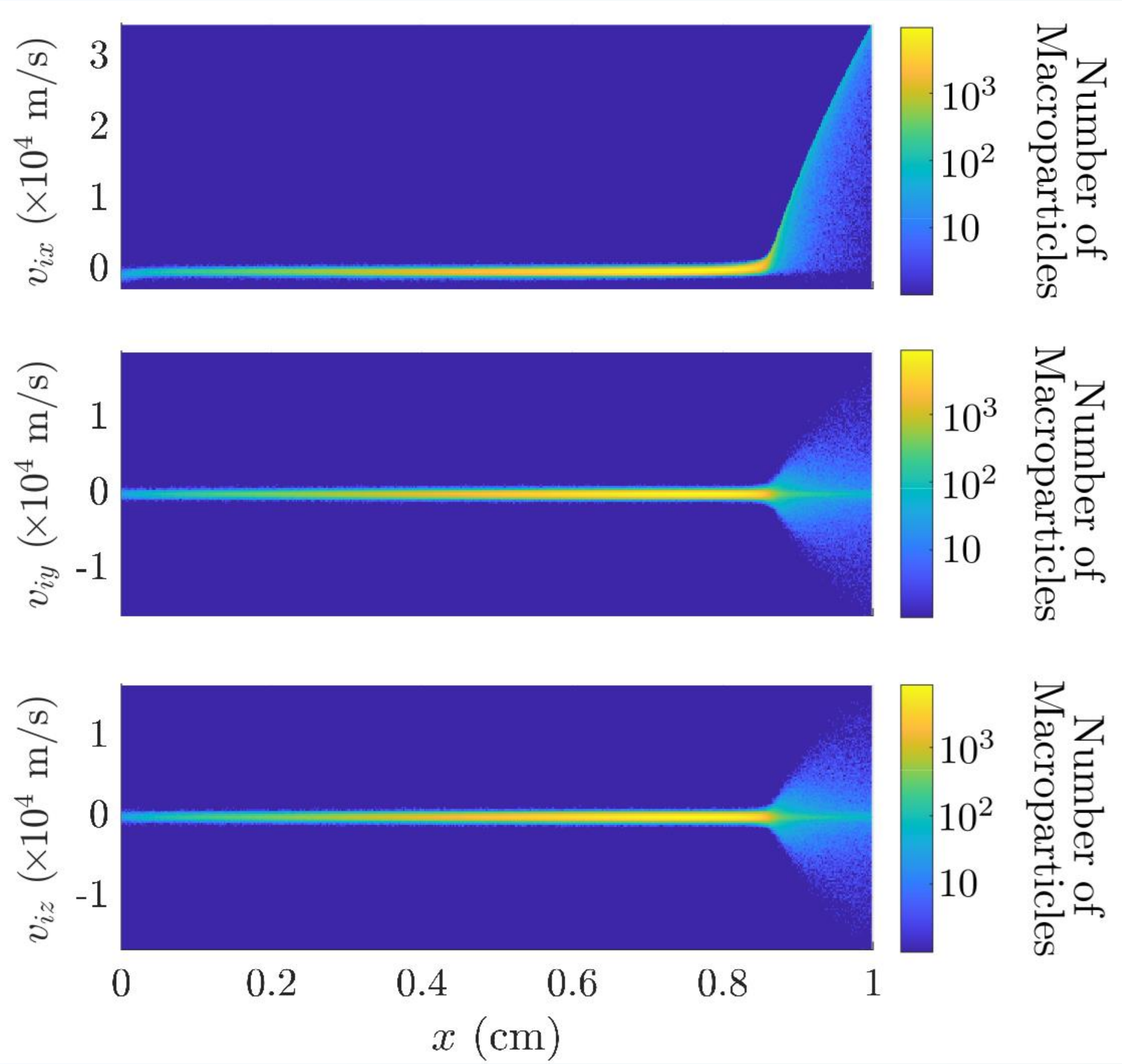


Ion sheath density

Sheath width

Ion sheath velocity

III. Comparison with fluid model from the literature and PIC results

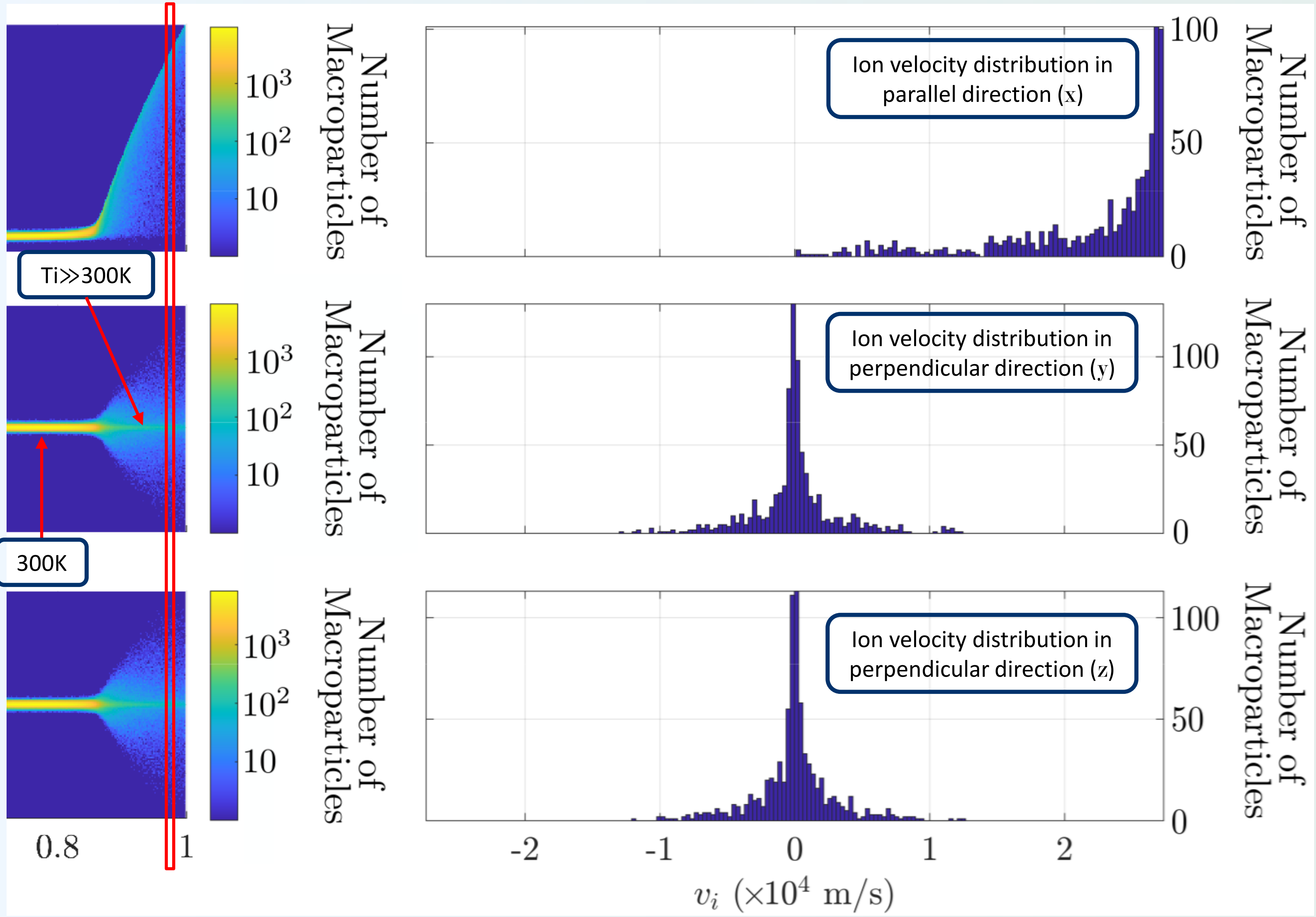


- 1D3v PIC code simulation using VSIM

- Plasma discharge simulation using the same parameters as the fluid code, following the (x) direction

