SAND2022-13270C

How sheath properties change with gas pressure: modeling and simulation

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4th October 2022

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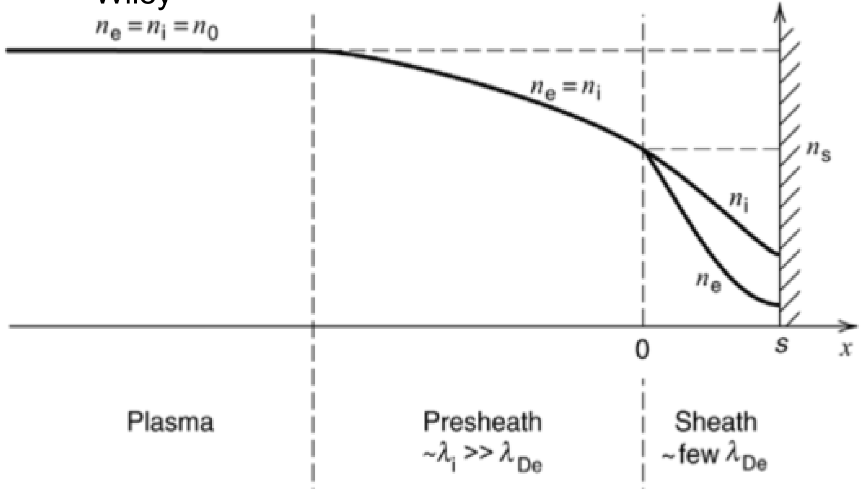
The sheath determines how the plasma and wall interact

- 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

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

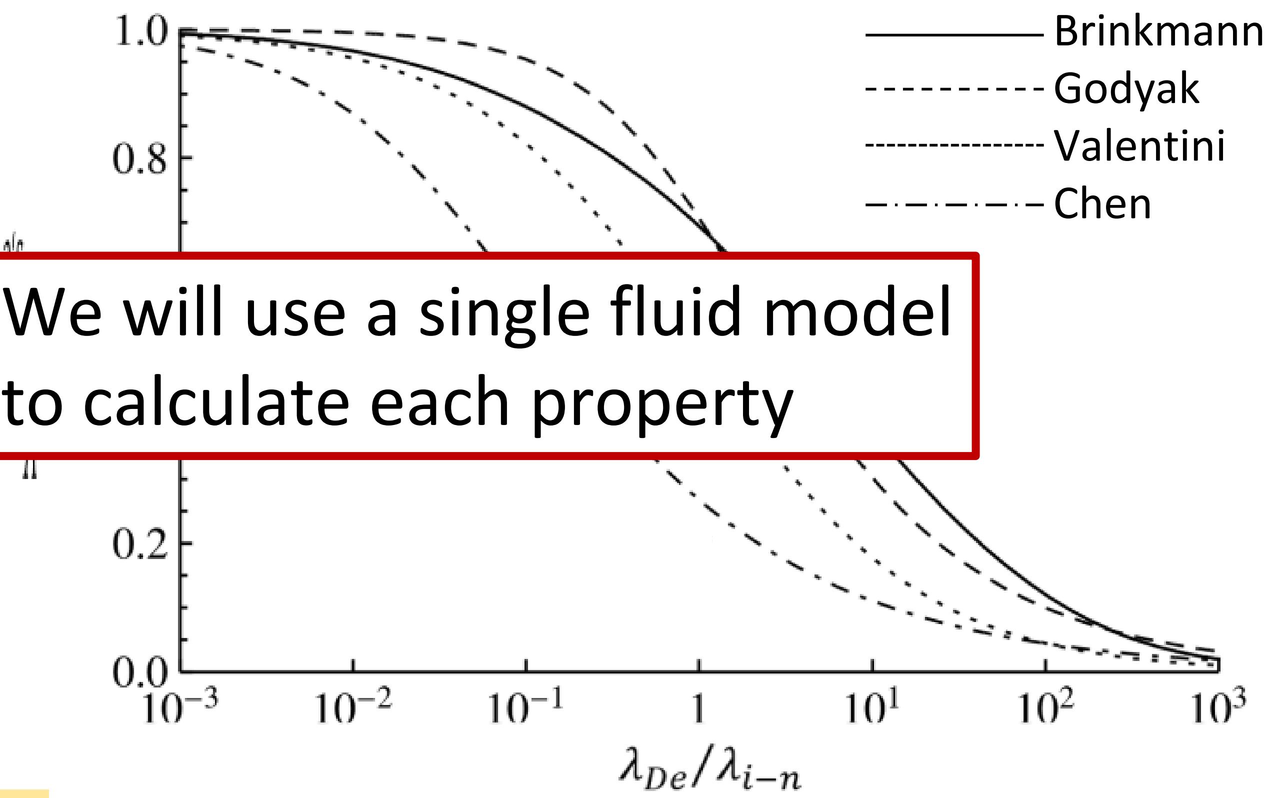
Models of sheath properties have been developed for a range of conditions, including p_n

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*

Edge-to-center density ratio $h_l = \frac{n_{se}}{n_0}$

- J.H. Palacio Mizrahi et al. (2013) *Physics of Plasmas*
- J-L Raimbault et al. (2009) *Plasma Sources Science and Technology*
- M. Lieberman and A. Lichtenberg (2005) Wiley



We will use a single fluid model to calculate each property

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

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

However, few experiments and incompatible assumptions limit the utility of the models

- Most experimental measurements rely on low pressure diagnostics
  - Laser induced florescence ~ 10mTorr
- Plasmas are found/used at higher pressures 1s → 10,000s of mTorr
- Collisional Bohm a_l models
  - Break down in quasineutrality
  - $\frac{|n_e - n_i|}{n_e} = P_\rho \sim 0.01 \rightarrow 0.1$
- Edge-to-center density ratios
  - $V_i = c_{s,c} \rightarrow \; a_l = 1$ for all pressures

Particle-in-cell simulations can study the sheath over a large pressure range $10^{-2} \rightarrow 10^4$mTorr and measurements can be made at many sheath edge locations

My goals are:

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

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

(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 $\frac{d(n_s V_s)}{dx} = \nu_{iz} n_e$

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

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

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

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

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

$p_n[mTorr]$	$\lambda_{\mathrm{De,c}}/\lambda_{in,c}$
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}

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

- 1D-3V simulations using Aleph
  - 1 cm domain
  - 500 to 5,000 cells to resolve $\lambda_{in,c} = 1/(n_n\sigma_s)$
  - 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

Add values of Prho min and max

Next are the results where

represents data from PIC simulations,

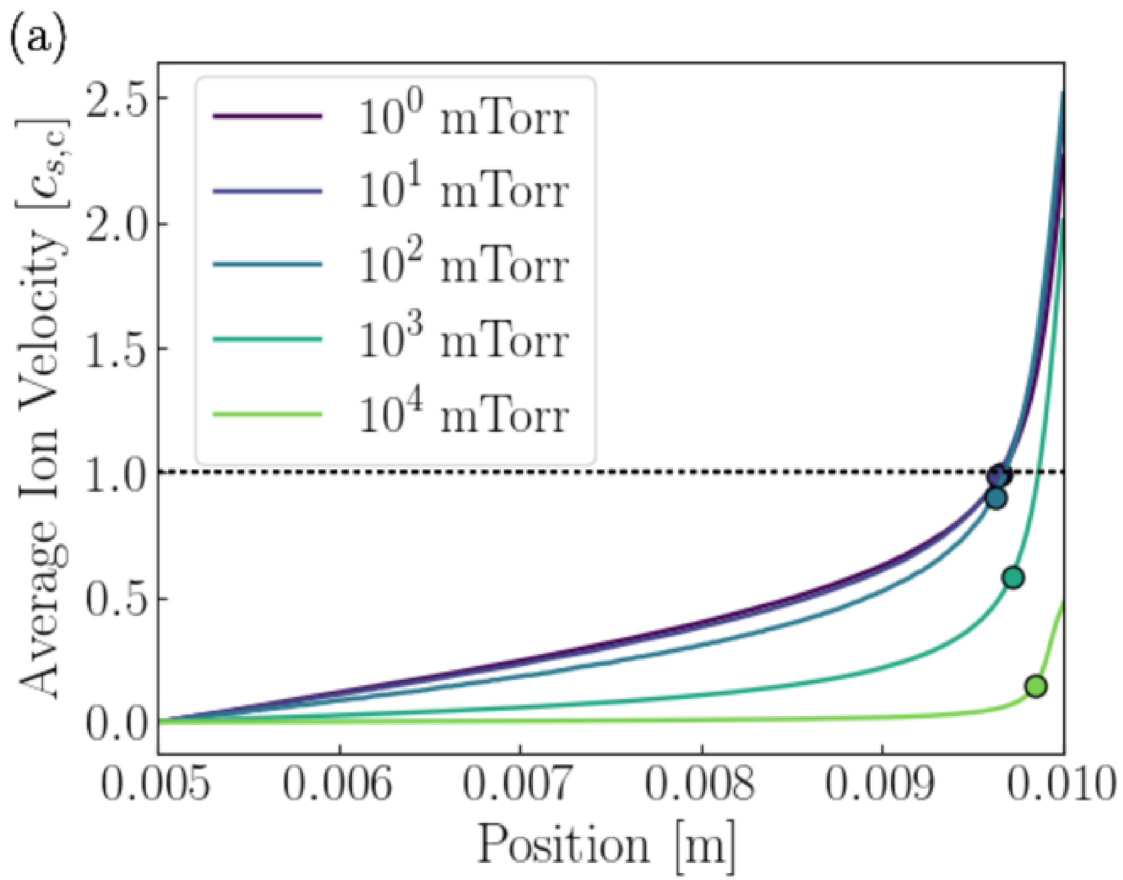
represents the numerical solutions to the fluid model,

