One-dimensional Particle Simulations of Knudsen-layer Effects on D-T Fusion

Presented to Kinetic Physics 2016 Workshop

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April 5-7, 2016

LLNL-CONF-683497
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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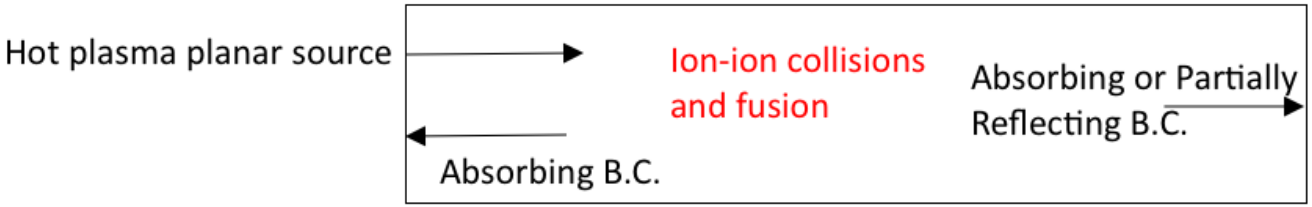
1D Particle Simulations of Knudsen-Layer (KL) Effects on D-T Fusion

- Motivation:
  - **High-energy DT ions** are less collisional $\nu_{coll} \sim v^{-3}$, have longer collisional-mean-free paths $l_{mfp} \sim v^4$, spatially diffuse faster $D_z \sim v^5$, and thus are preferentially lost to absorbing boundaries (**Knudsen-Layer effect**)
  - Given that the D-T fusion cross-section increases with energy up to ~70 keV, **do KL effects degrade inertial fusion reaction rates?**
- 1Dx-3Dv slab PIC simulations are used to study KL effects for conditions relevant to inertial fusion



- **Our simulations show that flow & endloss effects are dominant, and KL effects on the tail of the velocity distribution are sub-dominant in affecting fusion reaction rates for the conditions studied**

Journal article: Cohen, Dimits, Zimmerman, Wilks, Phys. Plas. ***21****, 122701 (2014).*

1D Particle Simulations of Knudsen-Layer (KL) Effects on D-T Fusion

- 1Dx-3Dv slab PIC simulations with ICEPIC are used to study KL effects
  - solves fully nonlinear collisional kinetic equation for $f(z,v_x,v_y,v_z)$

$$\frac{\partial f_s}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f_s + \mathbf{a}\cdot\nabla_{\mathbf{v}} f_s = C(f_s, f_s) + C(f_s, f_{s'})$$

with Takizuka-Abe-Nanbu Coulomb collisions

  - fluid electrons and ambipolar fields (electric fields have little effect)
  - Bosch-Hale kinetic and Maxwellian fusion computations
  - absorbing b.c. and explicit kinetic plasma source at z=0
  - partially or fully absorbing b.c. at z=L
- Verification and convergence of collision and fusion routines
- Base case and matrix of simulations
- PIC and simplified 1D hydro simulations obtain qualitatively similar results

- **KL effects modify velocity distributions (loss of highest axial energy ions) but have little influence on fusion rates for the conditions in our simulation if you accurately calculate the overall cooling and loss of plasma density**

PIC Simulation Methodology - Verification and Convergence of Collision and Fusion Computations