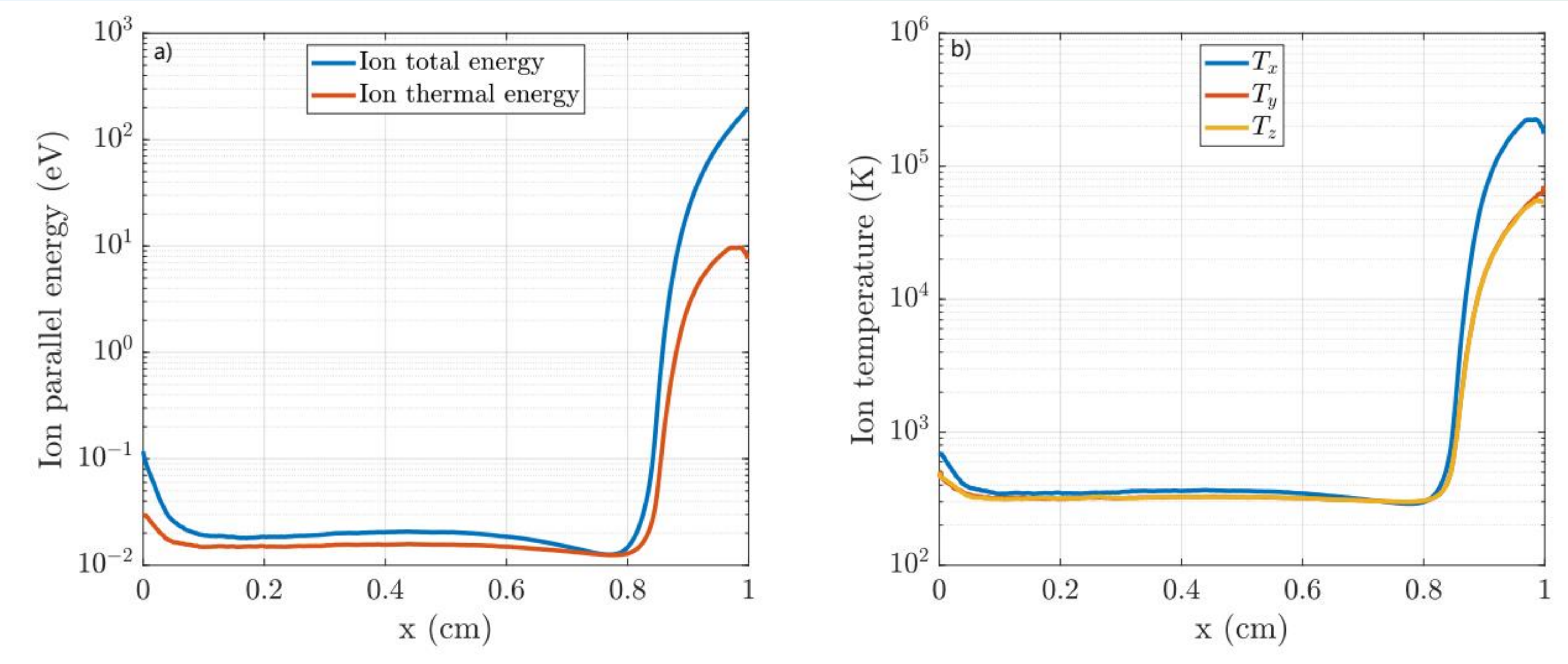
- Ion macroparticle velocities in parallel (x) and perpendicular (y, z) directions

III. Comparison with fluid model from the literature and PIC results



- Ion velocity distribution inside the cathode sheath (red box at 9.6mm)
- Symmetric perpendicular direction
- Asymmetric parallel direction – electric field acceleration
- Width of the distribution proportional to “temperatures”

III. Comparison with fluid model from the literature and PIC results



- Noticeable heating of the ions within the cathode sheath
- Anisotropy, parallel/perpendicular directions

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IV. Expansion of the plasma fluid model

Ion thermal energy equation

$\boxed{\varepsilon_{i,th}(t)}$

$$\boxed{\frac{\partial n_i \varepsilon_i^{th}}{\partial t} + \nabla \cdot (n_i \varepsilon_i^{th} \vec{v}_i) + p_i (\nabla \cdot \vec{v}_i) + \nabla \cdot \vec{q}_i = \nu_i n_i \left[\varepsilon_i^{kin} - \left(\varepsilon_i^{th} - \varepsilon_{gas}^{th}\right)\right]}$$

- The ion momentum equation is already solved
- Ion thermal energy equation implemented
- $\boxed{\nu_i = \nu_{in} + \nu_{iz} \frac{n_e}{n_i}}$ reflects the elastic collisions (ν_{in}) and the creation of cold, immobile ions from neutrals by impact ionization ($\nu_{iz} \frac{n_e}{n_i}$)
- Anisotropy in ion velocity distribution -> 1D fluid model along the parallel direction (of interest) calculating the ion parallel kinetic temperature

$$\boxed{\varepsilon_i^{th} = \frac{1}{2} k_B T_i}$$

- The closure relation on the heat flux assumes a Fick's law-like condition [11], but in 1D configuration

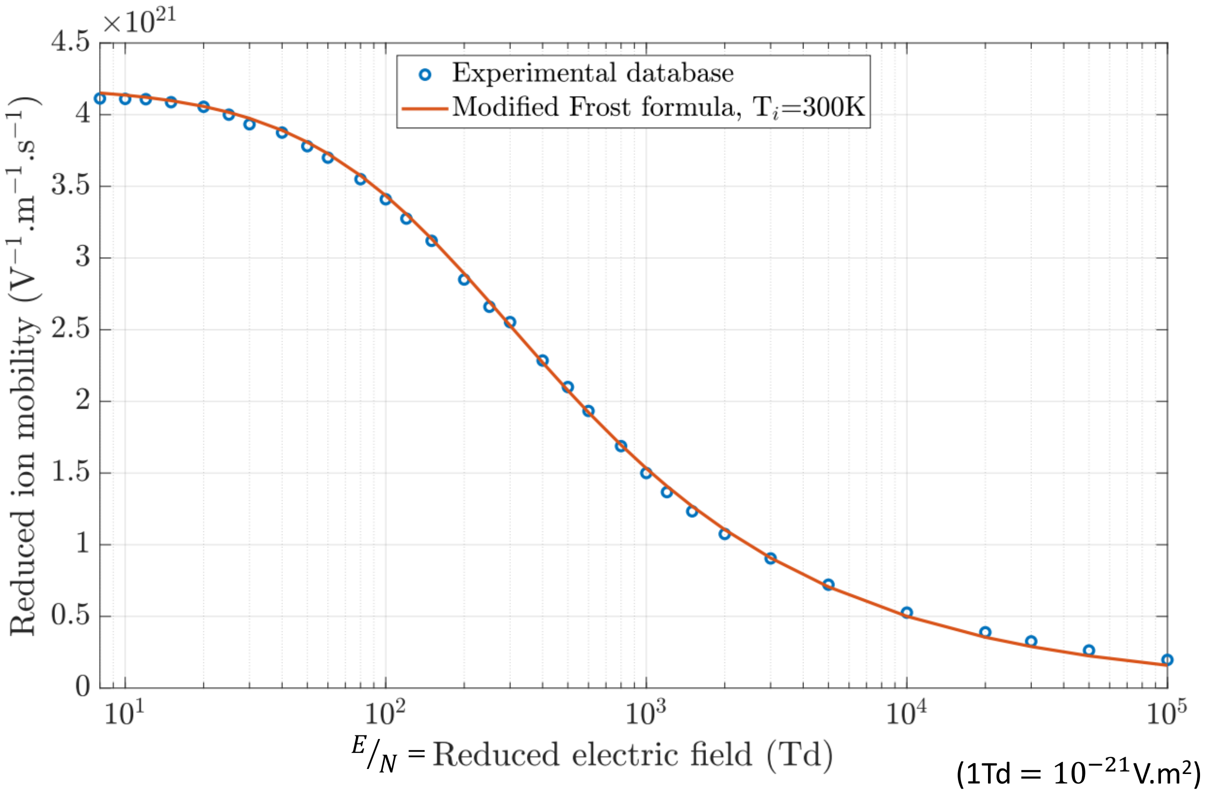
$$\boxed{\vec{q}_i = -\frac{5}{6} \frac{n_i k_B T_i}{m_i \nu_i} \nabla (k_B T_i)}$$

Bittencourt. Fundamentals of Plasma Physics. 3rd ed. Springer New York (2004)

[11] Hunana, Passot, Khomenko, et al., The Astrophysical Journal Supplement Series 260.2 (2022)

Kinetic Theory of Mobility and Diffusion: Section 5.3

IV. Modified ion mobility formula



(1Td = 10^{-21}V.m^2)

Figure II.8. – Comparison of the experimental database of argon ion mobility and the numerical results found using Khrapk's empirical formula (neutral temperature set to 300K).