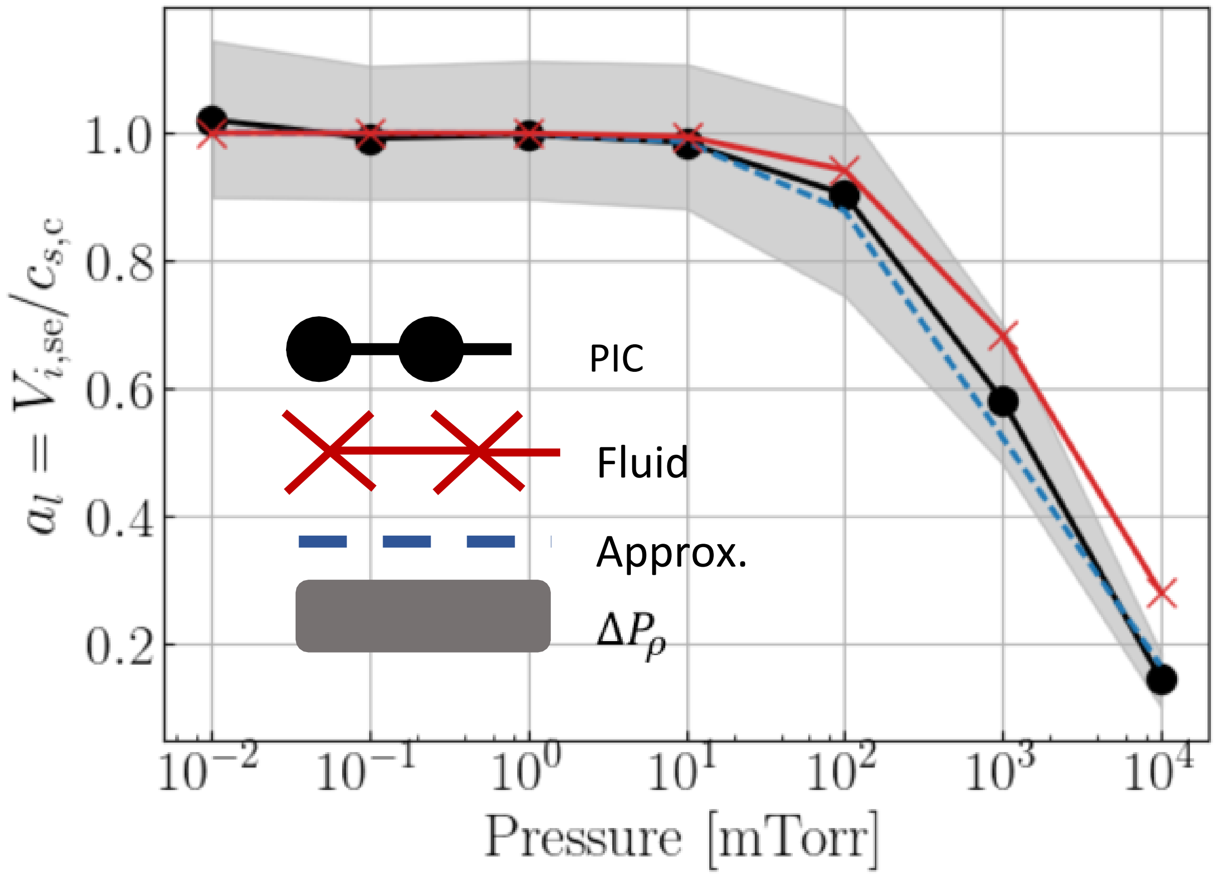
represents the analytic approximations to the fluid model, with modifications based on PIC, and

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

$$\frac{|n_e - n_i|}{n_e} = P_\rho$$

We observe a collisionally modified Bohm criterion



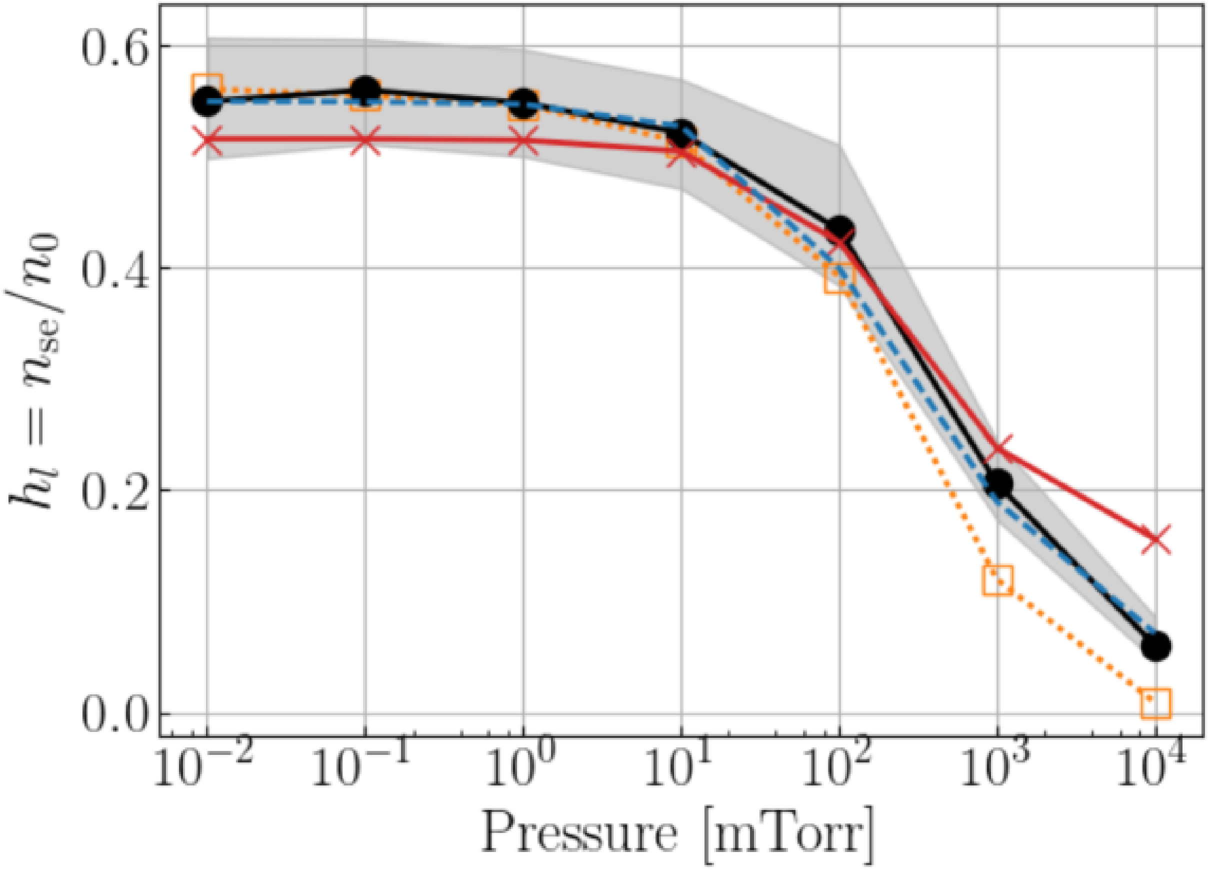


$$a_l = -10(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}}) + \sqrt{1 + 100(\lambda_{\mathrm{De,c}}/\lambda_{in,\mathrm{c}})^2}$$

