SAND2022-14022C

How sheath properties change with gas pressure: modeling and simulation

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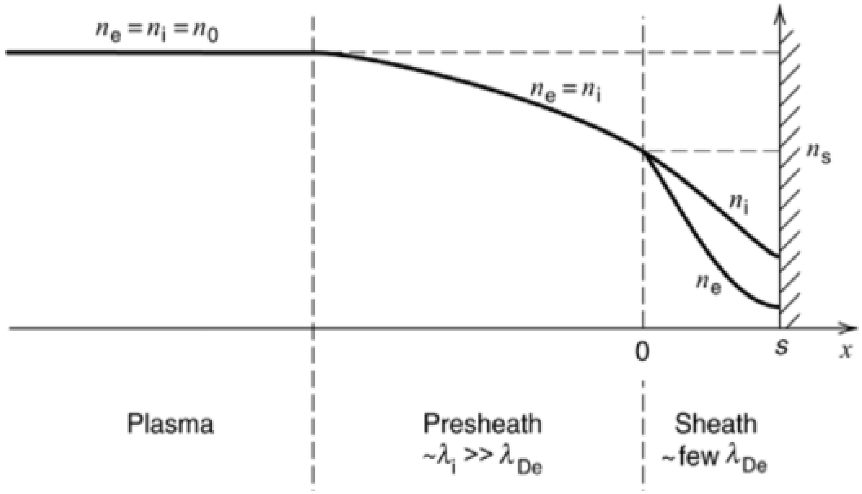
The sheath determines how the plasma and wall interact

- The flux of particles to the wall is related to n_{se} and $V_{i,se} \rightarrow \Gamma_w = n_{se} V_{i,se}$
  - In etching $\Gamma_w \rightarrow$ rate of etch
  - In global models $\Gamma_w \rightarrow$ Bulk T_e
    - $\overline{n_e} n_g K_{iz}(T_e) = \frac{2\Gamma_w}{L}$

M. Lieberman and A. Lichtenberg (2005) Wiley



Want to know $n_{se}, V_{i,se}$ in terms of bulk quantities

$$\Gamma_w = a_l h_l n_0 c_{s,c} \quad c_{s,c} = \sqrt{T_{e,c}/m_i} \quad a_l = \frac{V_{i,se}}{c_{s,c}} \quad h_l = \frac{n_{se}}{n_0}$$

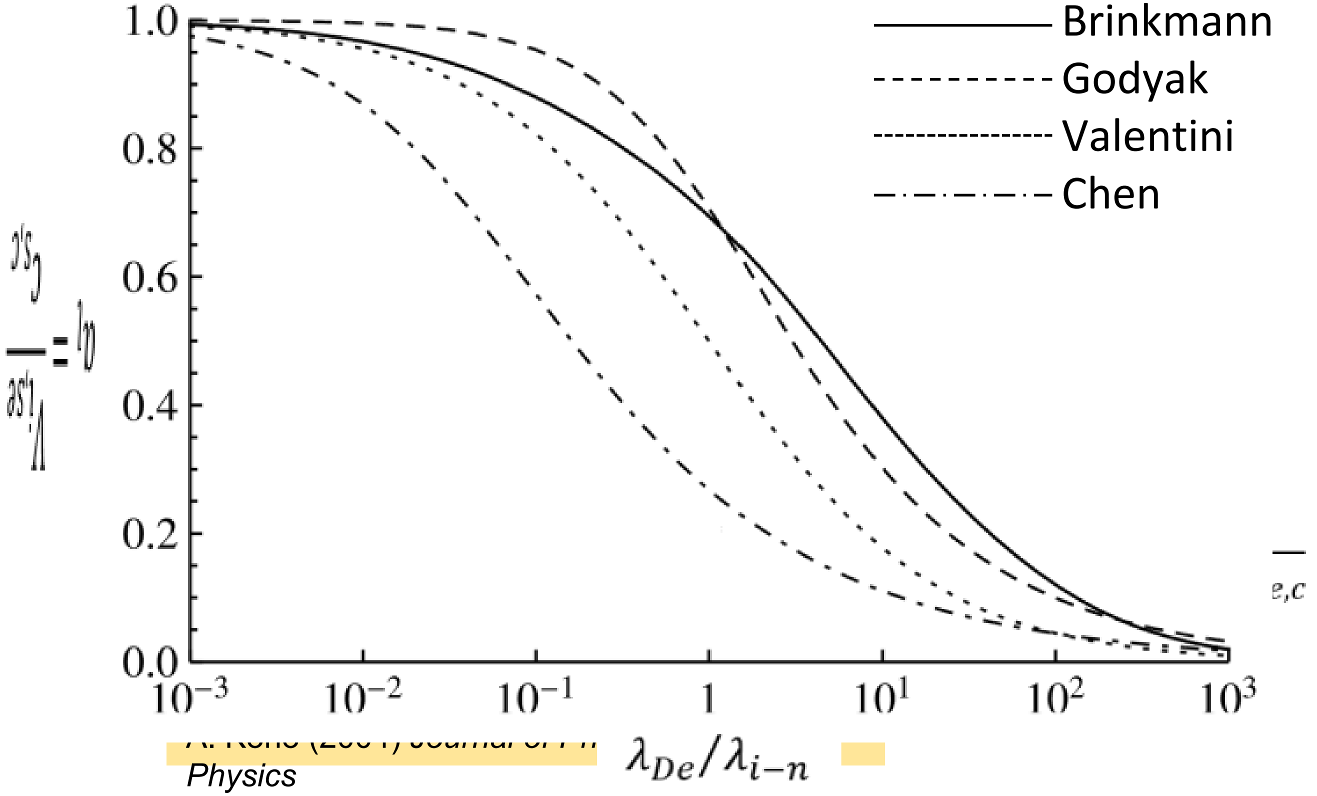
Many current models, but …

1. Use inconsistent assumptions (R_{in}) and only compute a few sheath properties
2. Use different definitions of the sheath edge
3. Few experimental test only at low pressure

Models of sheath properties have been developed for a range of conditions, including p_n

Sheath edge velocity (Collisional Bohm) $a_l = \frac{v_{i,se}}{c_{s,c}}$

- V. A. Godyak (1982) *Physics Letters A*
- H.B. Valentini (1996) *Physics of Plasmas*
- X.P. Chen (1998) *Physics of Plasmas*
- R.P. Brinkmann (2011) *Journal of Physics D: Applied Physics*
- J-Y Liu et al. (2003) *Physics of Plasmas*