- Temperature gradient term and ion-neutral collision frequency

$$\frac{\partial \vec{v}_i}{\partial t} + (\vec{v}_i \cdot \nabla)\vec{v}_i + \frac{\nabla(n_i k_B T_i)}{n_i m_i} = \frac{e}{m_i}\vec{E} - (\boxed{\nu_{in}} + \nu_{iz}\frac{n_e}{n_i})\vec{v}_i$$

- Theoretical calculations suggest one, two or three temperature models for ion mobility [12,13,14]

- Experimental data base at 300K, ion temperature dependency can be added using empirical formula [15, 16]

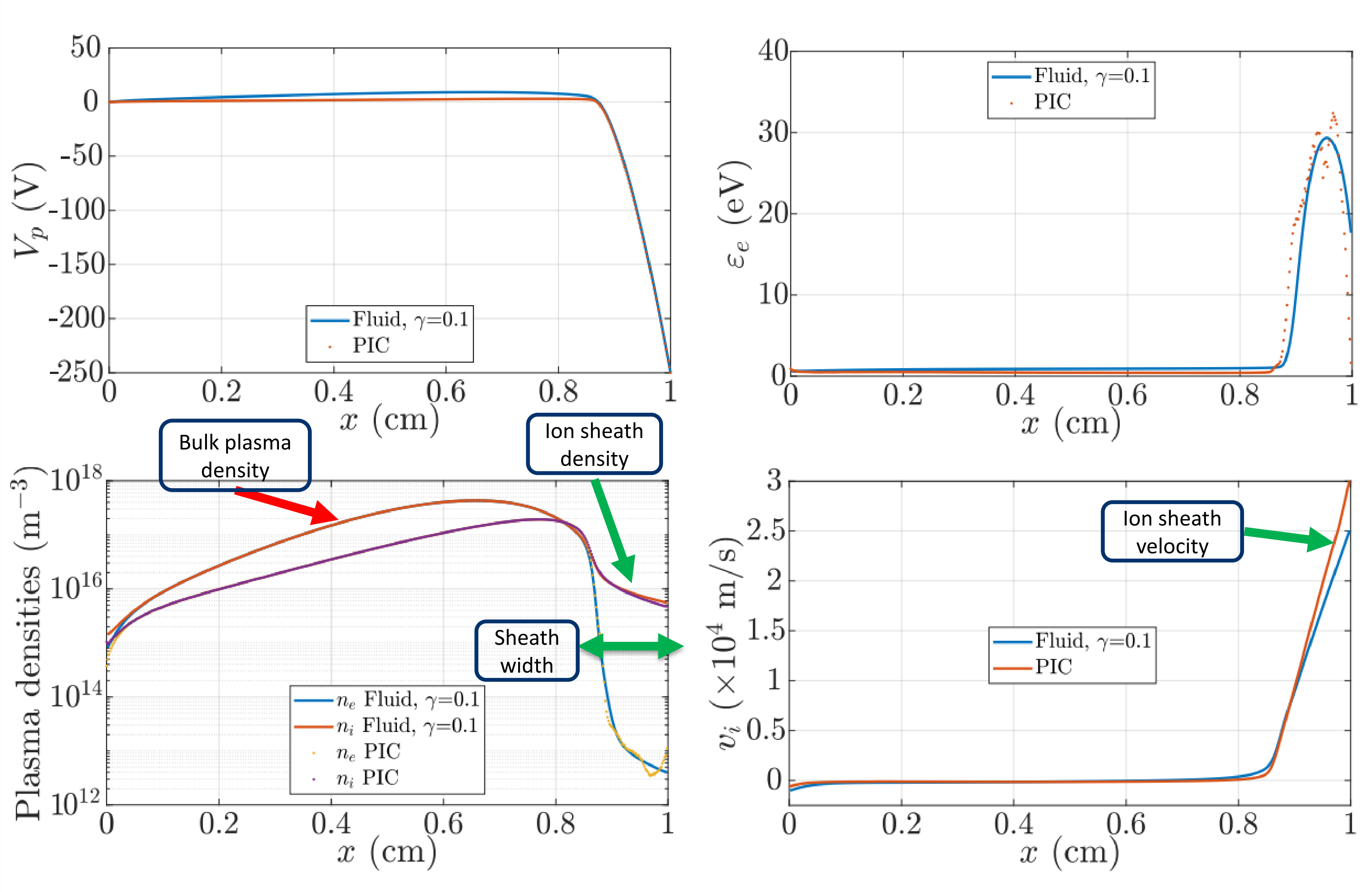
$$\frac{\mu_i E}{v_{T_i}} = A_t\left[1 + \left(B_t\frac{E}{N}\right)^{C_1}\right]^{-\frac{1}{2C_2}}\frac{E}{N}$$

- This impacts our fluid model through the ion-neutral elastic collision frequency ν_{in} which is obtained from the ion mobility

$$\nu_{in}(T_i, T_N, \frac{E}{N}) = \frac{e}{m_i \mu_i(T_i, T_N, \frac{E}{N})}$$

[12] Viehland and Mason, Annals of Physics, Volume 110, Issue 2 (1978)
[13] Lin, Viehland and Mason, Chemical Physics, Volume 37, Issue 3 (1979)
[14] McDaniel and Mason, *Transport Properties of Ions in Gases,* John Wiley & Sons, Inc. (1988)
[15] Khrapak et. Al., *High Temp.*, 2020
[16] Frost, *Phys. Rev.*, 1957

IV. Comparison of fluid results with self-consistent ion temperature computation and PIC results



- Improved agreement between fluid and PIC results in the cathode sheath
- Higher secondary electron emission rate in fluid model for fit
- Semi-collisional regime particularly sensitive to the assumptions of the model

IV. Comparison of fluid results with self-consistent ion temperature computation and PIC results

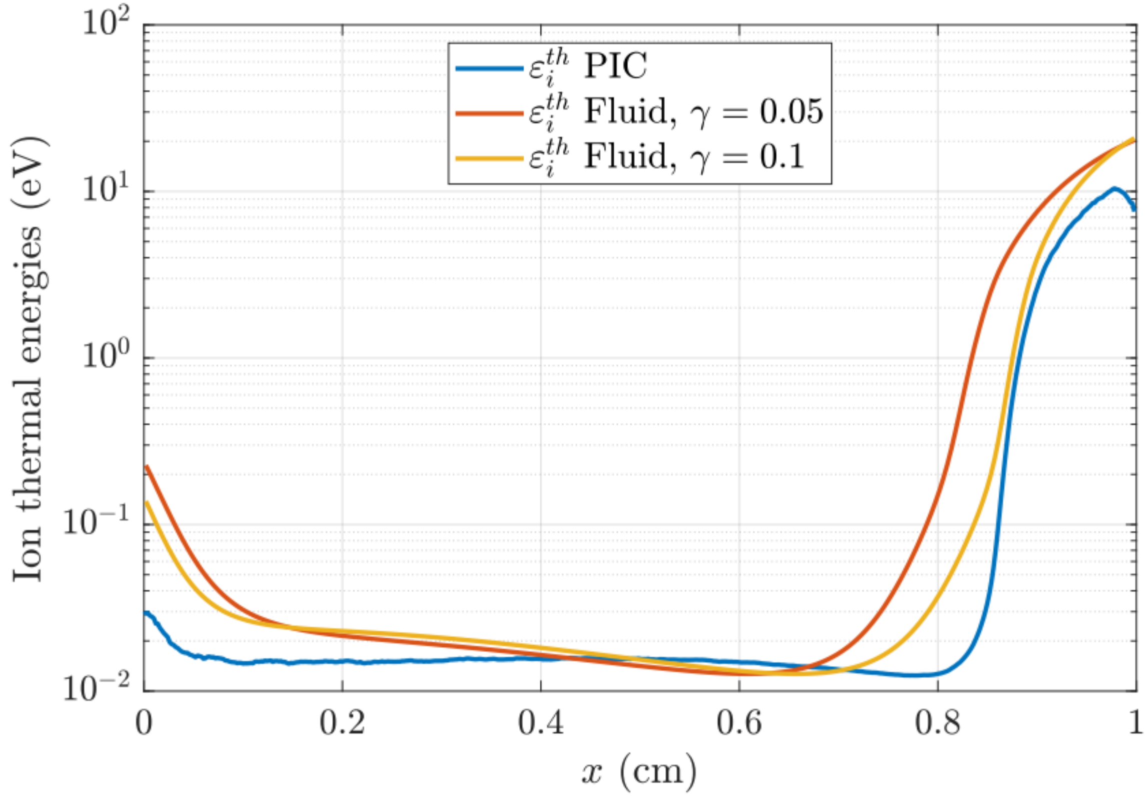
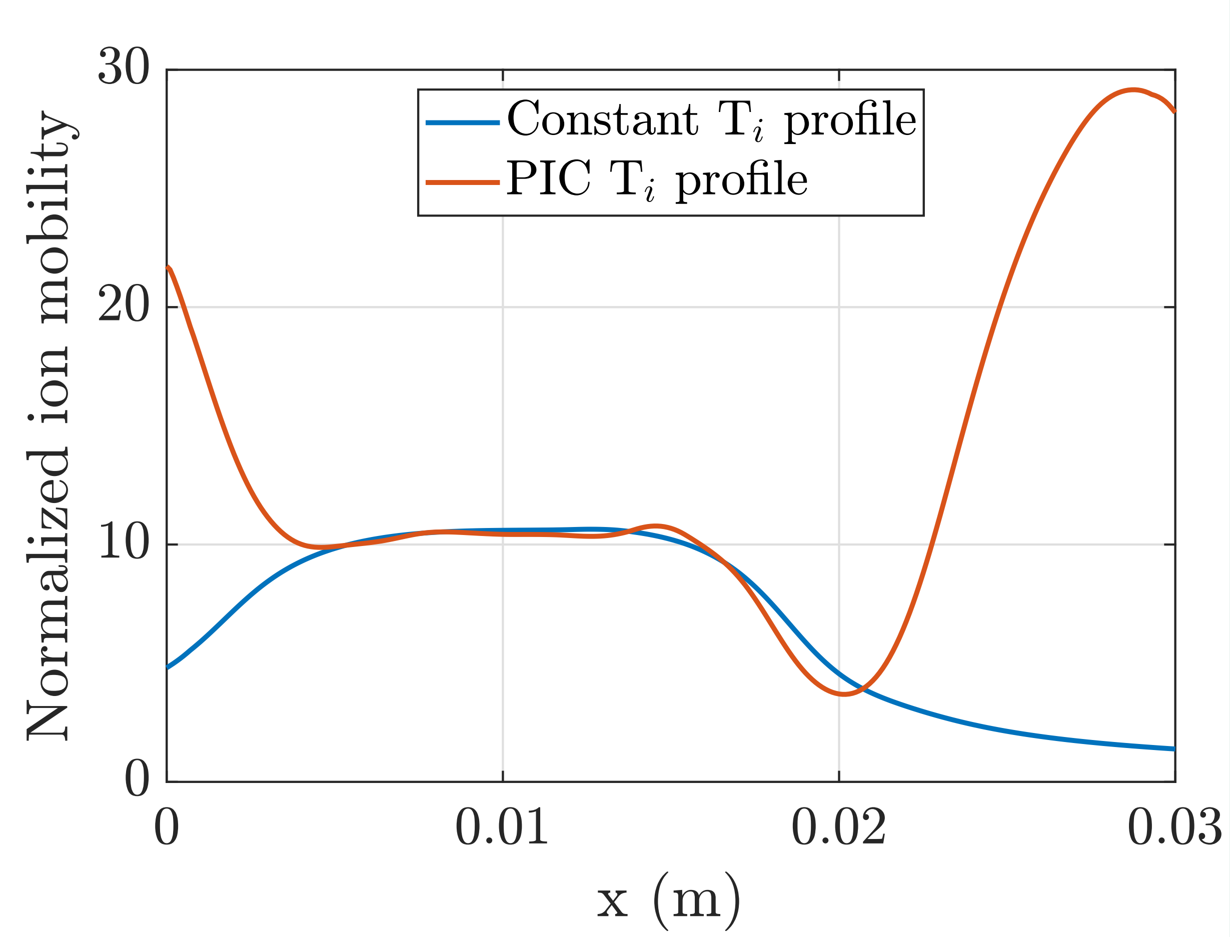