The edge-to-center density ratio decreases

- PIC
- Fluid
- Approx.
- ΔP_ρ
- $a_l = 1$

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



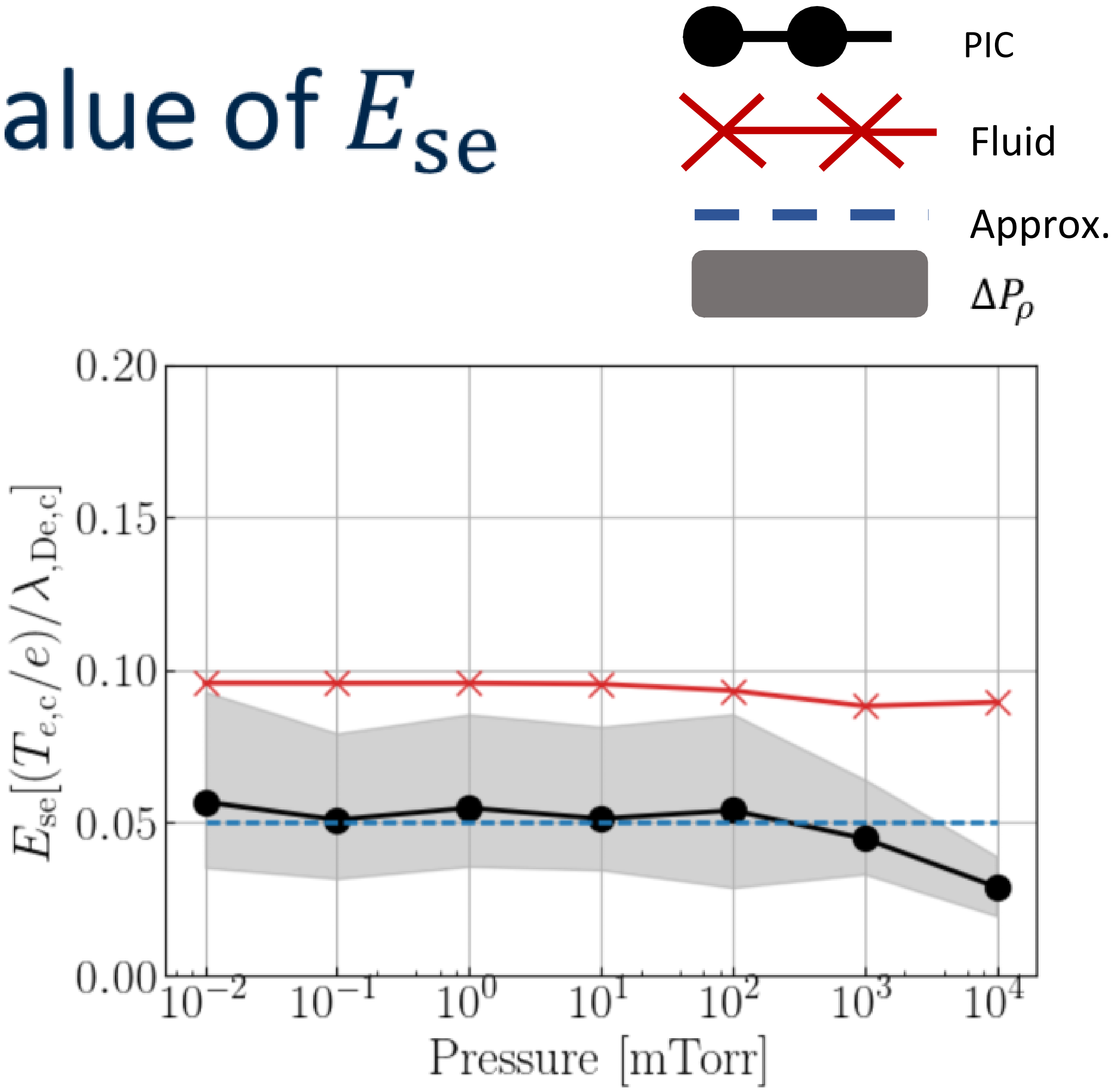
We observe a critical value of E_{se}

- 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*

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

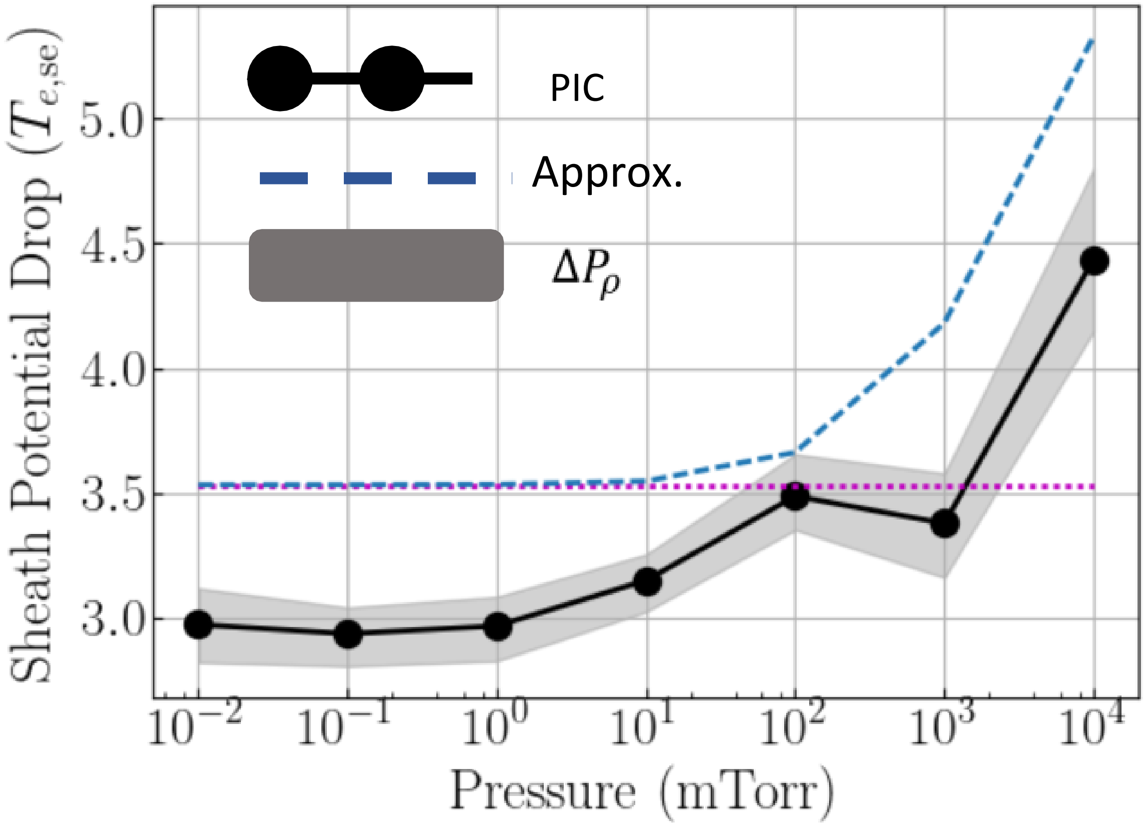


The sheath potential is determined by a_l

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

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

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



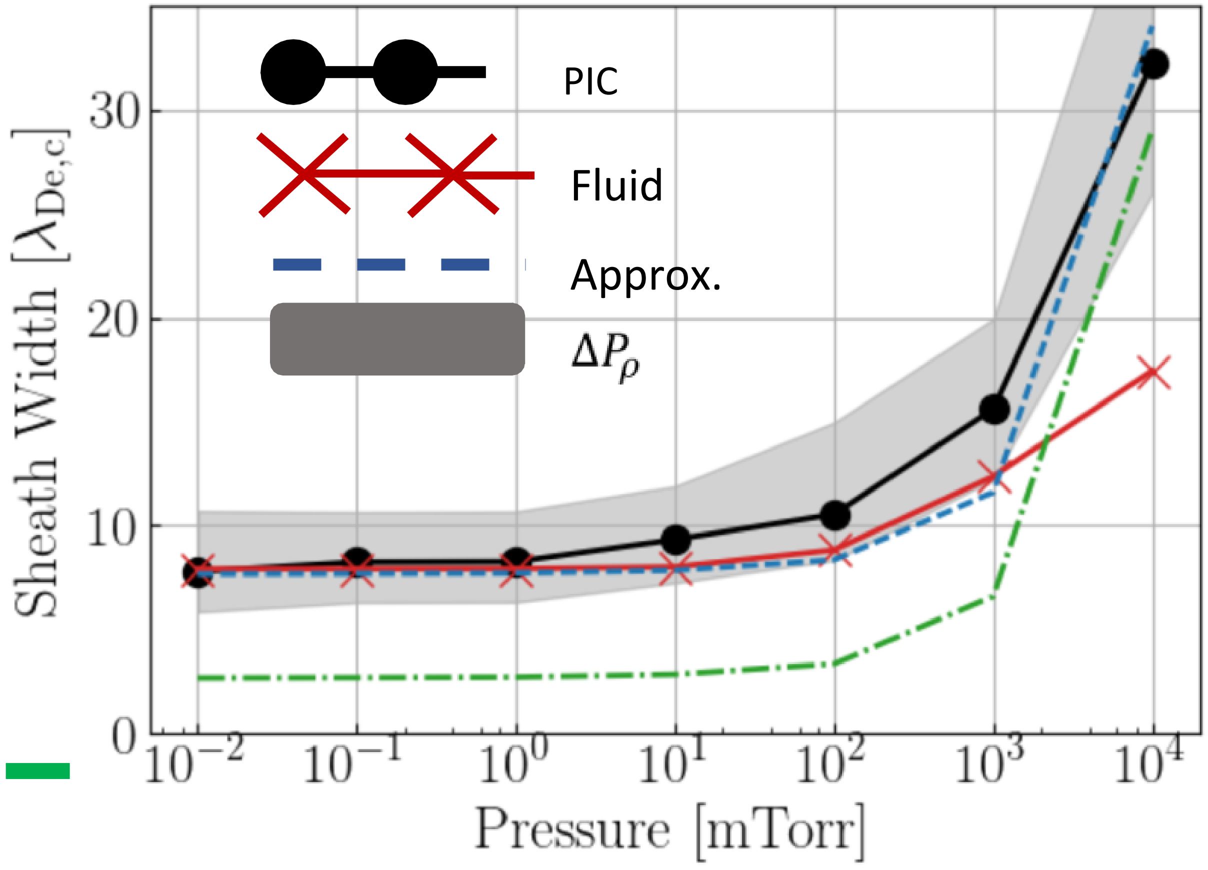
The sheath becomes wider and can be modeled with the Child-Langmuir law