Physics

T.E R.P. Brinkmann (2011) *Journal of Physics D: Applied Physics*

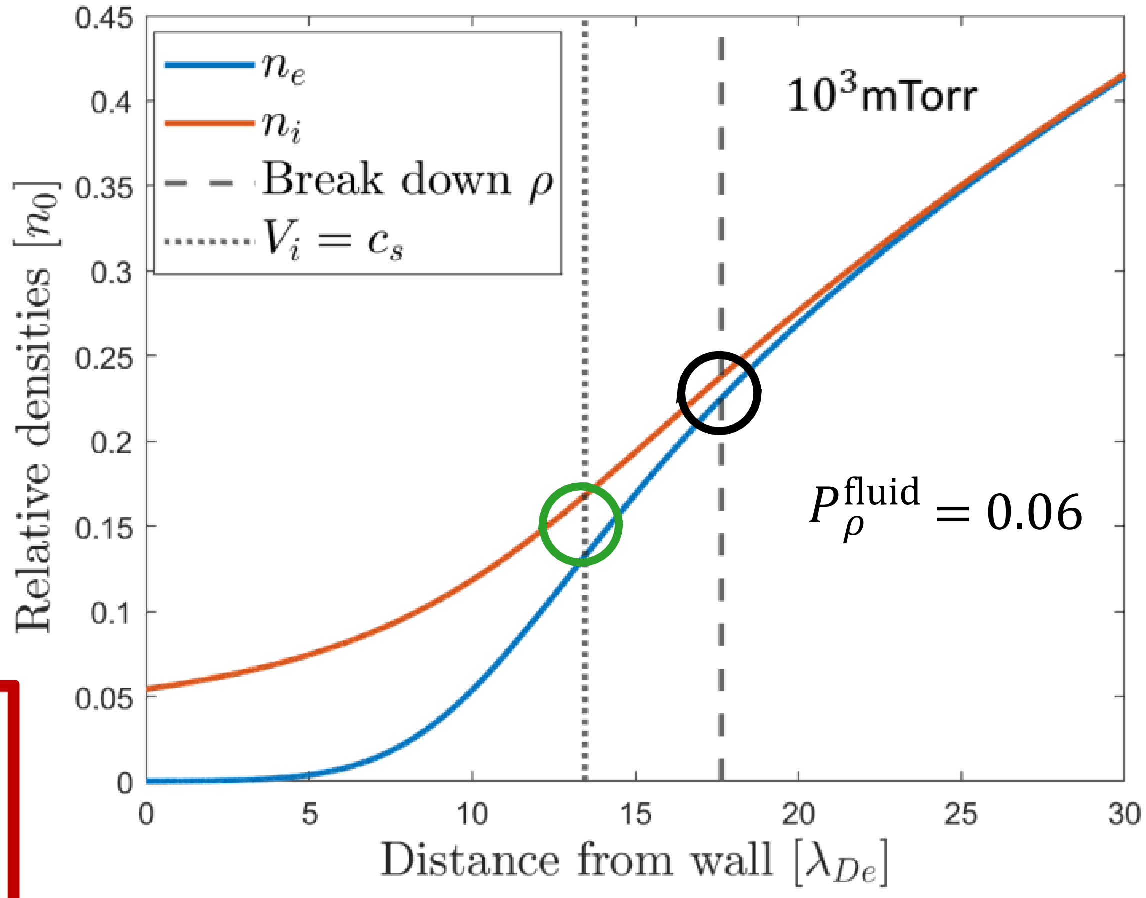
I.D. Kaga *Plasmas*

$$\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}} = (\lambda_{\mathrm{De,c}}\sigma_s)p_n/T_n$$

We will use a single fluid model to calculate each property

Different definitions of the sheath edge location leads to inconsistency between models

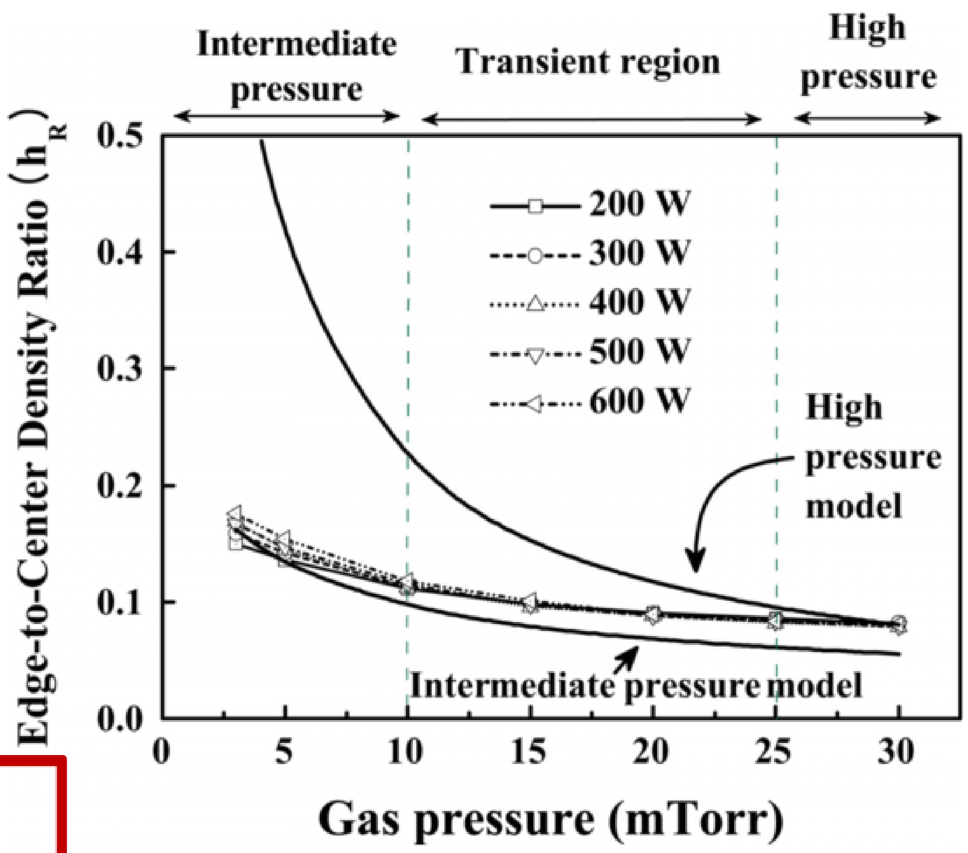
- Collisional Bohm models
  - Break down in quasineutrality
  - $\frac{|n_e - n_i|}{n_e} = P_\rho \sim 0.01 \rightarrow 0.1$
  - Or critical value of E_{se}
- Edge-to-center density ratios
  - $V_i = c_{s,c} \rightarrow \; a_l = 1$



We will use the breakdown in quasinetrality, where $P_\rho^{\mathrm{fluid}} = 0.06$ and $P_\rho^{\mathrm{PIC}} = 0.02$ are chosen so Bohm's criterion is filled at the lowest pressure

Also, experimental validation for these models is focused on relatively low pressures

- Edge-to-center density ratios have been measured in an inductively coupled device up to 30 mTorr
  - Used floating harmonics method at center and edge of device
  - $T_e \approx 1 \rightarrow 4$ eV, $n_0 \approx 10^{16}/\mathrm{m}^3$
  - Compared to models in M. Lieberman and A. Lichtenberg (2005) Wiley for cylindrical plasmas
- Plasmas are found/used at higher pressures 100s → 10,000s of mTorr



G-H Kim et al. (2010) *Physics of Plasmas*

Particle-in-cell simulations can study the sheath over a large pressure range $10^{-2} \rightarrow 10^4$ mTorr

My goals are:

(1) Extract all sheath edge properties using a single fluid model and sheath edge def.