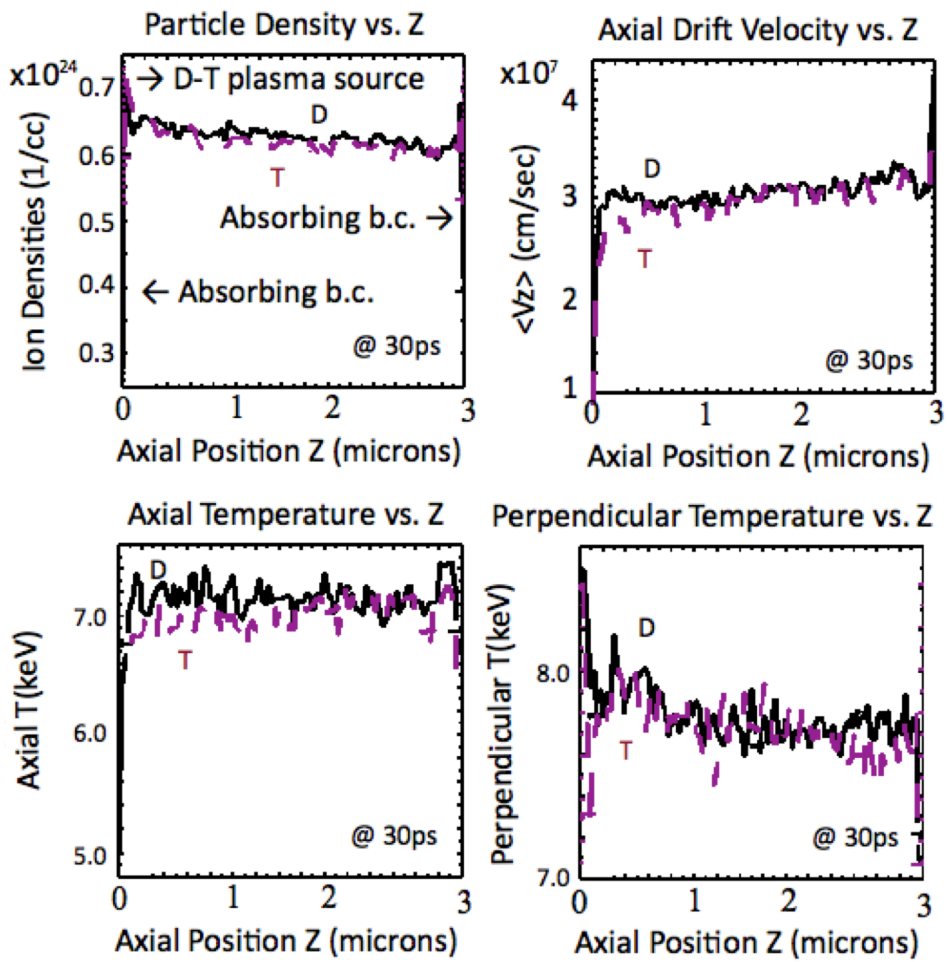
- **Collision algorithms**
  - Inter-species and intra-species collision routines in ICEPIC have been documented in B. I. Cohen, A. M. Dimits, A. Friedman, and R. E. Caflisch, IEEE Trans. Plasma Sci. 38, Issue 9 Part 1, 2394 2010, which provides guidance on Δt, $\nu_{coll}\Delta t \sim O(1)\times 10^{-2}$ for good accuracy. There is no simplification of the collision operator.
  - **Verified on test cases**: preserve a Maxwellian, momentum/energy conservation in binary collisions, relaxation rates of (i) weak temperature anisotropy and (ii) relative drift, …

- **Implementation of Bosch-Hale fusion cross sections**
  - Based on H.-S. Bosch, G. M. Hale, Nuc. Fusion 32, 611 (1992) : $\langle\sigma v\rangle$ thermal Eqs.(12-14) and σ kinetic Eqs.(8-9)+Table IV
  - **Verification** of D(t,n)α computation in code vs. Bosch and Hale tables
  - **Convergence** wrt particle statistics ➔ 10^4 ions per species per cell reduces error to < 0.5% in kinetic fusion rate recovering Maxwellian rate

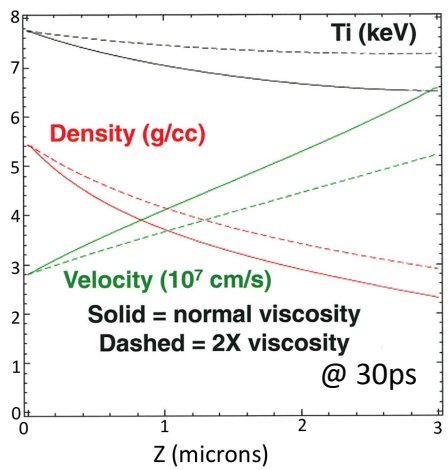
Typical Results from 1D PIC Simulation of Knudsen-Layer (KL) Effects on D-T Fusion – Base Case

- $K_n = l_{mfp}/L = 0.1$, T_0=9keV, n_0=1x10^{24}cm^{-3} (D & T), 10^4 particles/cell per ion species, L=3 micron, 100 cells, 30 ps, $\nu_{coll}t$~60
- **Steady flow** increasing from source to sink at $z=L$, **cooling** due to flow gradient and end loss; axial gradients in $T_{z,\perp}$, ion densities, and **fusion reduction**; anisotropy of $f(v_z, v_\perp)$ and $T_{z,\perp}$; and **KL effects**: depletion of velocity tail in v_z.

