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

Presented to Kinetic Physics 2016 Workshop


April 5-7, 2016
1D Particle Simulations of Knudsen-Layer (KL) Effects on D-T Fusion

• Motivation:
  – **High-energy DT ions** are less collisional $v_{\text{coll}} \sim v^{-3}$, have longer collisional-mean-free paths $l_{\text{mfp}} \sim v^4$, 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 $\sim 70$ 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

![Diagram](image)

• **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 $f(z,v_x,v_y,v_z)$
    \[
    \frac{\partial f_s}{\partial t} + v \cdot \nabla_x f_s + a \cdot \nabla_v f_s = C(f_s,f_s) + C(f_s,f_s') \] 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
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 $\Delta t$, $\nu_{\text{coll}} \Delta t \sim O(1) \times 10^{-2}$ 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) : $<\sigma v>$
  thermal Eqs.(12-14) and $\sigma$ kinetic Eqs.(8-9)+Table IV

- **Verification** of $D(t,n)\alpha$ computation in code vs. Bosch and Hale tables

- **Convergence** wrt particle statistics $\Rightarrow 10^4$ 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

- $K_n/l_{mfp}/L=0.1$, $T_0=9\text{keV}$, $n_0=1\times10^{24}\text{cm}^{-3}$ (D & T), $10^4$ particles/cell per ion species, $L=3$ micron, 100 cells, 30 ps, $\nu_{\text{coll}}t\sim60$

- 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 $v_{z}$.

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 $T_z, T_\perp < T_{\text{source}} = 9$ keV and $n(z) < n_0 = 1 \times 10^{24}$ cm$^{-3}$ → Not a K-L effect!

- For $T=9$ keV, $\varepsilon_{\text{Gamow peak}}/T \sim 3.2$; $f(v_z, v_\perp)$ 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 $T_2 = 1/3 \left[ <v_z^2> - <v_z^2> + <v_x^2> + <v_y^2> \right]$ agree to within $\sim 10\%$.

\begin{itemize}
  \item $T_1 = \text{initial/source temperature}$
  \item $T_2 = \text{local temperature}$
  \item $T_2 < T_1$
  \item Fusion rate = fusions per 1 ps per cell
\end{itemize}
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

- 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 $T_1 \rightarrow \text{not a KL effect}$!
- The kinetic and Maxwellian fusion rates agree within $\sim \pm 10\%$ using the local density and local temperature $T_2 = 1/3 \text{ m} [\langle v_z^2 \rangle - \langle v_z \rangle^2 + \langle v_x^2 \rangle + \langle v_z^2 \rangle]$
1D PIC Simulation of Knudsen-Layer (KL) Effects on D-T Fusion – Comparison to Albright et al PoP 2013

- 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 $f_{\text{ion}}(v)$ at constant density and temperature.

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 $T_z < T_{\text{source}}$ 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 $\Rightarrow$ 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 ($\sim 10\%$), 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.

# Suite of 1D PIC Simulations of Knudsen Layer Effects

122701-7 Cohen *et al.*  

Phys. Plasmas 21, 122701 (2014)

## TABLE I. Suite of simulations for 30 ps.

<table>
<thead>
<tr>
<th>Case No.</th>
<th>Description and Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>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</td>
</tr>
</tbody>
</table>
| 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 x 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 end loss; so more fusion; KL modification of f(v_z) is much weaker |
| 7        | Variation from base case: Adds fusion alpha particles at 0.001 x 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 ~ 0.8v_{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, more fusion, higher axial drift velocity, strong KL effect on f(v_z) |
| 11       | Variation from base case: Increased source rate, x 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 = 1.5μm  
Results: 3 x 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.

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

\( ^a \)Cases 3 and 4 are not in steady state at 30 ps.