$$a_l = \frac{V_{i,se}}{c_{s,c}} \qquad h_l = \frac{n_{se}}{n_0} \qquad \frac{w_s}{\lambda_{De,c}} \qquad \frac{e\Delta\phi_s}{T_{e,c}} \qquad \frac{e\Delta\phi_{ps}}{T_{e,c}} \qquad \frac{eE_{se}}{T_{e,c}/\lambda_{De,c}}$$

(2) Provide simple expression for sheath edge properties using the fluid model

(3) Test the viability of the model with particle-in cell simulations

The fluid model uses a constant volumetric source and constant collision frequency

$$\frac{\mathrm{d}}{\mathrm{d}x}(n_i V_i) = S$$

Most other models use $\frac{d(n_s V_s)}{dx} = \nu_{iz} n_e$,
Ultimately this leads to small differences

$$m_i n_i V_i \frac{\mathrm{d}V_i}{\mathrm{d}x} = e n_i E - R_{in} - m_i V_i S$$

$$R_{in} = m_i n_i V_i (c_{\mathrm{s,c}}/\lambda_{in,\mathrm{c}})$$

$$\lambda_{in,\mathrm{c}} = 1/(n_n \sigma_s)$$

$$\epsilon_0 \frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = -e(n_i - n_0 e^{-e\phi/T_{e,\mathrm{c}}})$$

Analytic expressions can be derived using approximations of the fluid model

To model a_l: $S \approx 0$

J-Y Liu et al. (2003) *Physics of Plasmas*

$$\frac{\mathrm{d}}{\mathrm{d}x}(n_i V_i) = 0$$

$$a_l = -\frac{(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}})}{2E'_{\mathrm{se}}} + \sqrt{1 + \left(\frac{(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}})}{2E'_{\mathrm{se}}}\right)^2}$$

$$\lambda_{\mathrm{De,c}} = \sqrt{T_{e,\mathrm{c}}\epsilon_0/n_0 e^2}$$

To model h_l: $n_i = n_e$

$$n(V) = \frac{-s(1+V^2) + \sqrt{s^2(1+V^4) + 2s(s + (\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}}))V^2}}{(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}})V^2}$$

J-L Raimbault et al. (2009) *Plasma Sources Science and Technology*

Using a single definition of the sheath edge: $h_l = n(a_l)$

Other properties ($\frac{e\Delta\phi_s}{T_{e,c}}$) are functions of h_l or a_l

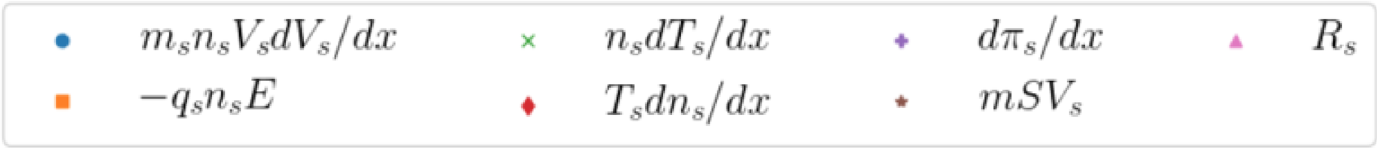
Particle-in-cell direct-simulation Monte Carlo simulations can be used to test our model

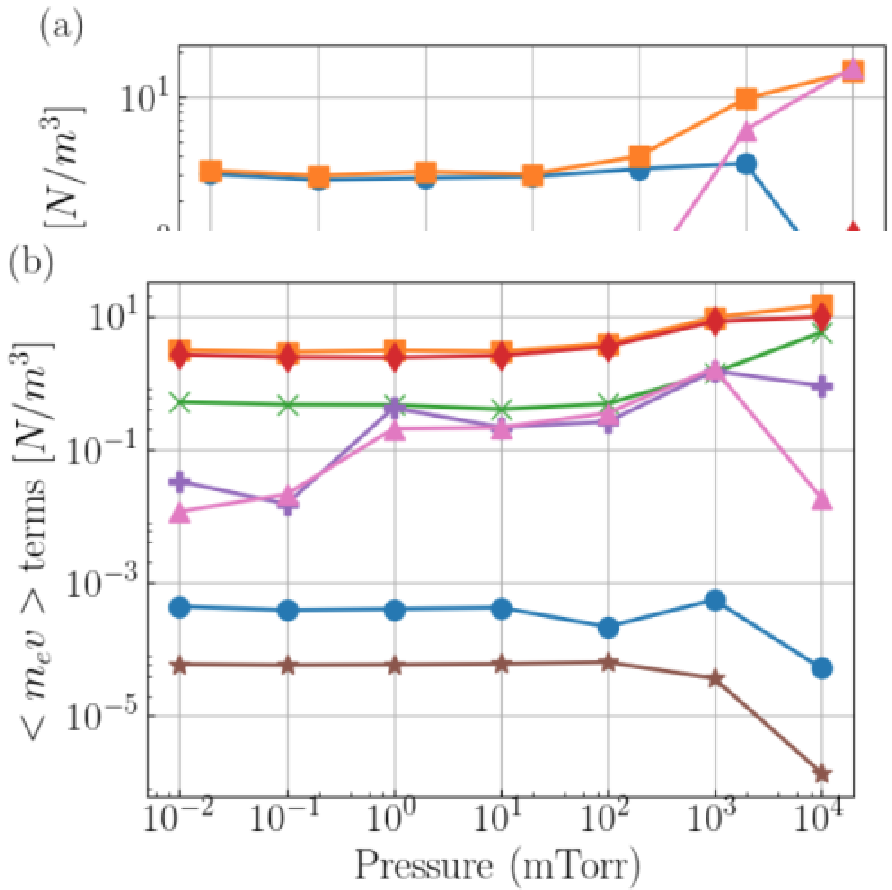
$p_n [mTorr]$	$\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}}$
10^{-2}	1.53×10^{-6}
10^{-1}	1.53×10^{-5}
10^{0}	1.52×10^{-4}
10^{1}	1.46×10^{-3}
10^{2}	1.30×10^{-2}
10^{3}	6.95×10^{-2}
10^{4}	2.93×10^{-1}

$$\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}} = (\lambda_{\mathrm{De,c}}\sigma_s)p_n/T_n$$

- 1D-3V simulations using Aleph
  - 1 cm domain
  - 500 to 5,000 cells to resolve $\lambda_{in,\mathrm{c}} = 1/(n_n \sigma_s)$
  - Absorbing boundary condition
  - Constant and uniform volumetric source
  - He ions (He+), electrons (e-), and He atoms
  - Isotropic ion-neutral collisions with from lxcat $\sigma = \sigma_s(c_{\mathrm{s,c}}/V_i)$
  - And elastic electron-neutral collision model from lxcat

The fluid model is consistent with simulations





$$m_s n_s V_s \frac{dV_s}{dx} = q_s n_s E - T_s \frac{dn_s}{dx} - n_s \frac{dT_s}{dx} - \frac{d\pi_s}{dx} - m_s V_s S - R_s$$

He+ ions

$$m_s n_s V_s \frac{dV_s}{dx} = q_s n_s E - \cancel{T_s \frac{dn_s}{dx}} - \cancel{n_s \frac{dT_s}{dx}} - \cancel{\frac{d\pi_s}{dx}} - m_s V_s S - R_s$$

electrons

$$\cancel{m_s n_s V_s \frac{dV_s}{dx}} = q_s n_s E - T_s \frac{dn_s}{dx} - \cancel{n_s \frac{dT_s}{dx}} - \cancel{\frac{d\pi_s}{dx}} - \cancel{m_s V_s S} - \cancel{R_s}$$