1D particle simulation

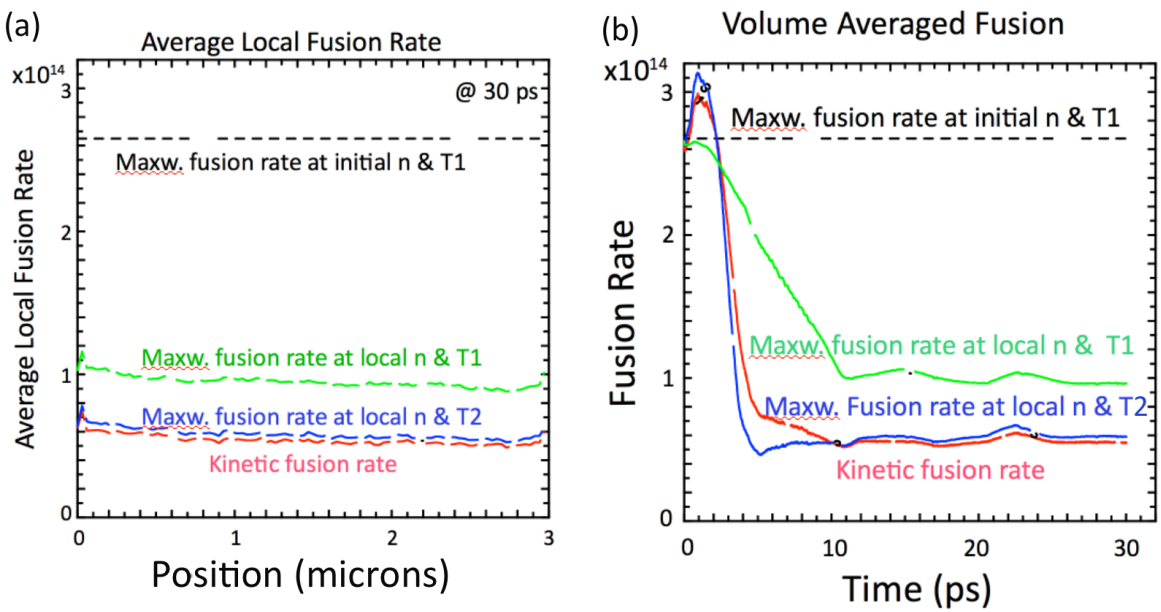


Simplified 1D hydro simulation (single species ion fluid, scalar pressure, no thermal conduction) **obtains qualitatively similar results**



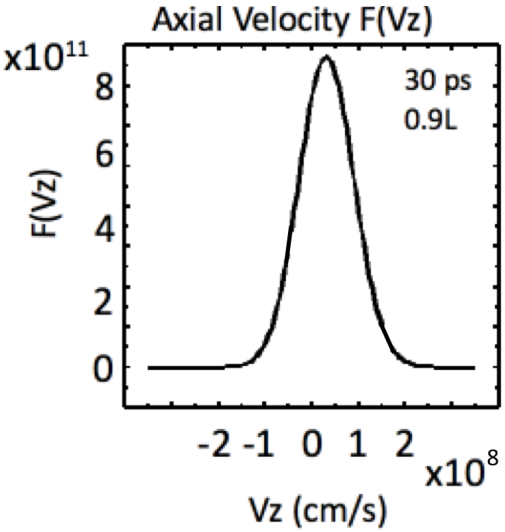
1D PIC Simulation of Knudsen-Layer (KL) Effects on D-T Fusion – Base Case

- Flow and end loss produce density and temperature gradients that **decrease *n*, *T*, and fusion reactivity** across the domain and relative to t=0 fusion rates : $T_z < T_\perp$ and $T_z, T_\perp < T_{source}$=9 keV and $n(z) < n_0 = 1\times10^{24}$ cm^{-3} ➔ **Not a K-L effect!**
- For T=9 keV, $\varepsilon_{Gamow\ peak}/T \sim 3.2$; $f(v_z, v_\perp)$ is colder and remains close to a Maxwellian near the Gamow energy where the fusion is maximized. The **kinetic and Maxwellian fusion rates** using the local n and local temperature $T_2 = 1/3\ [\langle v_z^2\rangle - \langle v_z\rangle^2 + \langle v_x^2\rangle + \langle v_y^2\rangle]$ **agree to within ~10%**.