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. Sheath edge properties at different pressures can be predicted 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 fluid model works well until about 10,000 mTorr, where temperature gradients become important

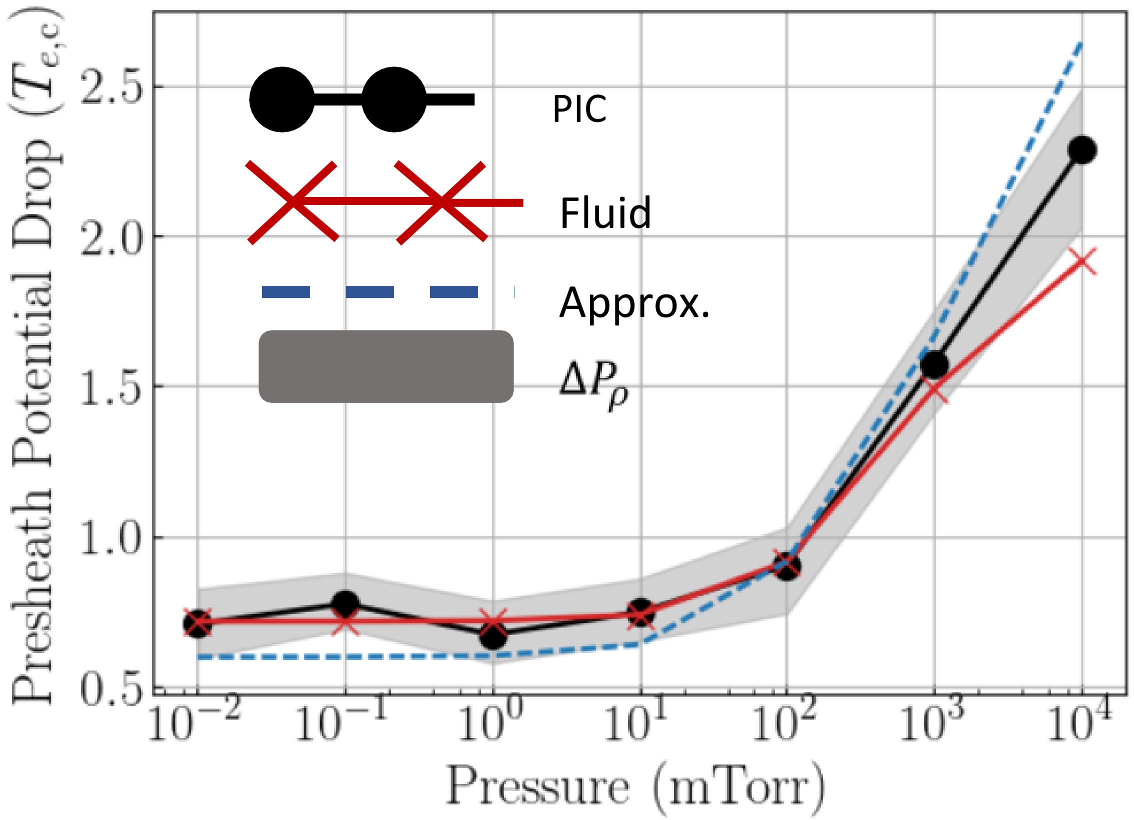
Acknowledgements

- Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
- This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences under contract number DE-NA0003525. This research used resources of the Low Temperature Plasma Research Facility at Sandia National Laboratories, which is a collaborative research facility supported by the U.S. Department of Energy, Office of Science, Office of Fusion Energy Sciences.

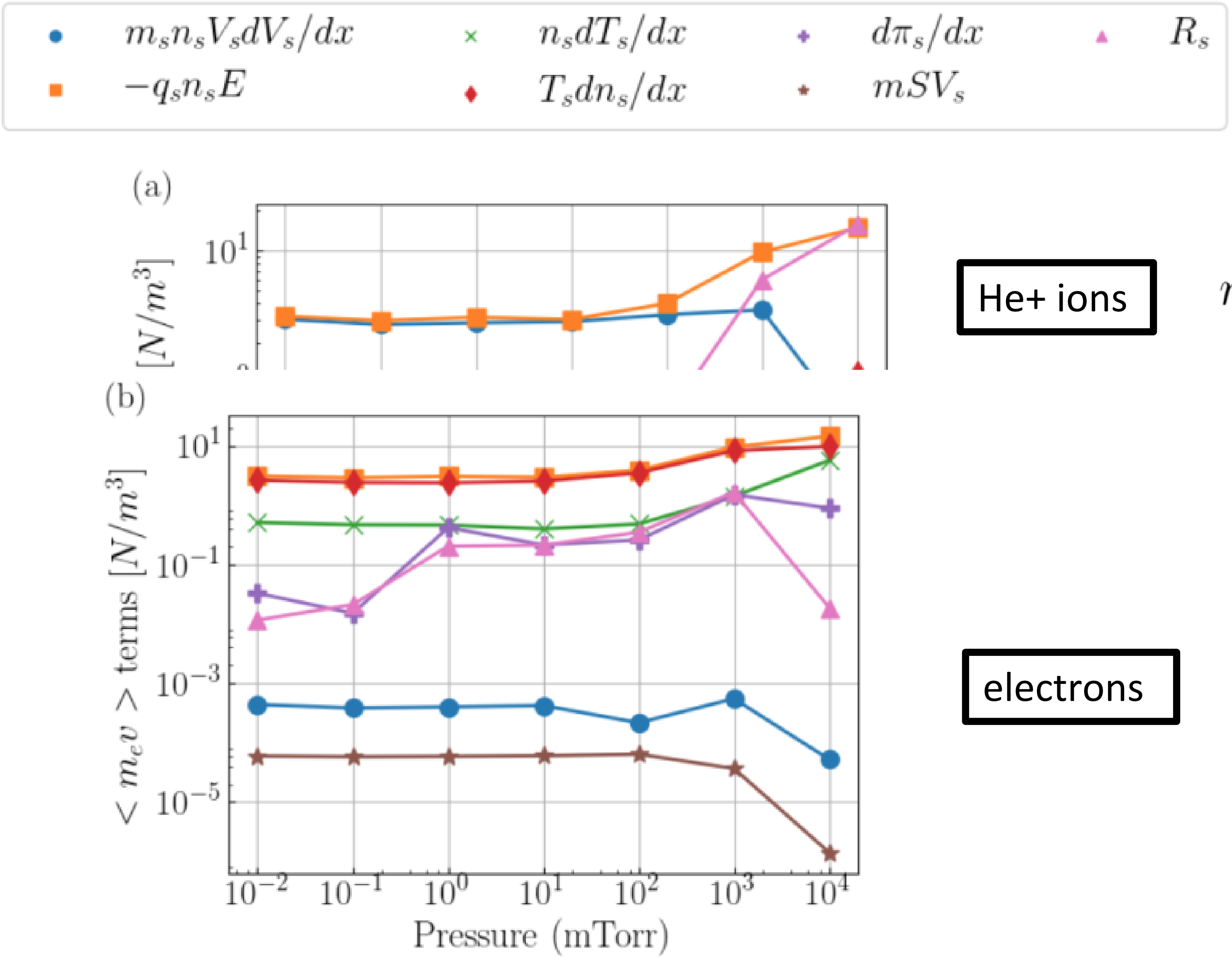
The presheath potential drop is related to h_l