Next are the results where

represents data from PIC simulations,

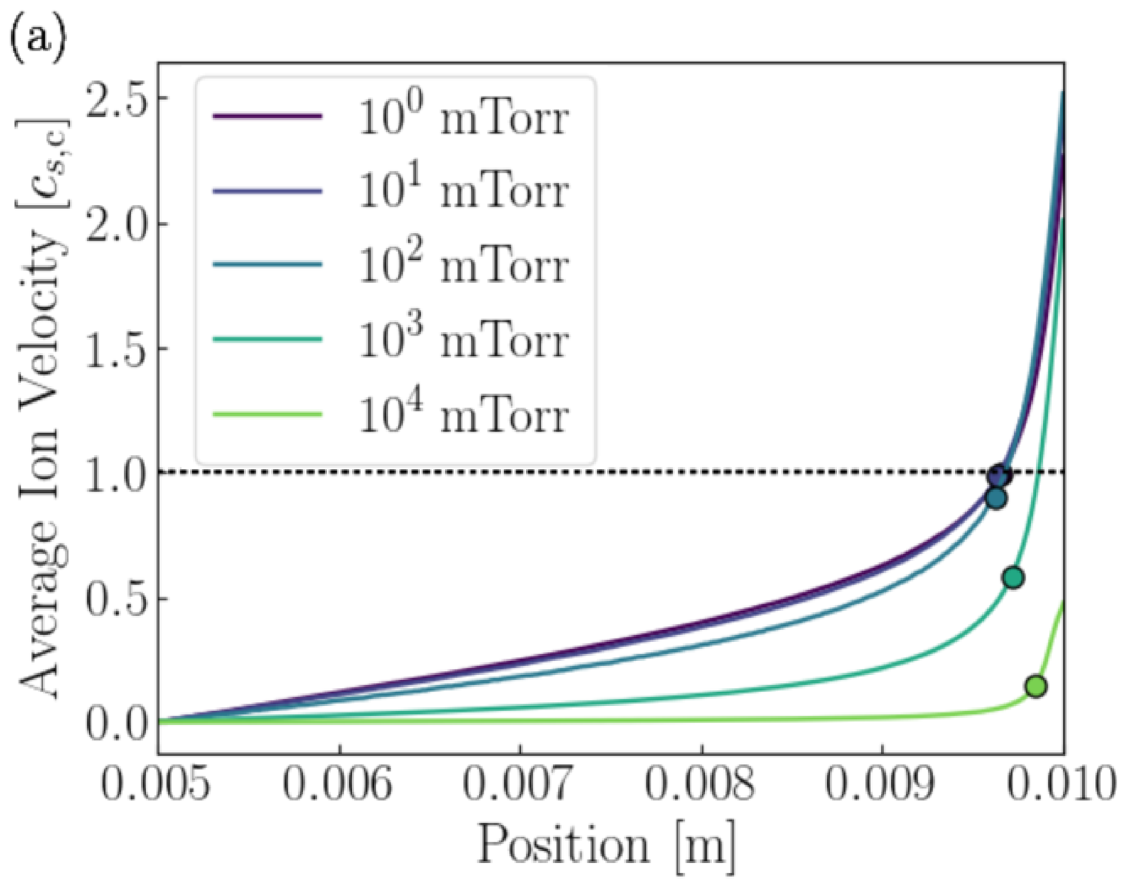
represents the numerical solutions to the fluid model,

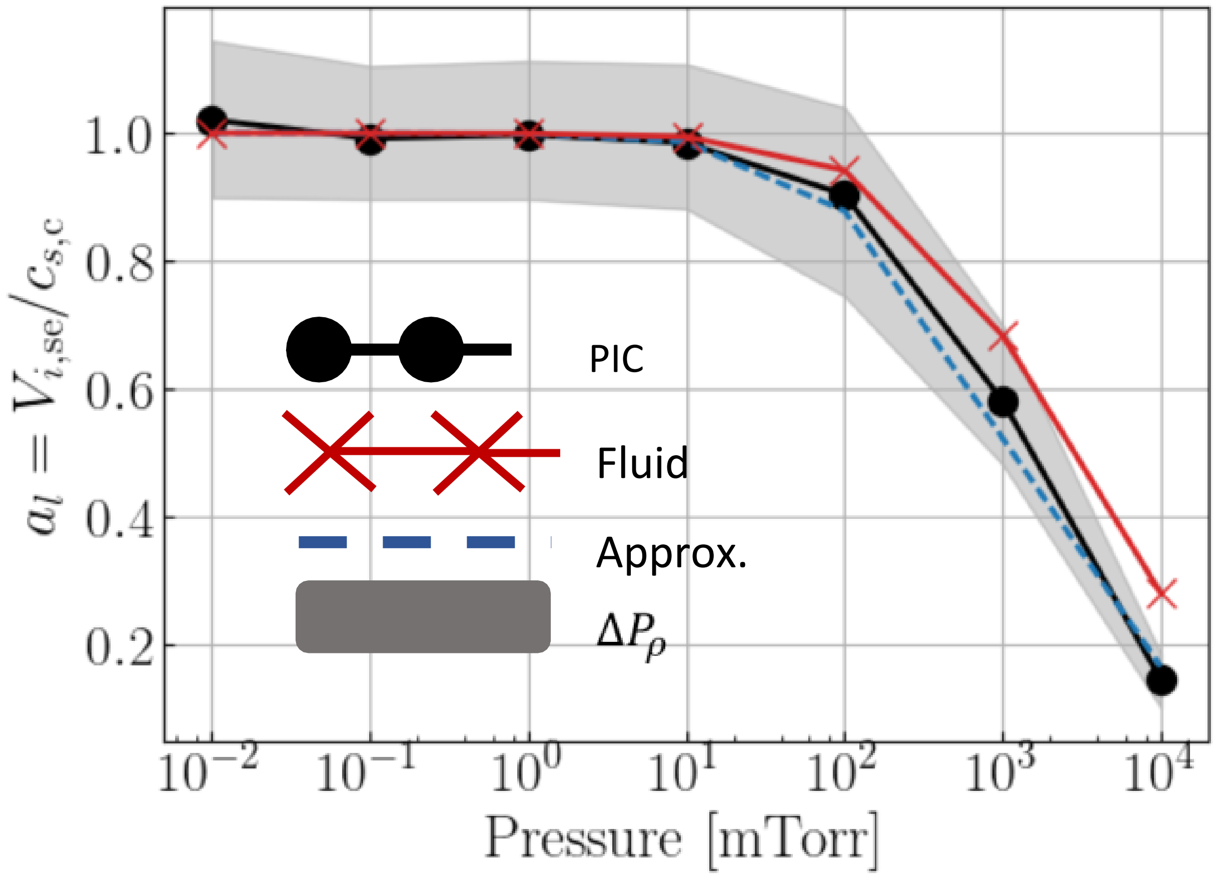
represents the analytic approximations to the fluid model, with modifications based on PIC, and

represents PIC data where the sheath edge location was varied to the left and right