Figure IV.3. – Comparison of Ar^+ ion thermal energy profiles in the parallel direction to the electric field calculated by the PIC and fluid codes.

- Fluid model approximately recovers PIC results in a qualitative and a quantitative way under similar modeling assumptions
- Further improvement of the model for other ion-neutral collisional processes

Some problematics concerning the fluid results with Khrapak's formula

- The higher the electric field amplitude is, the lower the ion mobility should be
- Ion-neutral charge exchange collisions are important for such energetic ions
- Empirical formula, at equilibrium: validity in the current simulation?



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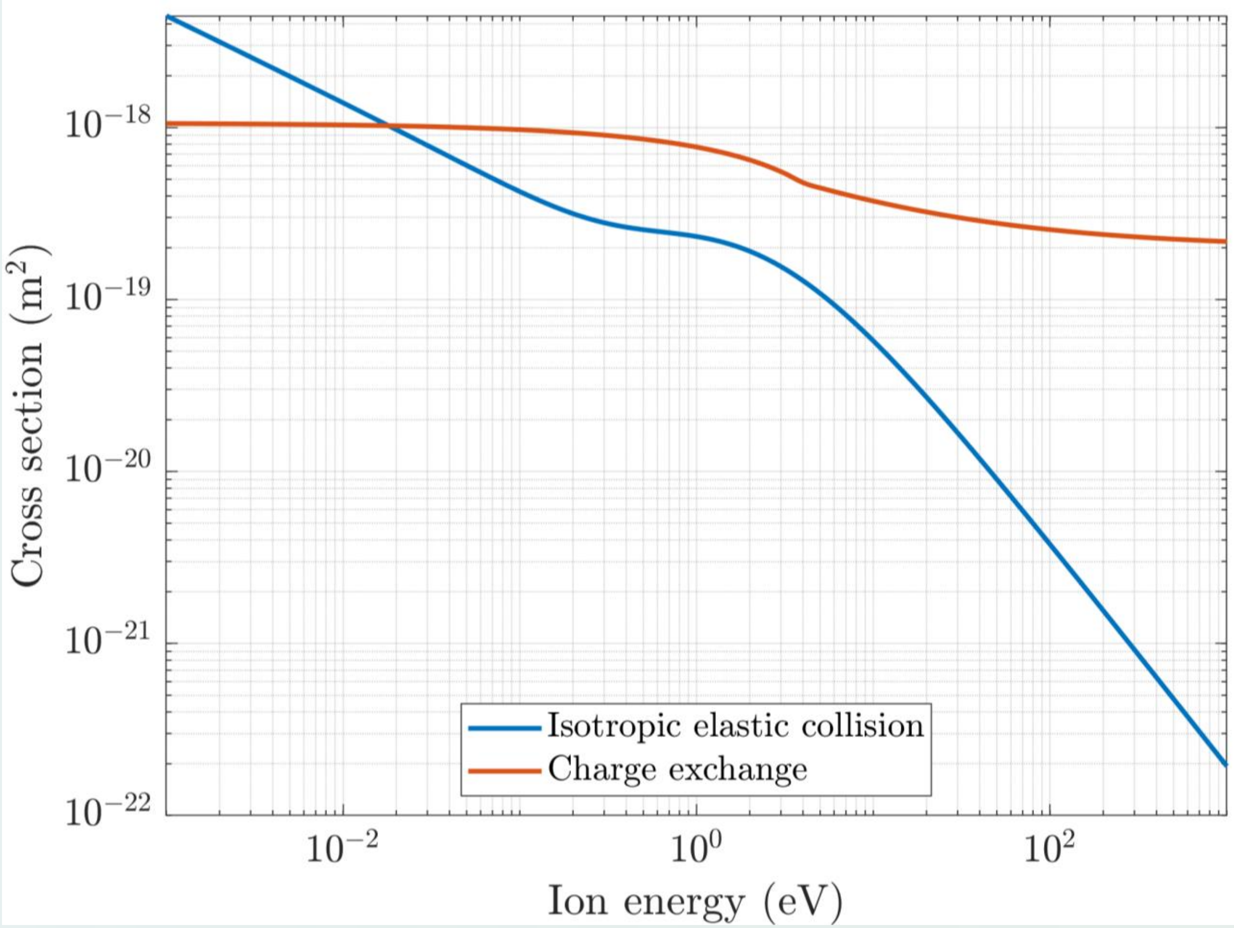