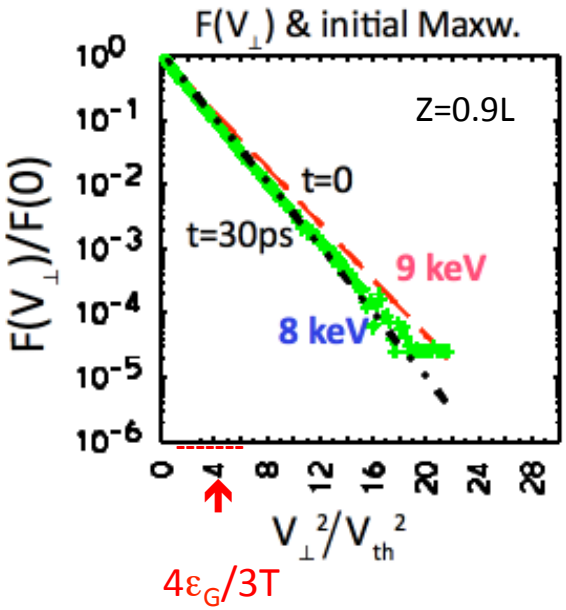


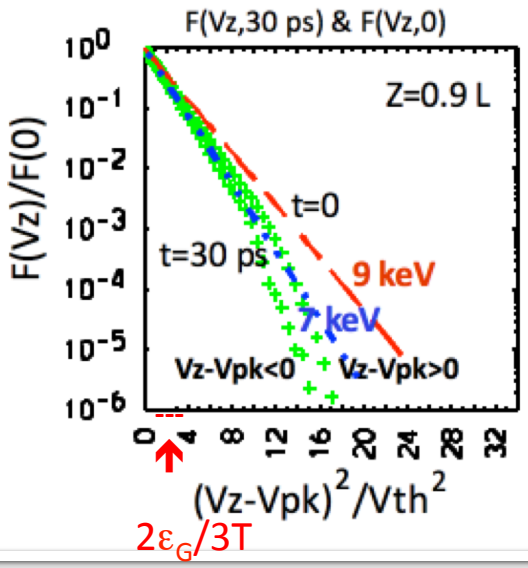
- T_1 = initial/source temperature
- T_2= local temperature
- $T_2 < T_1$
- Fusion rate = fusions per 1 ps per cell

1D PIC Simulation of Knudsen-Layer (KL) Effects on D-T Fusion – Base Case



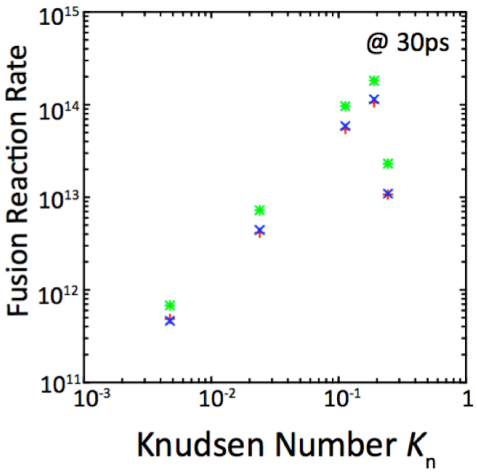
Deuterium velocity distributions





- $F(V_z)$ acquires a drift and cools more than does $F(V_\perp)$
- $F(V_z)$ loses tail ions forming a KL distribution
- $F(V_z, V_\perp)$ is close to Maxwellian around Gamow peak

1D PIC Simulation of Knudsen-Layer (KL) Effects on D-T Fusion – Matrix of Simulations