$$\frac{|n_e - n_i|}{n_e} = P_\rho \in [0.0077, 0.048]$$

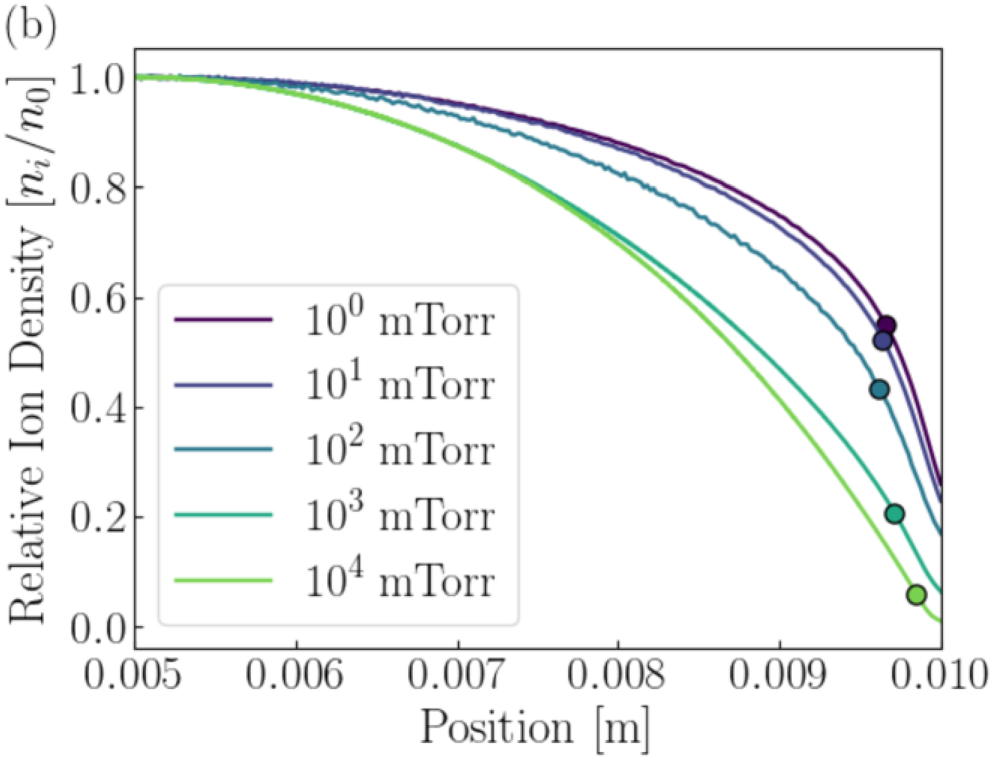
We observe a collisionally modified Bohm criterion

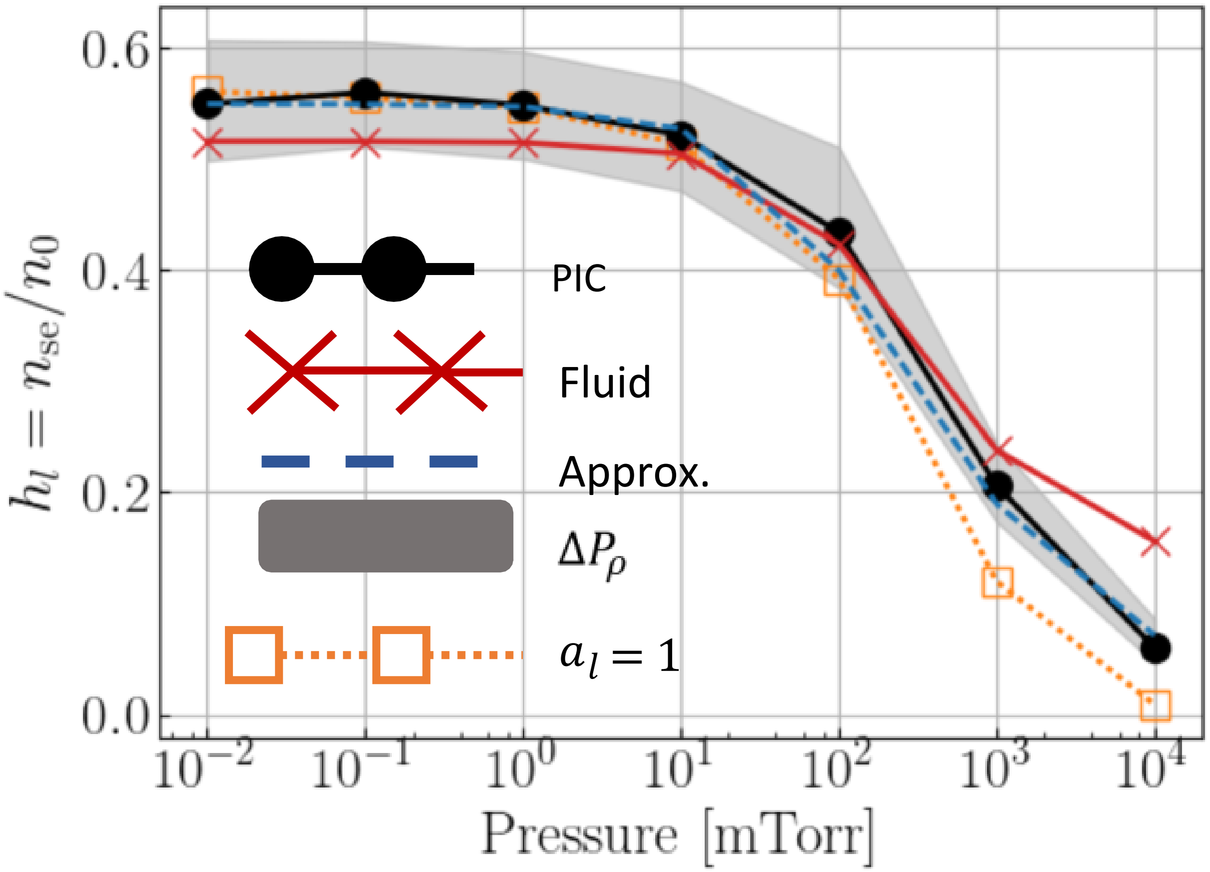




$$a_l = -10(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}}) + \sqrt{1 + 100(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}})^2}$$

The edge-to-center density ratio decreases





$$h_l = \frac{0.55 + 0.5(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}})}{1 + 30(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}})}$$