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

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



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

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

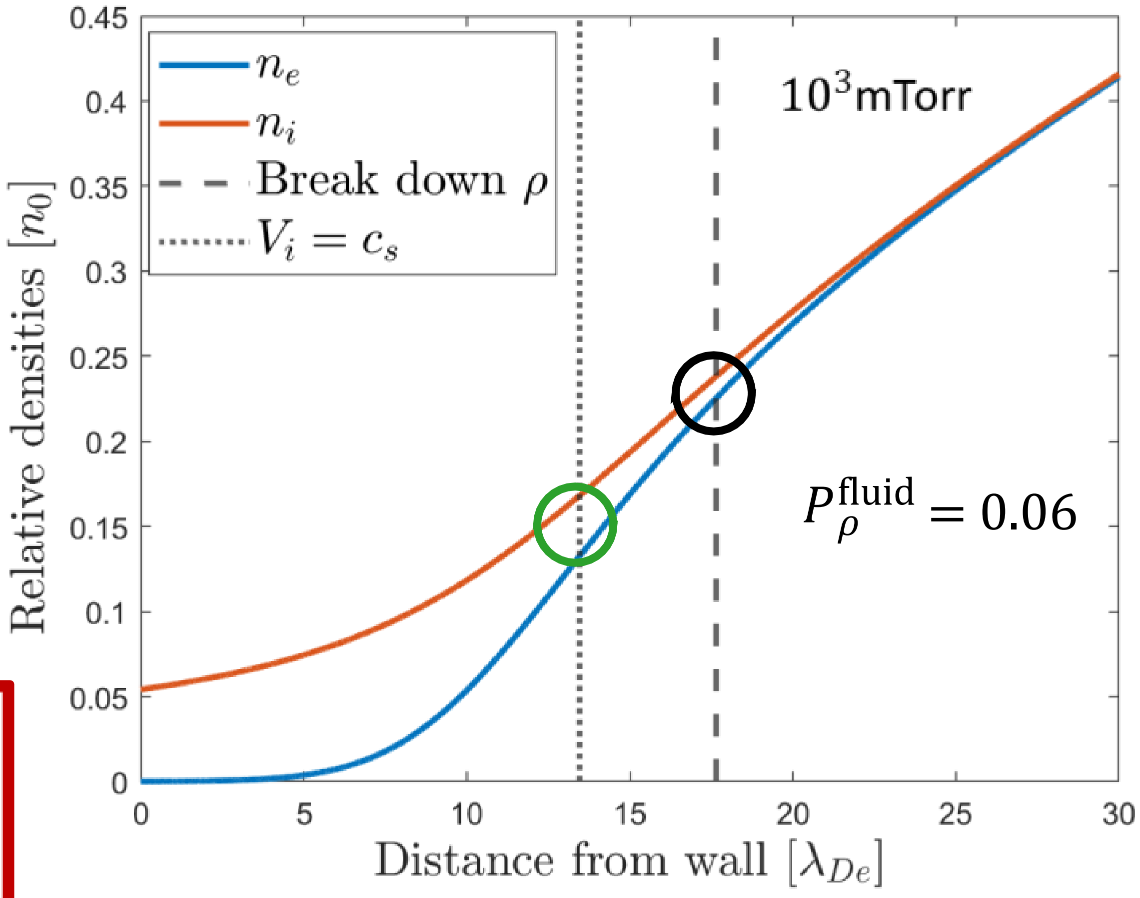
electrons

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

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
  - $V_i = c_{s,c} \rightarrow \; a_l = 1$

Was #5

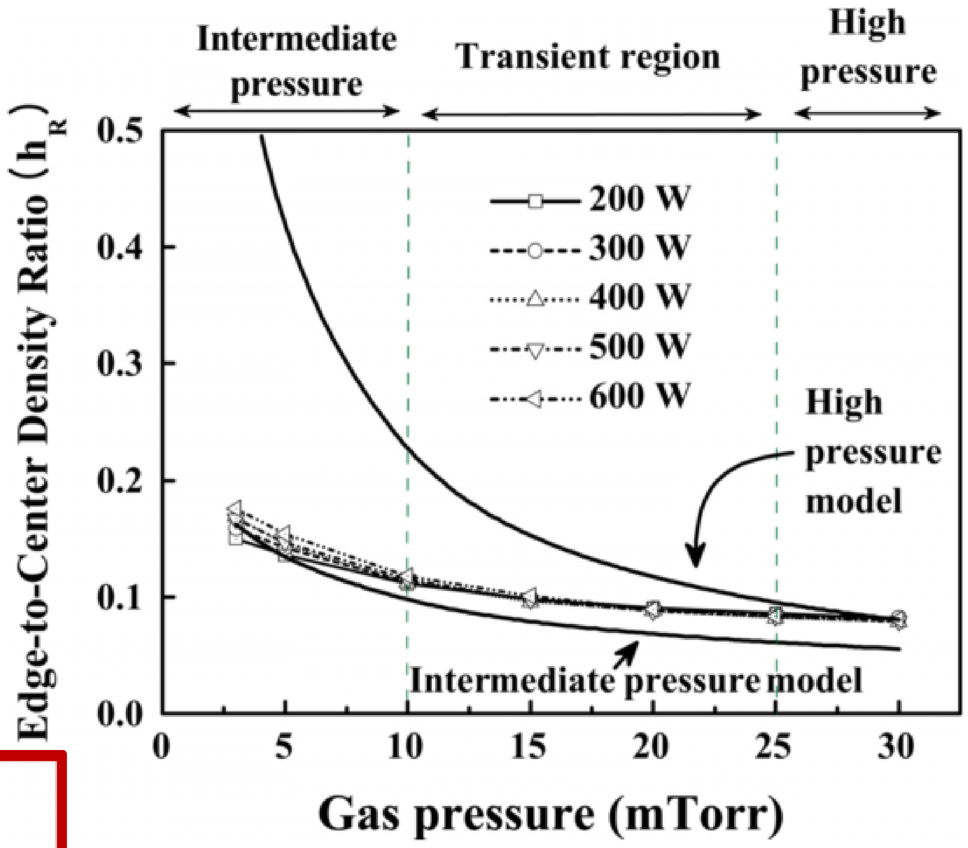


We will use the breakdown in quasineutrality, where $P_\rho^{\text{fluid}} = 0.06$ and $P_\rho^{\text{PIC}} = 0.02$ are chosen so Bohm's criterion is filled at the lowest pressure