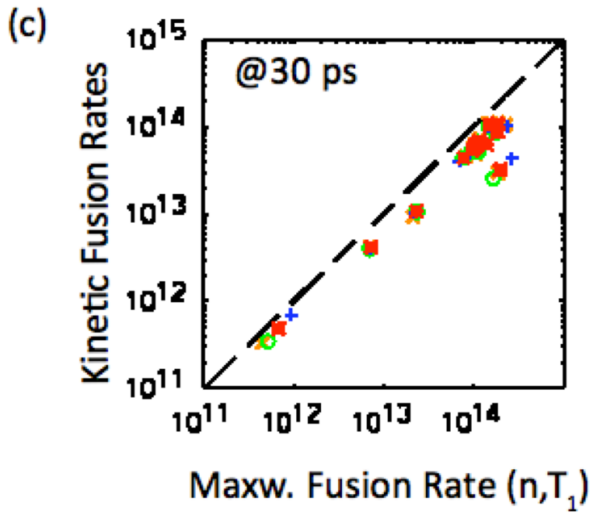


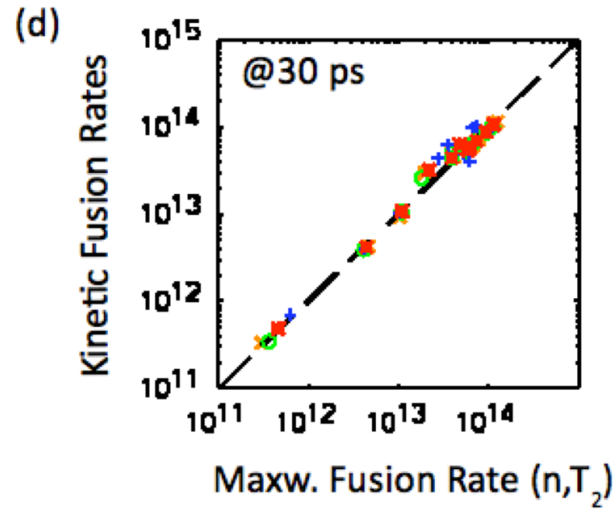
T_1 (keV) = [2, 4, 9, 12] & 3 μm and 9 keV & 1.5 μm

+ kinetic fusion rate

x thermal Maxwellian fusion rate using local n and T_2

* thermal Maxwellian fusion rate using local n and initial/source T_1





Results from suite of simulations

- Suite of simulations varying plasma and boundary conditions yields consistent results
- Bosch-Hale kinetic fusion rate in the simulations is **reduced 45-70%** below the Maxwellian rate using the local density and the initial/source temperature $\boldsymbol{T_1}$ **➔ not a KL effect**!
- The kinetic and Maxwellian fusion rates agree within ~±10% using the local density and local temperature $\boldsymbol{T_2}$=1/3 m[$\langle v_z^2\rangle - \langle v_z\rangle^2 + \langle v_x^2\rangle + \langle v_z^2\rangle$]

1D PIC Simulation of Knudsen-Layer (KL) Effects on D-T Fusion – Comparison to Albright et al PoP 2013

Ref. B. J. Albright, Kim Molvig, C.-K. Huang, A. N. Simakov, E. S. Dodd, N. M. Hoffman,1 G. Kagan, and P. F. Schmit, Phys. Plasmas 20,122705 (2013)

- Our slab simulations observe a kinetic fusion reactivity reduction= **0.57** for K_n=0.11 (adjusted for the volume-average ion densities and temperatures) compared to a reactivity reduction=**0.62** for K_n=0.12 in the slab calculation of Albright et al.

- Albright et al use a linear collision operator, assume pitch-angle scattering is dominant in the tail, and hold the Maxwellian component of $f_{ion}(\mathbf{v})$ at constant density and temperature