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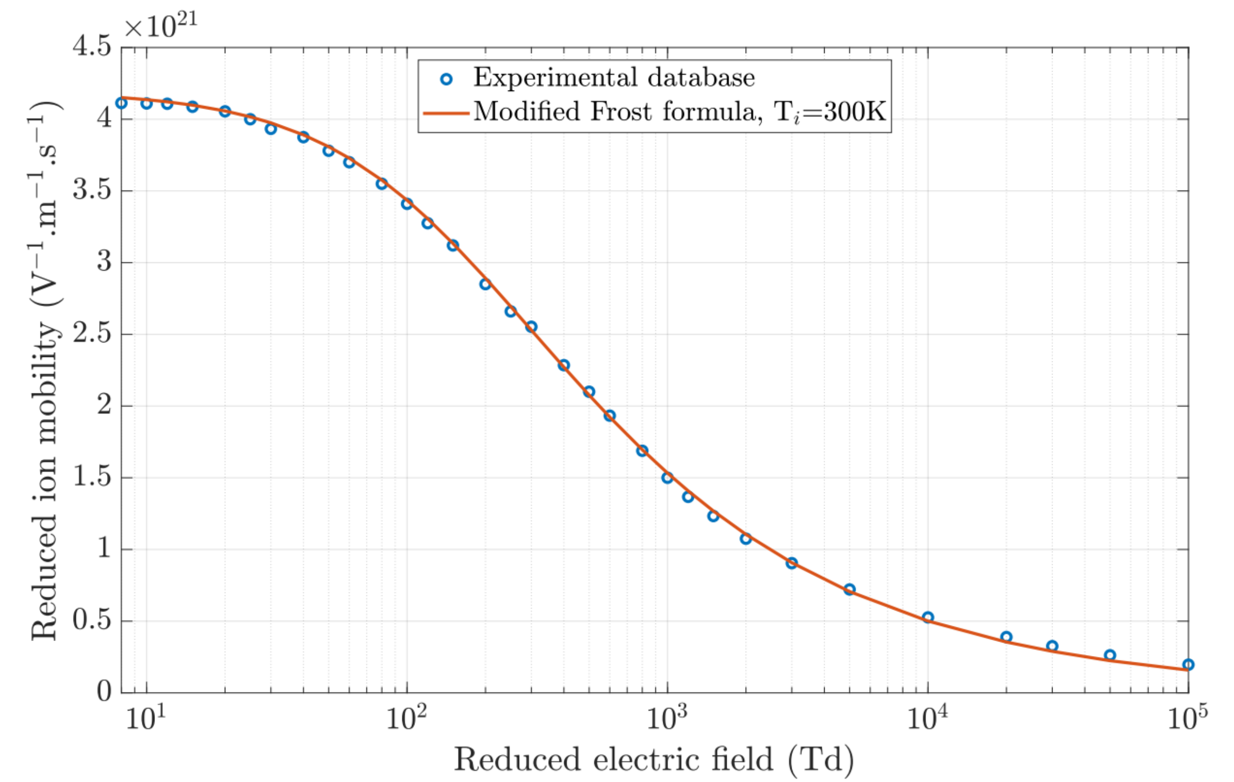
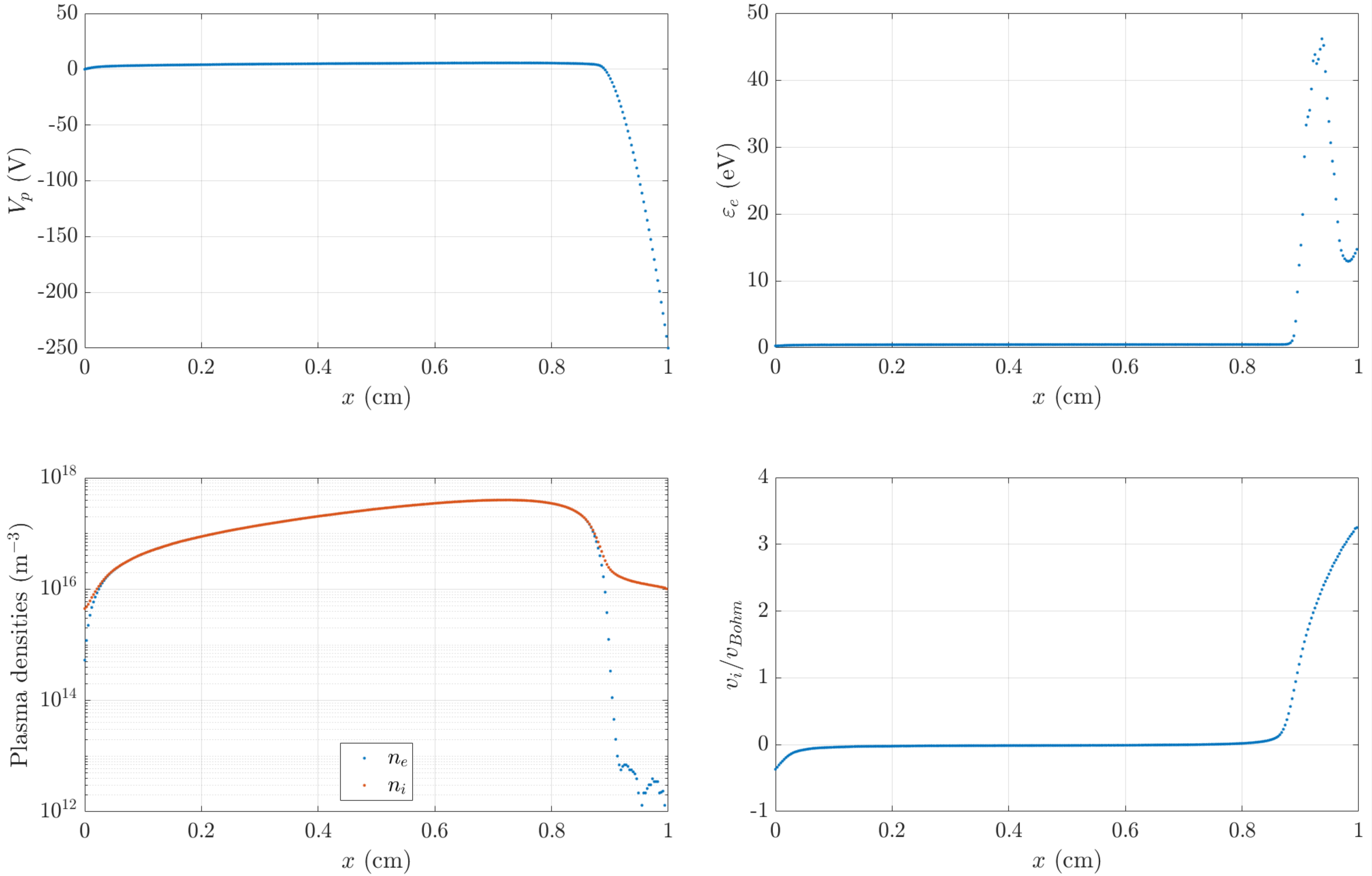
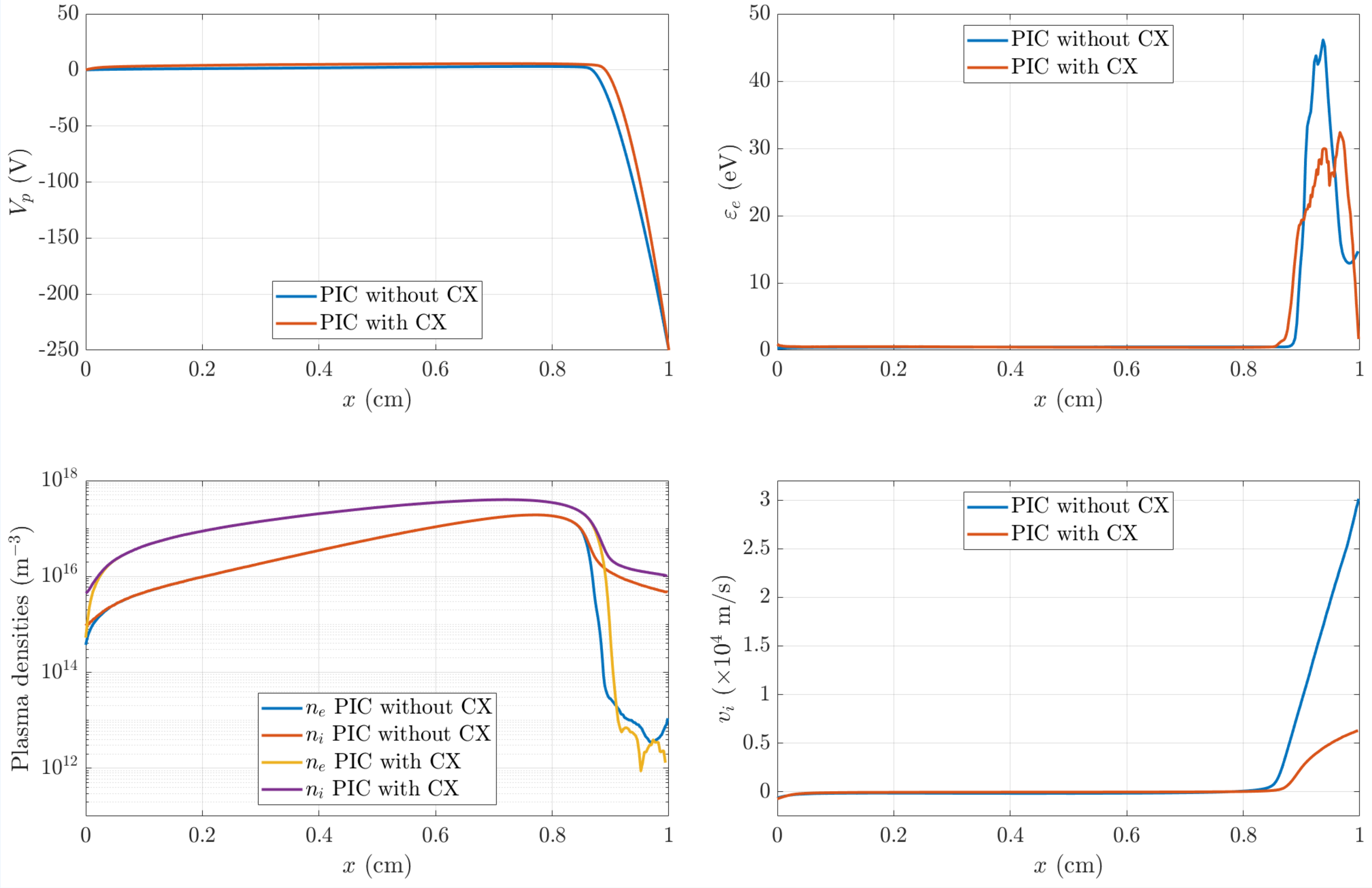