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

Was #4



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

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*

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

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

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

Was #8

To model h_l: $n_i = n_e$

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

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

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

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

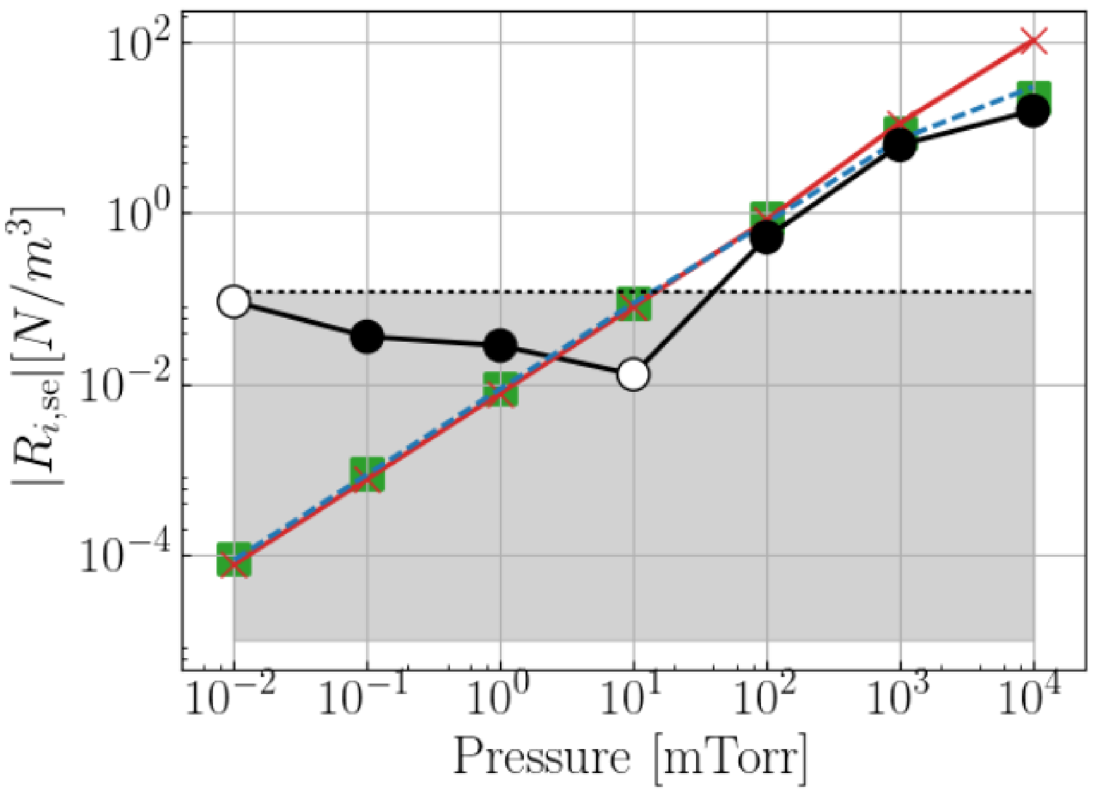
- Calculated R_i directly from PIC data using momentum equation (●, empty means $R_i < 0$):

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

- 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

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

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

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

- 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

$p_n[mTorr]$	$\lambda_{De,c}/\lambda_{in,c}$	$T_{e,c}[eV]$	$T_{e,se}[eV]$	$V_{i,se}[m/s]$	$n_{se}[\#/m^3]$	$n_0[\#/m^3]$	$\sigma_s(T_{e,c})[m^2]$
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}

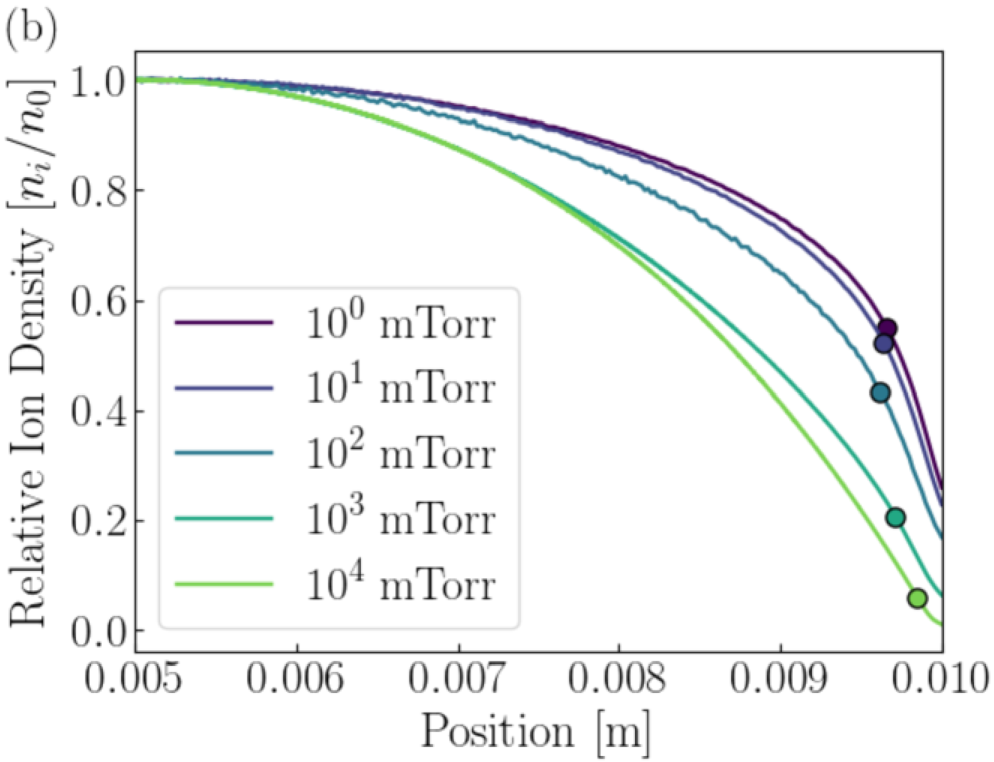
The model is easy to integrate because of S

$$nV = s\xi \quad \text{or}$$

$$h_l a_l = s(L - w_\mathrm{s})/\lambda_{\mathrm{De,c}}$$

$$n(V^2 + 1) + \frac{\lambda_{\mathrm{De,c}}}{\lambda_{in,\mathrm{c}}}\frac{s}{2}\xi^2 = 1 \quad \text{or}$$

$$h_l(a_l^2 + 1) + \frac{\lambda_{\mathrm{De,c}}}{\lambda_{in,\mathrm{c}}}\frac{s}{2}\left(\frac{L - w_\mathrm{s}}{\lambda_{\mathrm{De,c}}}\right)^2 = 1$$