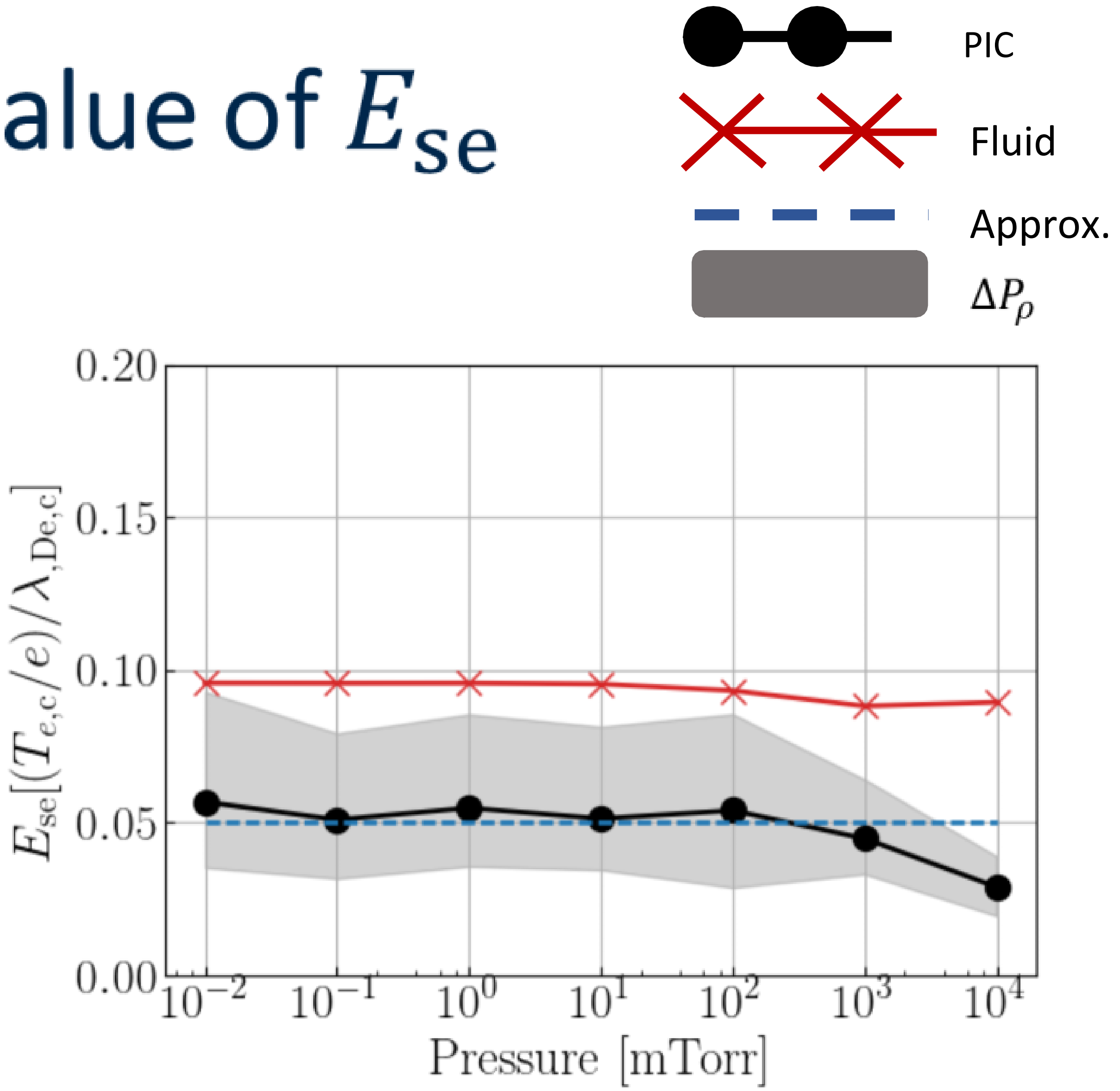
We observe a critical value of E_{se}

- Breakdown in quasineutrality↔ critical electric field

- Significantly, lower than previous predictions $E_1 = (T_{e,se}/e)/\lambda_{De,se}$

V. A. Godyak (1982) *Physics Letters A*

$$E_{se} = 0.05(T_{e,c}/e)/\lambda_{De,c}$$

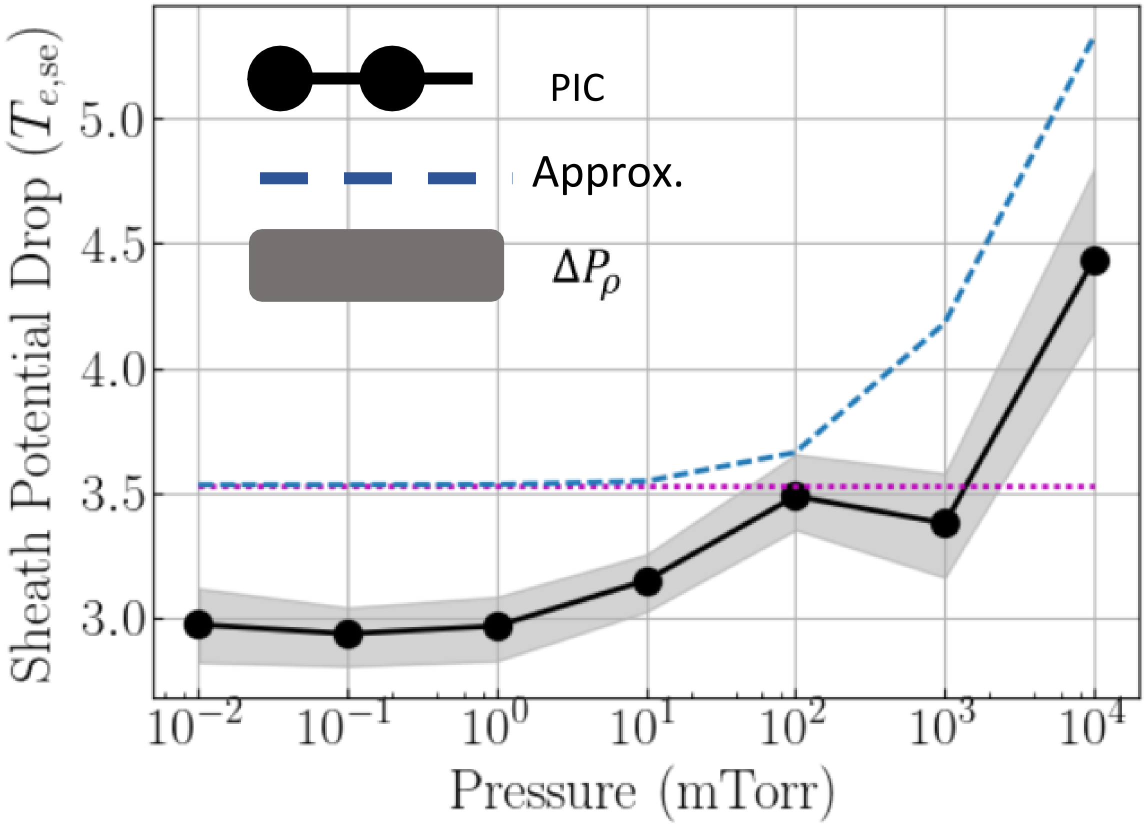


The sheath potential is determined by a_l

$$\Gamma_{e,\mathrm{se}} = \frac{1}{4} h_l n_0 \sqrt{8T_{e,\mathrm{se}}/\pi m_e} \exp(-e\Delta\phi_\mathrm{s}/T_{e,\mathrm{se}})$$