IV. Influence of ion-neutral charge exchange collisions



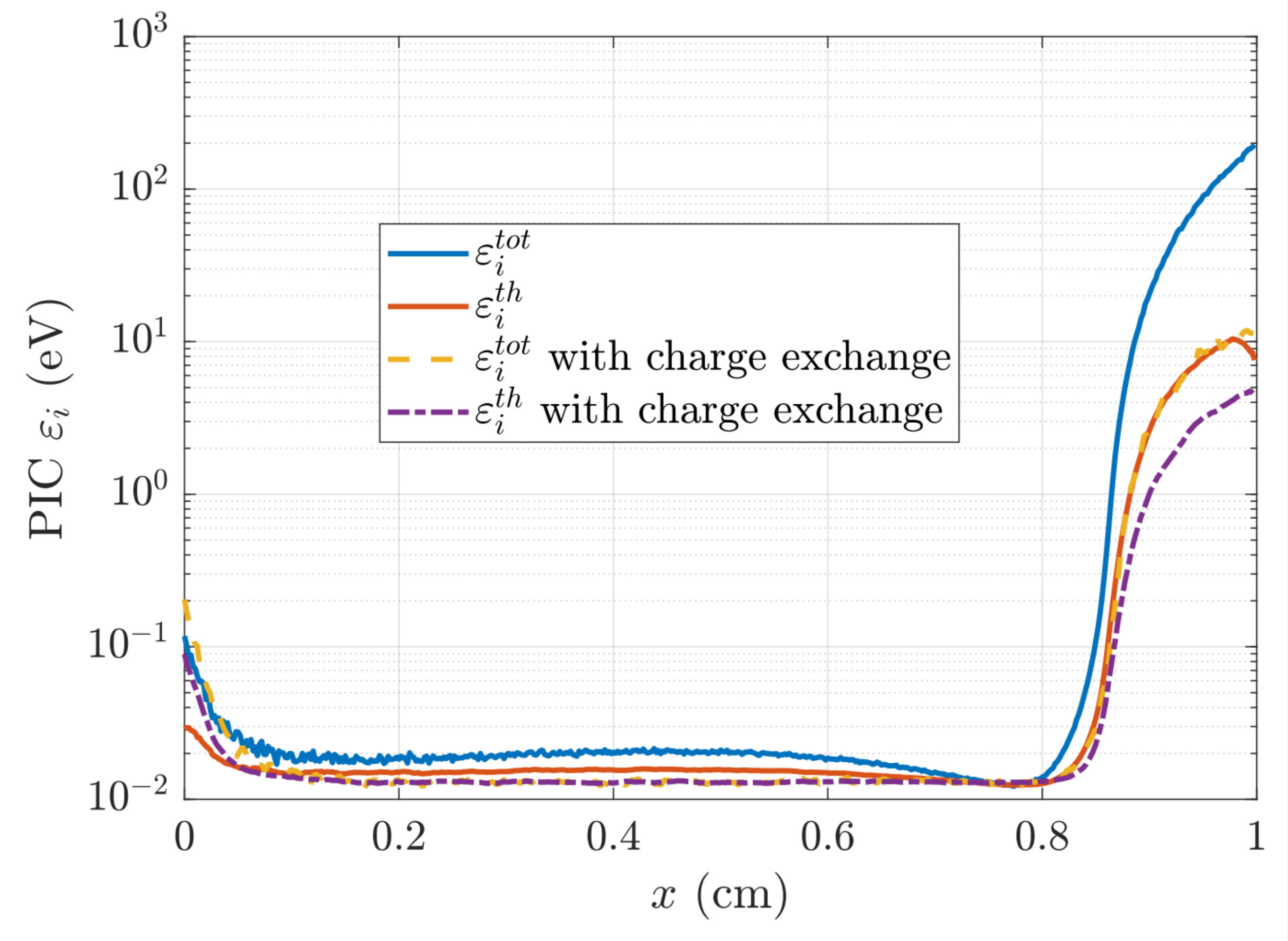
- PIC simulation result with ion-neutral elastic and charge exchange collisions
- Even though the ions are noticeably slowed down, there is still no accumulation of ions in the cathode sheath

IV. Influence of ion-neutral charge exchange collisions



- Noticeable discrepancy concerning ions – importance of charge exchange collisions
- A way to incorporate charge exchange collisions into the fluid model?

Influence of charge exchange collisions at 130Pa



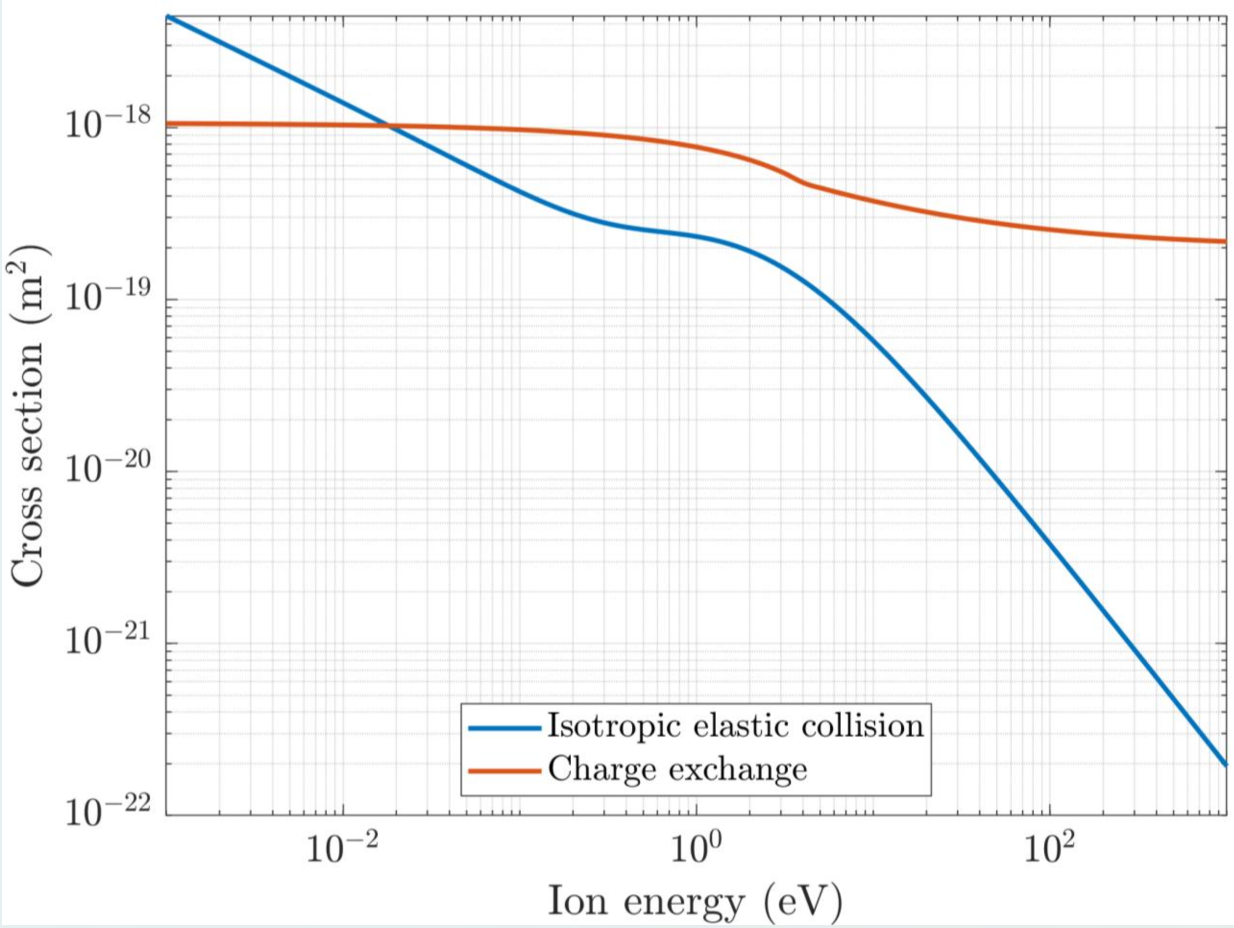
- Ion-neutral charge exchange collisions are important
- Ions slowed down, but still considerably heated in the cathode sheath
- Keep the ion thermal energy equation, but alternative way to compute total ion-neutral collision frequency