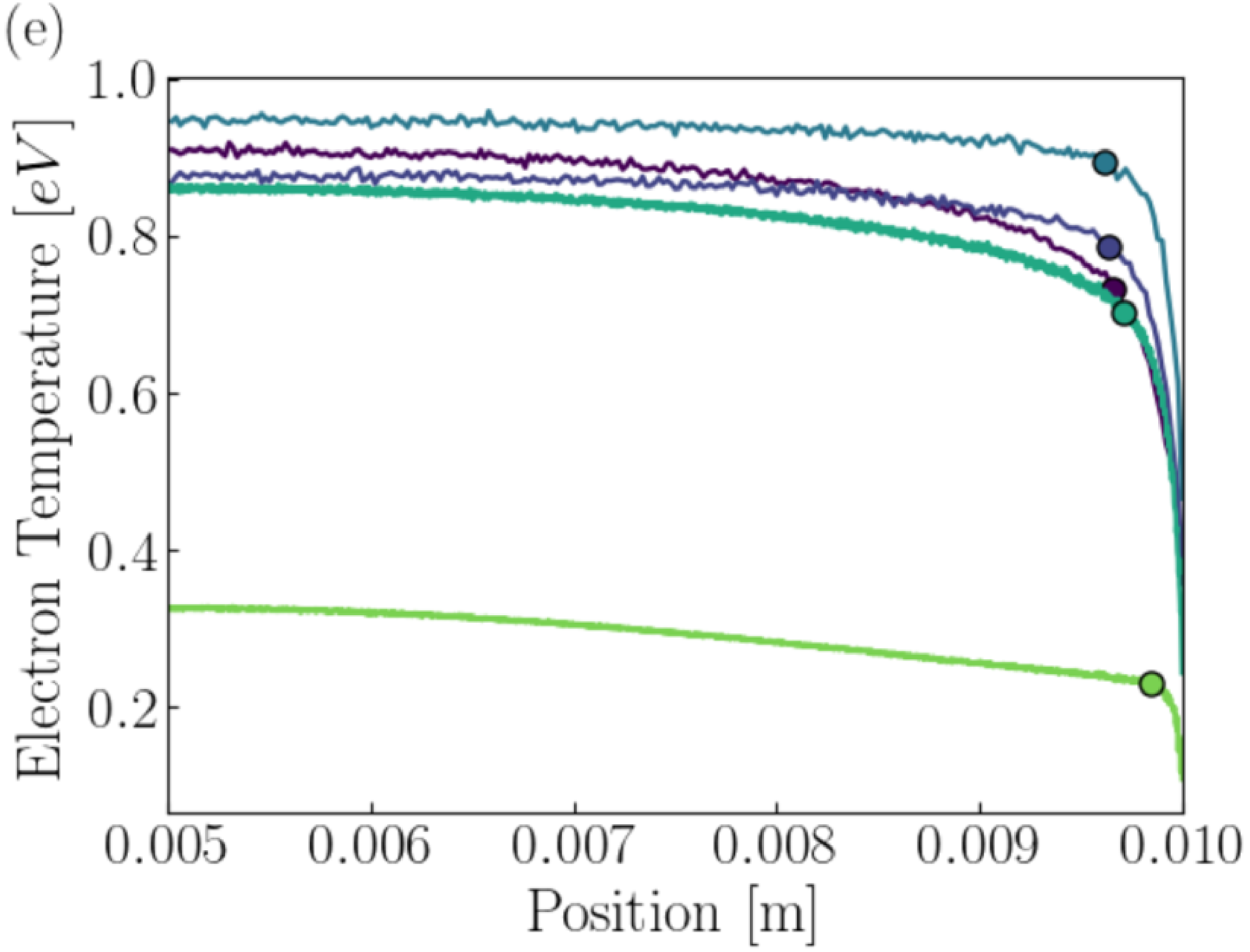


Electron temperature remains relatively constant in PIC

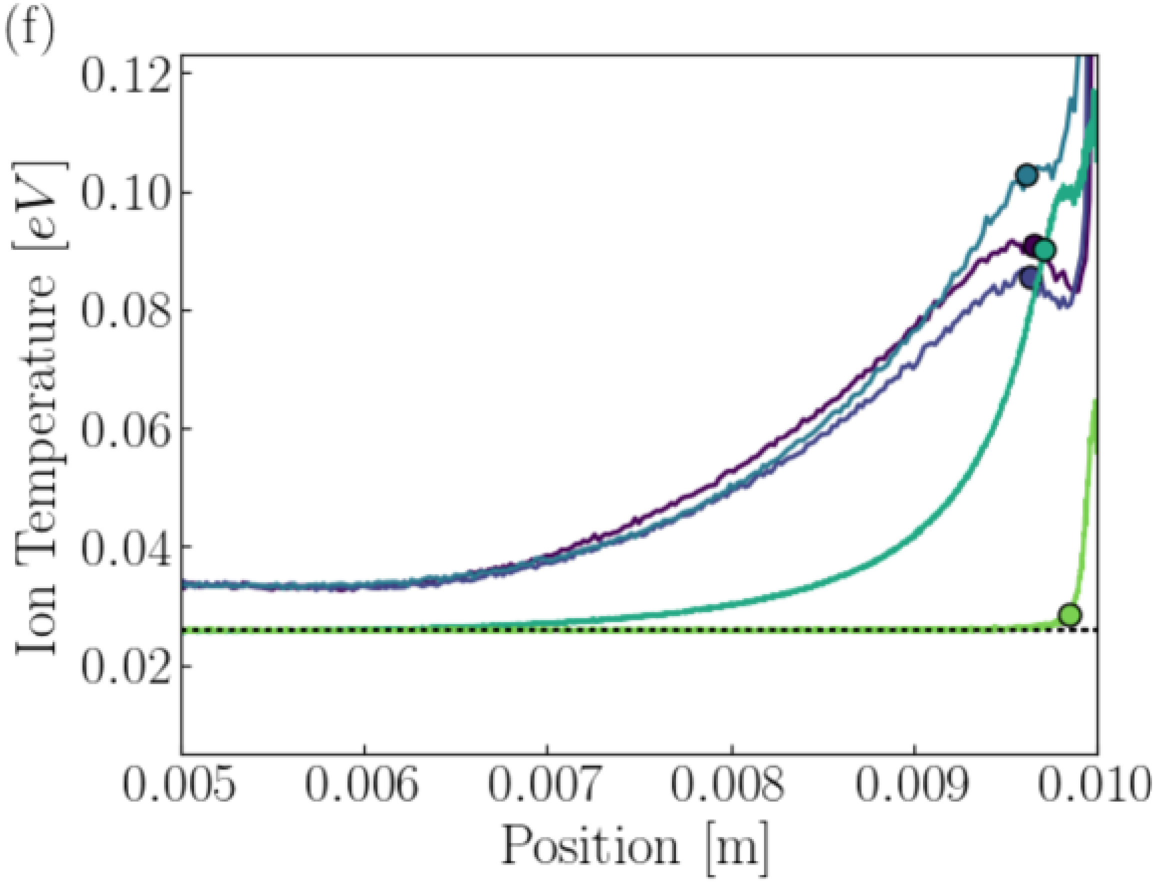
$$T_s = \frac{m_s}{n_s} \int (v_x - V_s)^2 f_{s,x}(v_x)\, \mathrm{d}v_x$$

$$f_{s,x}(v_x) = \int f_s(\mathbf{v}) \mathrm{d}v_y \mathrm{d}v_z$$

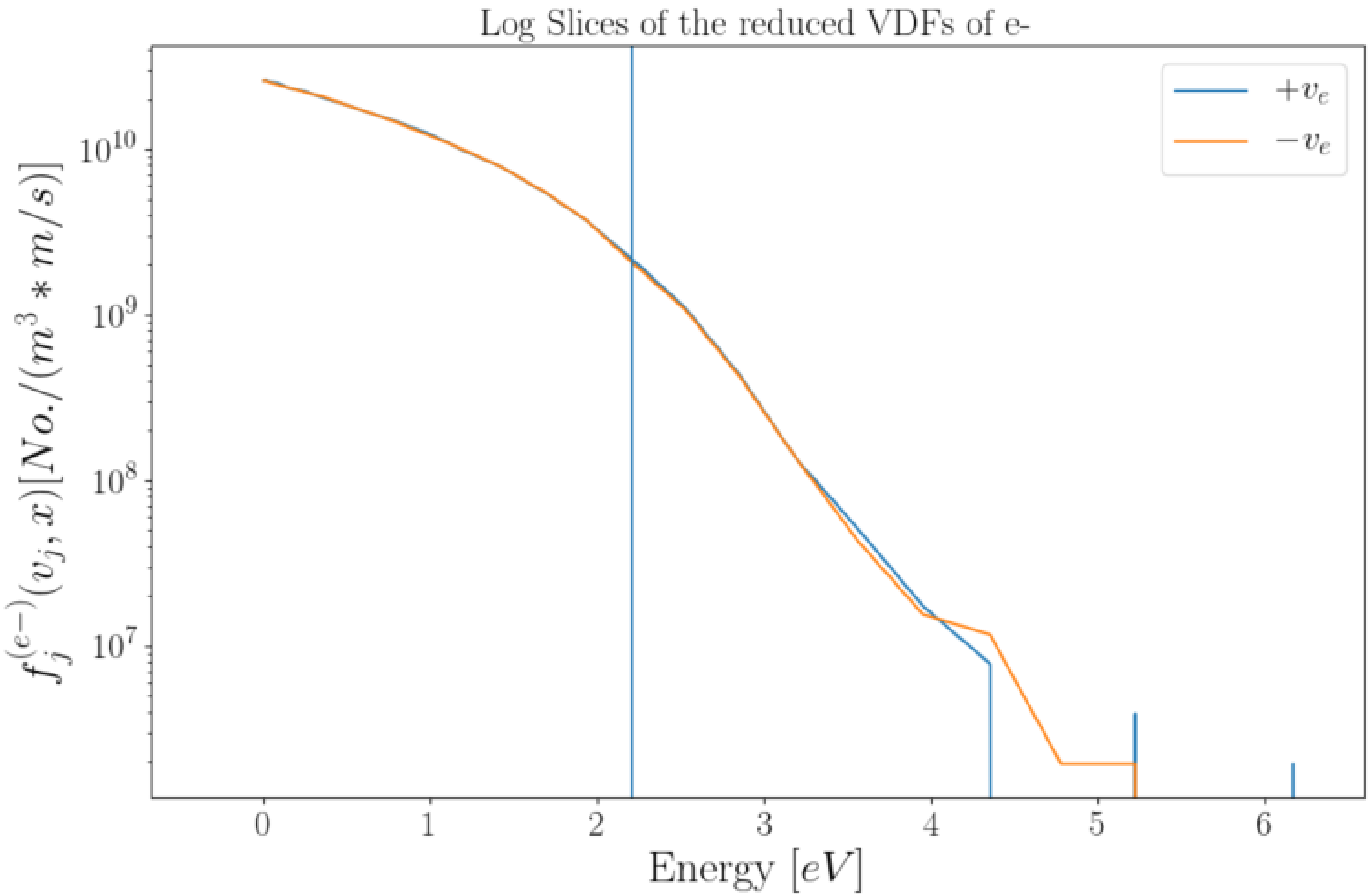
$$V_s = \frac{1}{n_s} \int v_x f_{s,x}(v_x)\, \mathrm{d}v_x$$