$$\Gamma_{i,\mathrm{se}} = h_l n_0 a_l c_{\mathrm{s,c}}$$

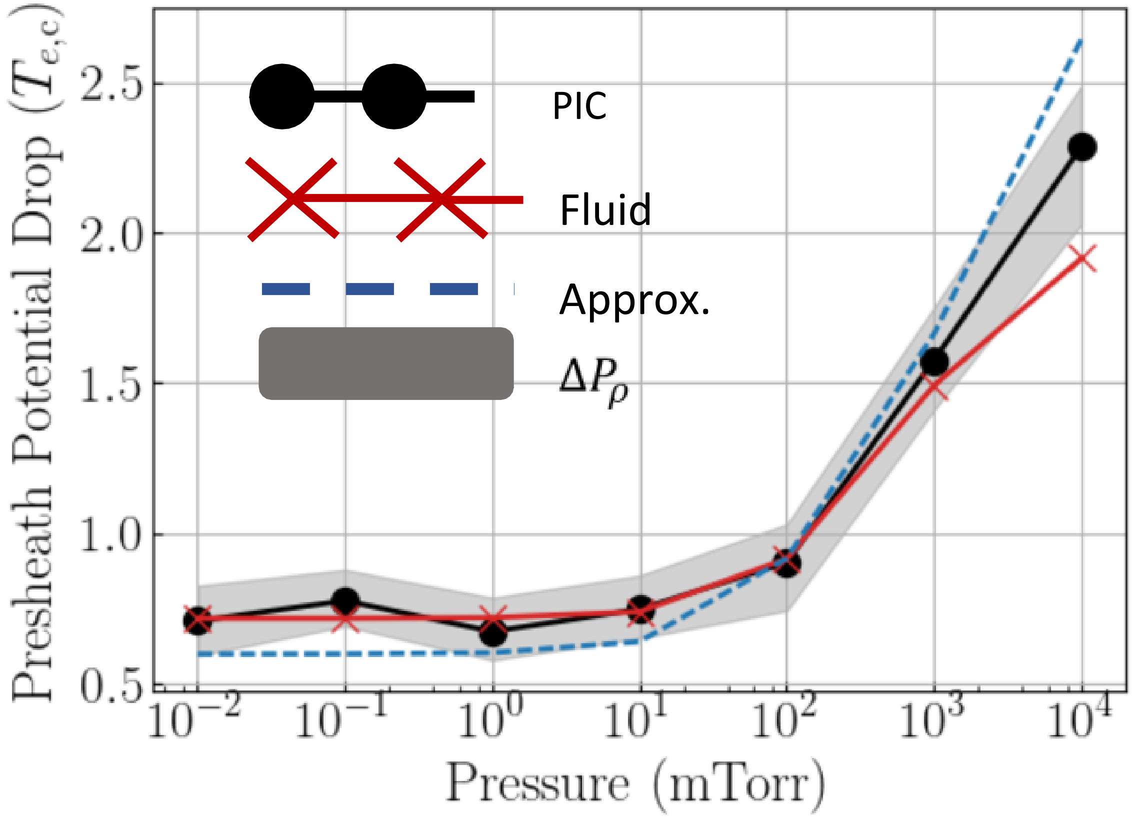
$$\frac{e\Delta\phi_\mathrm{s}}{T_{e,\mathrm{se}}} = -\frac{1}{2}\ln\left(a_l^2 2\pi \frac{m_e}{m_i}\frac{T_{e,\mathrm{c}}}{T_{e,\mathrm{se}}}\right) \approx -\frac{1}{2}\ln\left(a_l^2 2\pi \frac{m_e}{m_i}\right).$$



The presheath potential drop is related to h_l

$$n_e = n_0 e^{-e\phi/T_{e,c}}$$

$$\frac{e\Delta\phi_{\text{ps}}}{T_{e,c}} = -\ln\left(h_l\right)$$



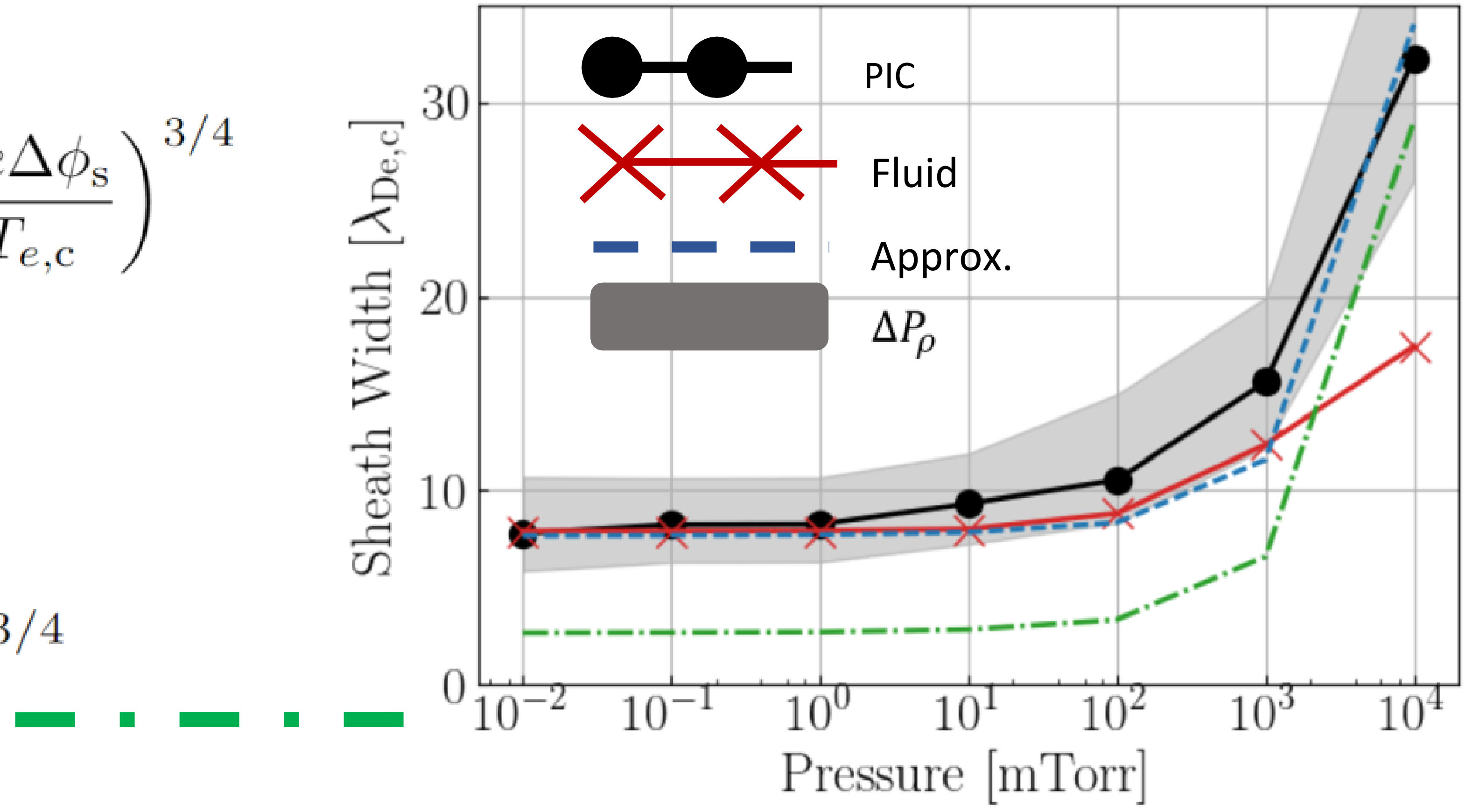
The sheath becomes wider and can be modeled with the Child-Langmuir law