Ion-neutral total collision frequency calculation

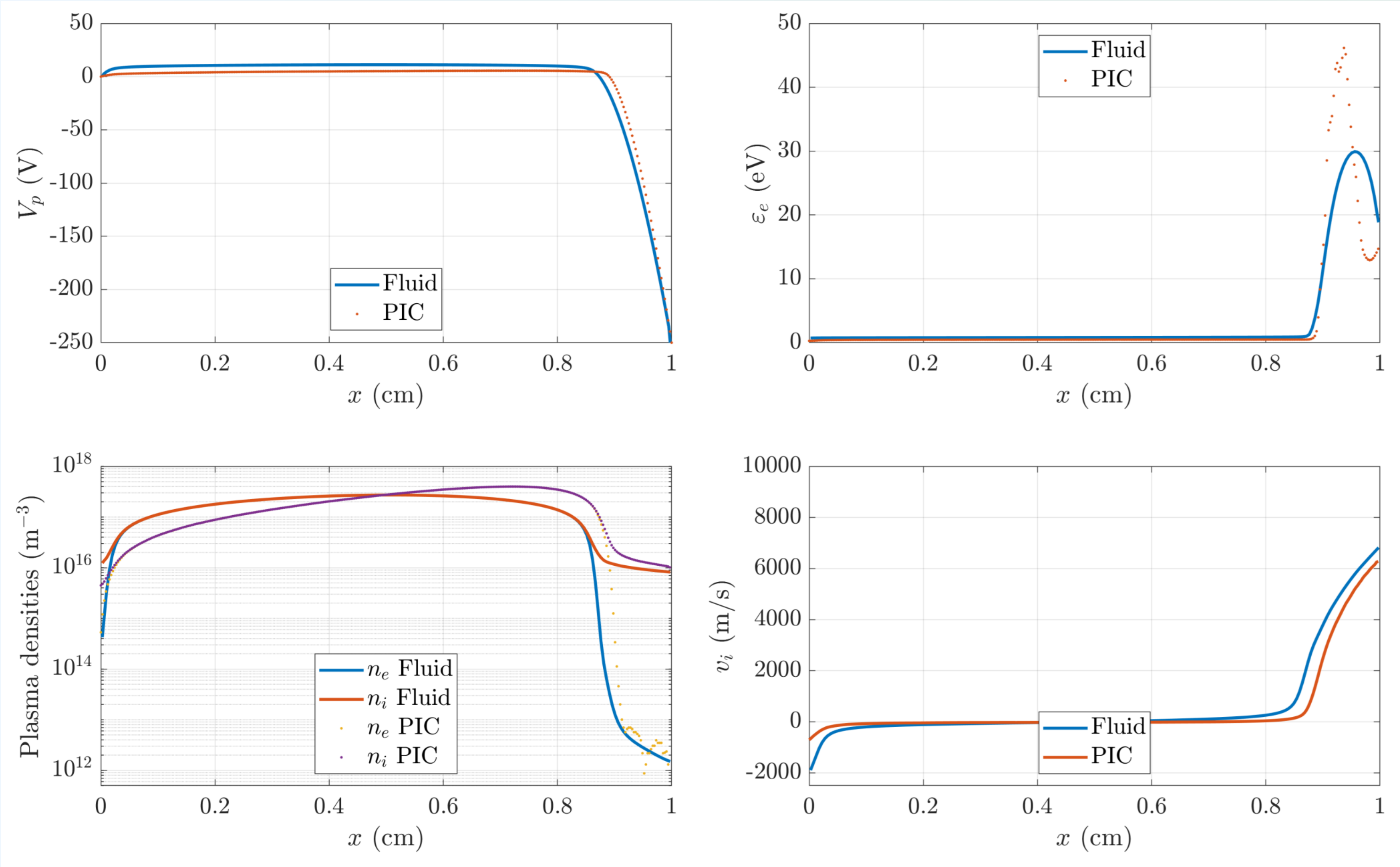
- Using both ion-neutral elastic and charge exchange collision cross section
- Assuming shifted Maxwellian distributions of ions inside the cathode sheath

$$\langle \nu_i \rangle = n_n \langle v_i \sigma_{i-n} \rangle = f\left(v_{d,i}, T_i\right)$$

$$\nu_{i-n,fluide} = \nu_{i,EL} + \nu_{i,CX}$$

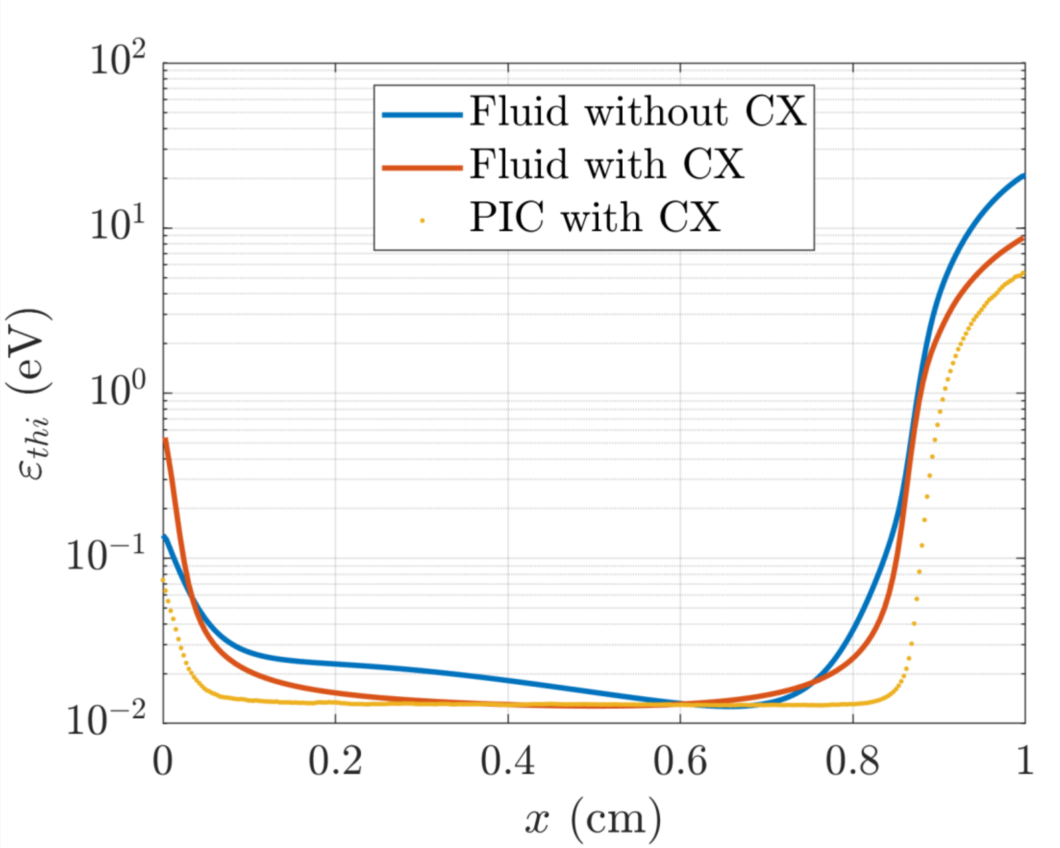


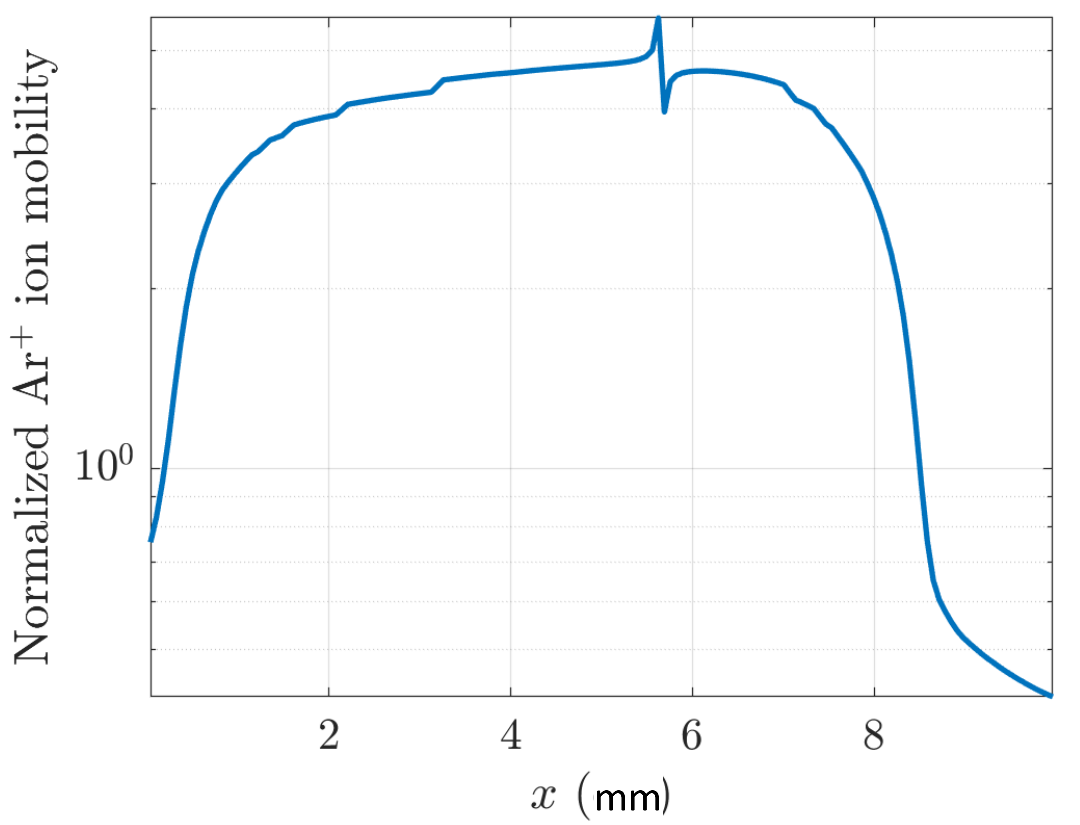
IV. Influence of ion-neutral charge exchange collisions