Ion temperature increases near sheath edge caused by instabilities and collisions



The model also lacks kinetic effects, specifically the depletion of high energy electrons



determined from Bohm's criterion

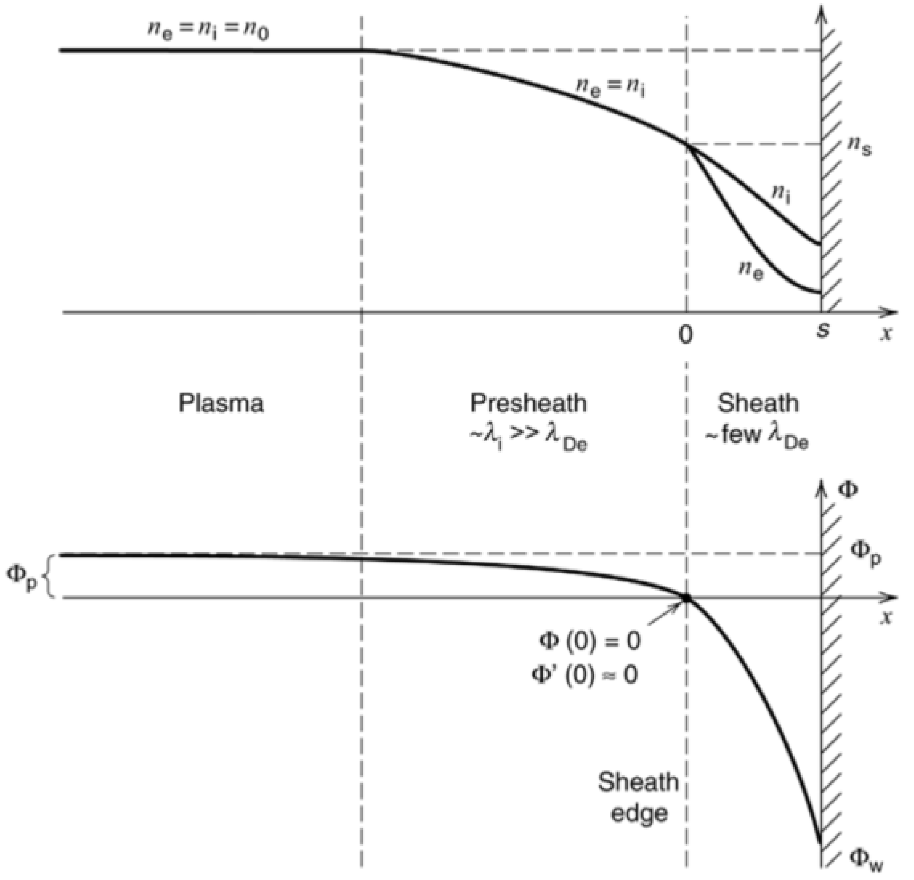
$$n_{se}V_{se}^{i} = h_l n_0 a_l c_s$$
$$= 0.61 n_0 c_s$$

- Bohm's criteria tells us
  1. $V_{se}^{i} \rightarrow c_s$
  2. Presheath potential drop is $\frac{T_e}{2e}$

$a_l = V_{se}^{i}/c_s = 1$

- The Boltzmann density relation tells us
  1. $n_e = n_0 e^{-e\phi/T_e}$
  2. $n_{se} = 0.61 n_0$

$h_l = n_{se}/n_0 = 0.61$



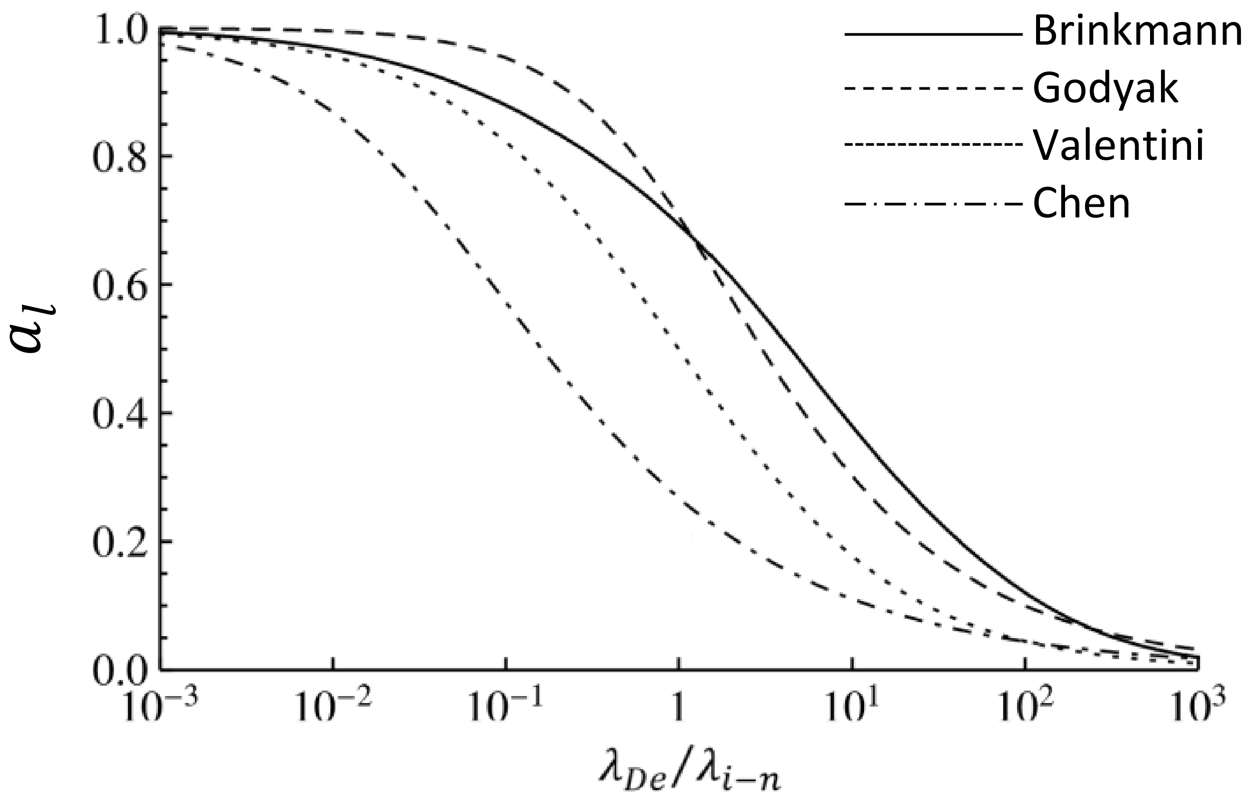
M. Lieberman and A. Lichtenberg. *Principles of Plasma Discharges and Materials Processing*, Wiley 2005

Increasing the pressure is predicted to decrease $a_l = V_{se}^i / c_s$

Godyak: $a_l = \left(1 + \frac{\pi \lambda_{De}}{2\lambda_{i-n}}\right)^{-1/2}$

Valentini: $a_l = \left(1 + \left(\frac{\lambda_{De}}{\lambda_{i-n}}\right)^{2/3}\right)^{-1/2}$

Chen: $a_l = \left(1 + 12.9\left(\frac{\lambda_{De}}{\lambda_{i-n}}\right)^{4/5}\right)^{-1/2}$



Brinkmann, R.P., 2011. Journal of Physics D: Applied Physics 44, 042002

The friction force is represented by a constant collision frequency model

$$R_{in} = m_i n_i V_i \nu_{in}$$

$$\nu_{in} = n_n \sigma V_i = c_{\mathrm{s,c}}/\lambda_{in,\mathrm{c}}$$

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

$$\sigma = \sigma_s (c_{\mathrm{s,c}}/V_i)$$

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

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