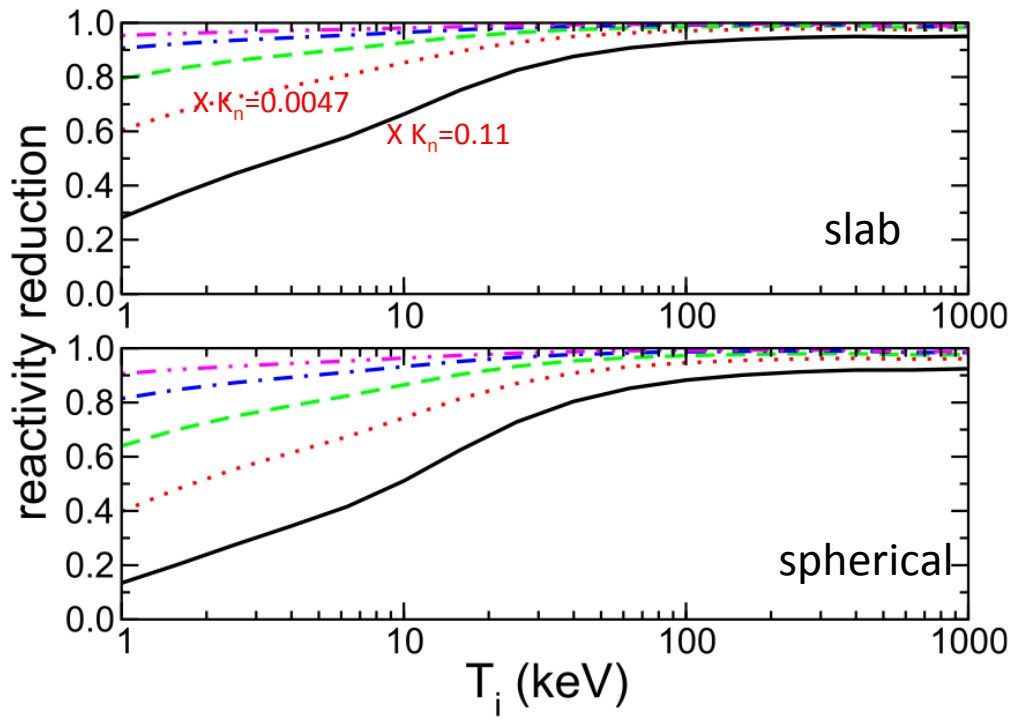


FIG. 5. DT fusion reactivity reduction factor $\langle\sigma_{\rm fus}v\rangle(T_i,N_K)/\langle\sigma_{\rm fus}v\rangle(T_i,0)$ averaged over plasma fuel volume for slab (top) and spherical (bottom) geometry for equimolar DT fuel at constant density and temperature across the cavity. Shown are results for $N_K^{\rm cav}=0.12$ (solid), 0.048 (dotted), 0.024 (dashed), 0.012 (dot-dashed), and 0.006 (dot-dot-dashed).

Knudsen Layer PIC Simulations: Observations and Conclusions

- PIC simulations solve fully nonlinear collisional kinetic equations with explicit source and absorbing or partially absorbing boundary conditions as an initial-value problem
- A steady-state flow is achieved for t > 20-25 ps in PIC and hydro simulations
- Energy from the injected source is partitioned between flow energy and parallel temperature resulting in $T_z < T_{source}$ and $T_z < T_\perp$
- Flows increase toward $z=L$, and densities and temperatures necessarily decrease to conserve mass and energy fluxes, which affect fusion rates ➔ **kinetics plays a role, but this is not a KL effect due to modifications just to the tail of $f(v_z,v_\perp)$!**
- There is qualitative agreement between the PIC and hydro simulations
- KL effects on $f(v_z)$ high energy tail are present in the PIC simulations but do ***not*** have a significant effect on the fusion reaction rates (~10%), but overall cooling and density evolution matter
- The ICEPIC simulations are solving a somewhat different physical problem than in the linearized Molvig *et al.* and Albright *et al.* calculations.

Journal article: Cohen, Dimits, Zimmerman, Wilks, Phys. Plas. ***21****, 122701 (2014).*

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Suite of 1D PIC Simulations of Knudsen Layer Effects

TABLE I. Suite of simulations for 30 ps.