- PIC and fluid simulation result with ion-neutral elastic and charge exchange collisions
- Ion fluid velocity comparable in both simulations, but still no ion accumulation inside the cathode sheath in fluid simulation

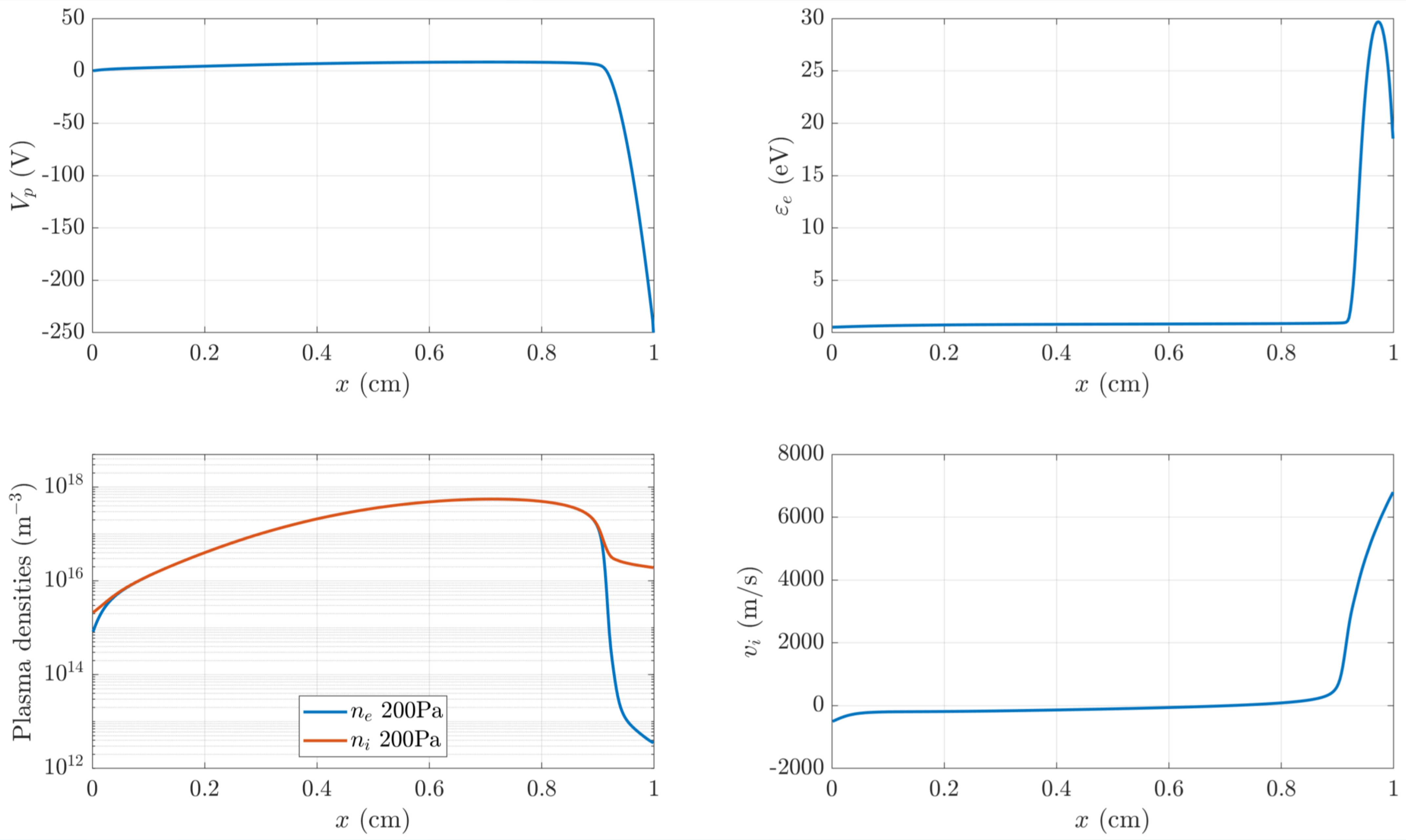
IV. Comparison of fluid results with self-consistent ion temperature computation and PIC results



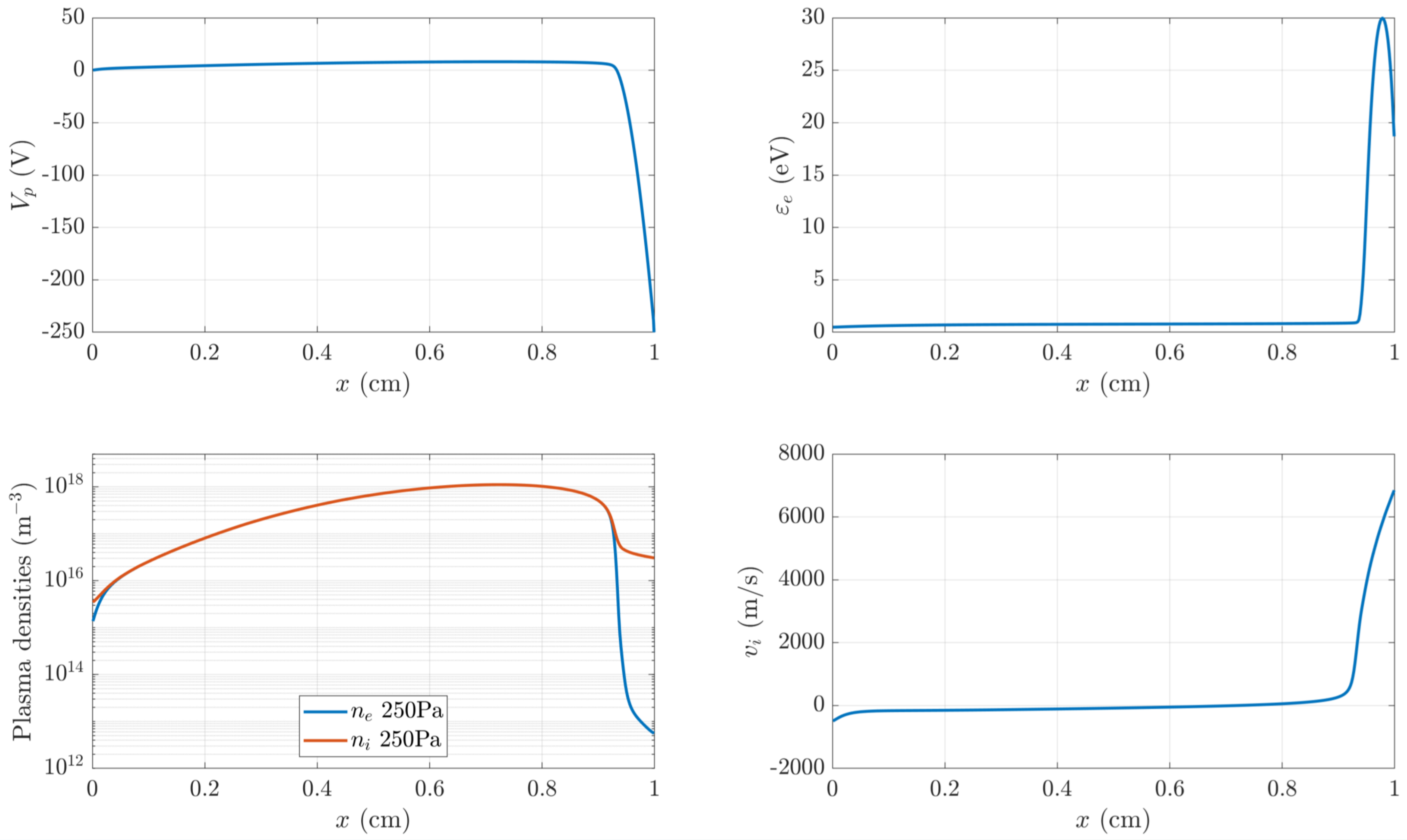


- Fluid ion temperature profile comparable to the PIC one
- The ion mobility (estimated as $\frac{v_i}{E}$ here) is decreasing as the electric field amplitude increases
- Further improvement of the model ongoing

IV. Influence of ion-neutral charge exchange collisions



IV. Influence of ion-neutral charge exchange collisions



Summary

Conclusions

- Starting from scratch, a 1D fluid DC discharge model including plasma sheath has been developed
- Our fluid models recovers other fluid results published in the literature
- Non negligible ion heating observed in kinetic simulation(moderate pressure range, intermediate collisional regime).
- The addition of the ion energy equation to improves the fluid model results with respect to the PIC results (very sensitive to the assumptions of the model)

Perspectives

- Implementation of other inelastic collisional processes
- Proper implementation of charge exchange collisions in fluid model
- Shifted/truncated distribution functions for charged species inside the sheath
- Extension of the model in 2D with magnetic field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Thank You For Your Attention
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