Child-Langmuir Law:

$$\frac{w_s}{\lambda_{De,c}} = \frac{\sqrt{2/(\Gamma_{i,se}/n_0 c_{s,c})}}{3}\left(\frac{2e\Delta\phi_s}{T_{e,c}}\right)^{3/4}$$

$$\Gamma_{i,se} = h_l n_0 a_l c_{s,c}$$

$$\frac{w_s}{\lambda_{De,c}} = \frac{\sqrt{2/h_l a_l}}{3}\left(\frac{2e\Delta\phi_s}{T_{e,c}}\right)^{3/4}$$



Conclusions

1. Can model the sheath edge properties at different pressures using a simple fluid model, where the sheath edge is where quasineutrality breaks down
2. There is a collisional Bohm speed a_l and edge-to-center density ratio h_l decrease with pressure.
3. The sheath potential only depends on a_l and increases with pressure
4. The electric field at the sheath edge is constant with pressure
5. The fluid model works well until about 10,000 mTorr, where temperature gradients become important

Acknowledgements

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The PIC friction force is accurately described by the model, except at low pressures

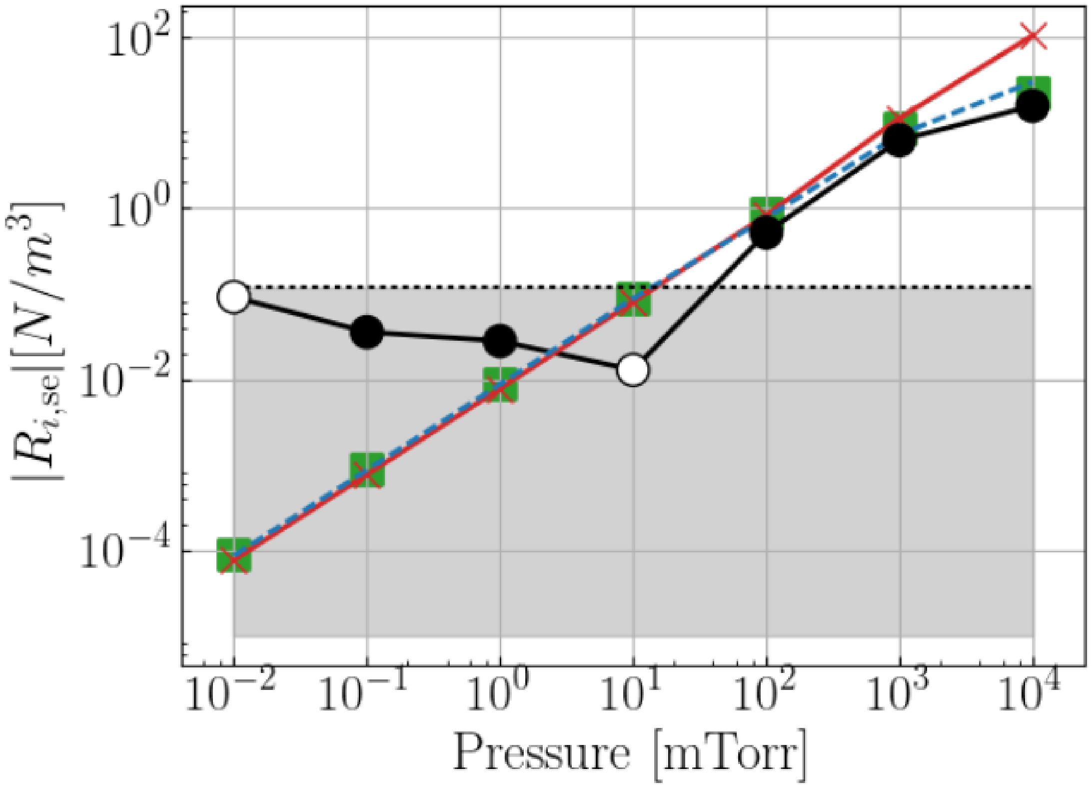
- Calculated R_i directly from PIC data using momentum equation (●, empty means $R_i < 0$):

$$m_s n_s V_s \frac{\mathrm{d}V_s}{\mathrm{d}x} = q_s n_s E - T_s \frac{\mathrm{d}n_s}{\mathrm{d}x} - n_s \frac{\mathrm{d}T_s}{\mathrm{d}x} - \frac{\mathrm{d}\pi_s}{\mathrm{d}x} - m_s V_s S - R_s.$$

- And compared to (■):

$$R_{in} = m_i n_i V_i (c_{\mathrm{s,c}} / \lambda_{in,\mathrm{c}})$$

- Where ··············· is an estimate of the statistical noise floor of R_i based on other term in the momentum equation



Also, each model makes different assumptions based on a general fluid model

$$\frac{d(n_s V_s)}{dx} = Source(x)$$

$$m_s n_s V_s \frac{\mathrm{d}V_s}{\mathrm{d}x} = q_s n_s E - T_s \frac{\mathrm{d}n_s}{\mathrm{d}x} - n_s \frac{\mathrm{d}T_s}{\mathrm{d}x} - \frac{\mathrm{d}\pi_s}{\mathrm{d}x} - m_s V_s S - R_s.$$

$$\epsilon_0 \frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = -e\left(n_i - n_0 e^{-e\phi/T_{e,c}}\right)$$

- Plasma source profiles
  - Often $\frac{d(n_s V_s)}{dx} = \nu_{iz} n_e$
  - Constant $\frac{d(n_s V_s)}{dx} = S$
- Models for ion-neutral friction
  - Constant ν_{in}, λ_{in}
  - Variable ν_{in}
- Sheath edge definitions

PIC simulation data

$p_n [mTorr]$	$\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}}$	$T_{e,\mathrm{c}} [eV]$	$T_{e,\mathrm{se}} [eV]$	$V_{i,\mathrm{se}} [m/s]$	$n_{\mathrm{se}} [\#/m^3]$	$n_0 [\#/m^3]$	$\sigma_s(T_{e,\mathrm{c}}) [m^2]$
10^{-2}	1.53×10^{-6}	0.895	0.701	4.72×10^3	1.60×10^{16}	2.92×10^{16}	1.29×10^{-19}
10^{-1}	1.53×10^{-5}	0.903	0.718	4.61×10^3	1.64×10^{16}	2.92×10^{16}	1.27×10^{-19}
10^{0}	1.52×10^{-4}	0.909	0.732	4.65×10^3	1.62×10^{16}	2.95×10^{16}	1.26×10^{-19}
10^{1}	1.46×10^{-3}	0.868	0.786	4.49×10^3	1.67×10^{16}	3.21×10^{16}	1.21×10^{-19}
10^{2}	1.30×10^{-2}	0.945	0.894	4.30×10^3	1.74×10^{16}	4.01×10^{16}	1.14×10^{-19}
10^{3}	6.95×10^{-2}	0.859	0.701	2.64×10^3	2.90×10^{16}	1.41×10^{17}	1.29×10^{-19}
10^{4}	2.93×10^{-1}	0.326	0.230	4.07×10^2	4.74×10^{16}	7.91×10^{17}	2.25×10^{-19}