Case No.	Description and Comments
1	Base Case: 9 keV initial and source plasma; no reflection at right side; D-D, T-T, and D-T collisions; no electric fields; no ion-electron collisions
2	Variation from base case: 4 keV initial and source plasma Results: Colder, more collisional, much less fusion, similar density, lower axial drift velocity, much weaker KL effect on $f(v_z)$
3	Variation from base case: 50% reflectivity from right side boundary (9 keV retherm) Results: A little colder but higher density, particularly near reflecting wall; slightly more fusion, weaker drift velocity, less end loss, much weaker KL effect on $f(v_z)$
4	Variation from base case: 50% reflectivity from right side boundary (4 keV retherm) Results: Colder, more collisional, much less end loss, and denser than 107 and 110; little or no KL effect on $f(v_z)$
5	Variation from base case: Adds fully ionized Cu at 0.001× number density of D & T Results: More collisional; smaller K_n; slightly higher density because end loss smaller; more fusion; weaker KL effect on $f(v_z)$
6	Variation from base case: Adds ion-electron collisions and ambipolar electric field, $T_e = 9$ keV Results: Slightly higher density and temperature; lower drift velocity and less endloss; so more fusion; KL modification of $f(v_z)$ is much weaker
7	Variation from base case: Adds fusion alpha particles at 0.001 × number density of D & T and ion-electron collisions (but electron fluid temperature held constant) Results: Lower drift velocity and less end loss, so slightly higher density; slightly hotter plasma; 20% more fusion; alphas contribute more collisionality; effective K_n is reduced leading to weaker KL effect on $f(v_z)$
8	Variation from base case: Collisionless plasma Results: Higher drift velocity $\sim 0.8 v_{th}$; $f(v_z, v_\perp)$ determined by source; more end loss, so density is ~20% less and fusion is reduced; $f(v_z, v_\perp)$ loses most $v_z < 0$ particles
9	Variation from base case: 2 keV initial and source plasma Results: Colder, more collisional, much less fusion, higher density, much lower axial drift velocity, very small KL effect on $f(v_z)$
10	Variation from base case: 12 keV initial and source plasma Results: Hotter, less collisional, similar density, more fusion, higher axial drift velocity, strong KL effect on $f(v_z)$
11	Variation from base case: Increased source rate, ×1.66 Results: Higher axial drift velocity, slightly colder, higher density, more collisional, more fusion, strong KL effect on $f(v_z)$
12	Variation from base case: System length reduced to $L = 1.5\mu$m Results: 3× axial drift velocity, slightly colder, 1/2 density, relatively flat spatial plasma profiles, reduced fusion, strong KL effect on $f(v_z)$

Suite of 1D PIC Simulations of Knudsen Layer Effects

TABLE II. Fusion reaction rates, temperatures, $\langle v_z \rangle$, and K_n for suite of simulations.

Case Nos.	Avg. kin Fusion	Kin/Maxw Fusion T_1	Kin/Maxw Fusion T_2	T_z (keV)	$T_\perp$ (keV)	$\langle v_z \rangle$ (cm/s)	K_n	KL $f(v_z)$
1	5.46×10^{13}	0.568	0.927	7.0	7.8	3.0×10^7	0.11	Yes
2	4.14×10^{12}	0.573	0.935	3.5	3.6	1.6×10^7	0.024	Weaker
3[a]	6.31×10^{13}	0.6 ± 0.1	1.3 ± 0.1	7.8 ± 1	6.7 ± 0.5	$9 \pm 5 \times 10^6$	0.067	Weaker
4[a]	3.19×10^{13}	N/A	1.4 ± 0.5	5 ± 0.5	4.7 ± 0.5	$9 \pm 3 \times 10^6$	0.031	No
5	6.20×10^{13}	0.585	0.938	7.0	7.9	3.0×10^7	0.075	Weaker
6	1.04×10^{14}	0.698	0.920	8.0	8.3	1.7×10^7	0.10	Weaker
7	6.91×10^{13}	0.606	0.934	7.3	7.9	2.4×10^7	0.097	Weaker
8	4.42×10^{13}	0.575	1.12	3.4	9.0	4.9×10^7	∞	No
9	4.85×10^{11}	0.717	1.05	1.9	1.9	7.5×10^6	0.0047	No
10	1.06×10^{14}	0.584	0.926	9.5	10.2	4.7×10^7	0.19	Yes
11	8.70×10^{13}	0.475	0.920	6.5	7.5	4.7×10^7	0.078	Yes
12	1.07×10^{13}	0.463	0.976	6.3	7.4	9.0×10^7	0.24	Yes

[a]Cases 3 and 4 are not in steady state at 30 ps.