Modeling an Iodine Hall Thruster Plume in the Iodine Satellite (iSAT)

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**USING IODINE FOR HALL-EFFECT THRUSTERS (HETs)**

- Iodine has been identified as an attractive alternative propellant to Xe for HETs
  - High storage density (2-3 times of Xe)
  - Efficient ionization (lower ionization potential, higher ionization cross section than Xe)
  - Similar mass for I and larger mass for I₂ than Xe
  - Comparable performance to Xe with higher T/P ratio at higher power operating condition

- A dearth of detailed knowledge of physical processes occurring in the plume

- Critical risk: High reactivity
  - Concern for spacecraft system integration
OBJECTIVE

• Simulate the iodine plasma plume generated by BHT-200 Hall thruster and its interaction with the spacecraft body/solar array in the iSAT

Busek’s BHT-200 Thruster

Basic configuration of iSAT
OVERVIEW OF NUMERICAL MODEL

• 3-D Hybrid-particle code, DRACO, developed at AFRL
  – Particle-in-cell (PIC) combined with Monte Carlo Collision (MCC)
• Quasi-neutrality
• Boltzmann relation with a polytropic temperature model:

\[ \phi = \phi_r + \frac{k_B T_{e,r}}{e} \left( \frac{\gamma}{\gamma - 1} \right) \left[ \left( \frac{n_e}{n_{e,r}} \right)^{\gamma - 1} - 1 \right] \]
Collision Cross Section Models (1)

- Neutral-neutral: Momentum-exchange (MEX)
  - Variable Hard-Sphere model
- Ion-neutral: Momentum- and charge-exchange (CEX)
  - Semi-empirical models based on measurements
- For iodine, CEX collision is also important in a Hall thruster plume
  - Consider: I-I⁺, I₂-I⁺, and I₂-I₂⁺
    - I₂-I⁺, and I₂-I₂⁺ available from measurement\(^1\)
    - I-I⁺ calculated using Sakabe’s formula\(^2\)

• Verify Sakabe’s formula using Xe-Xe⁺ data by Miller
\[ \sigma_{\text{C EX}} = A - B \log(E) \]

<table>
<thead>
<tr>
<th></th>
<th>( A )</th>
<th>( B )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Xe-Xe⁺</td>
<td>87.3</td>
<td>13.6</td>
</tr>
<tr>
<td>Xe-Xe</td>
<td>45.7</td>
<td>8.9</td>
</tr>
<tr>
<td>I₂-I₂⁺</td>
<td>66.0</td>
<td>4.7</td>
</tr>
</tbody>
</table>

\[ \sigma_{\text{C EX}}(I^+,I_2) = c_1 \log^3(E) + c_2 \log^2(E) + c_3 \log(E) + c_4 \]

<table>
<thead>
<tr>
<th></th>
<th>( c_1 )</th>
<th>( c_2 )</th>
<th>( c_3 )</th>
<th>( c_4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>I₂-I₂⁺</td>
<td>-0.47</td>
<td>3.5</td>
<td>-9.0</td>
<td>82.0</td>
</tr>
</tbody>
</table>

\[ \sigma(v) = [A - B \log_{10}(v)] \left( \frac{\varepsilon_I}{\varepsilon_{I_0}} \right)^{-1.5} \]

\[ A = 1.81 \times 10^{-14} \]

\[ B = 2.12 \times 10^{-15} \]

\[ \varepsilon_{I_0} = 13.6 \text{ eV} \]
Create the geometry & surface meshing in Cubit

Create the volume mesh using Volcar
PARAMETERS USED FOR SIMULATION

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Xenon</th>
<th>Iodine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Discharge voltage (V)</td>
<td>250</td>
<td>250</td>
</tr>
<tr>
<td>Discharge current (A)</td>
<td>0.75</td>
<td>0.74</td>
</tr>
<tr>
<td>Anode mass flow rate (mg/s)</td>
<td>0.84</td>
<td>0.82</td>
</tr>
<tr>
<td>Cathode mass flow rate (mg/s)</td>
<td>0.098</td>
<td>0.096</td>
</tr>
<tr>
<td>Mass (propellant) utilization efficiency</td>
<td>0.981</td>
<td>0.853</td>
</tr>
<tr>
<td>Ion mass flow rate (kg/s)</td>
<td>8.24E-07</td>
<td>6.99E-07</td>
</tr>
<tr>
<td>Species temperature (K)</td>
<td>700</td>
<td>700</td>
</tr>
</tbody>
</table>


• Use HPHall source to provide particle information
• Compare with measurement by Nakles (2007)
  – Facility backpressure: $5 \times 10^{-6} \text{Torr} \approx 1.6 \times 10^{17} \text{ m}^{-3}$
COMPARISON WITH EXPERIMENTAL DATA

- Generally good agreement
SIMULATION OF IODINE PLUME (1)

• Additional reactions due to molecular species ($I_2$, and $I_2^+$)
  – Including dissociative ionization, electron attachment, and inelastic energy exchange

• Accurate modeling requires these processes to be implemented in the model
  – However, the goal is to provide a first-order approximation of the iodine particle flux on spacecraft surfaces using the numerical tools available to us at this stage

• Atomic iodine species ($I$, $I^+$, and $I^{2+}$) are simulated using the HPHall

• Molecular species are introduced at the discharge channel exit assuming Maxwellian velocity distributions.
**SIMULATION OFIODINE (2)**

- Use iodine mole fraction measurement and mass utilization efficiency 85.3% to calculate I$_2$ and I$_2^+$ mass flow rates
  - Assumed 10% of the total neutral flow is I$_2$

<table>
<thead>
<tr>
<th>Species</th>
<th>Mole Fraction, Xe</th>
<th>Mole Fraction, I</th>
</tr>
</thead>
<tbody>
<tr>
<td>I$_2^+$</td>
<td>0.021</td>
<td>0.004</td>
</tr>
<tr>
<td>Xe$^+$, I$^+$</td>
<td>0.975</td>
<td>0.953</td>
</tr>
<tr>
<td>Xe$^{2+}$, I$^{2+}$</td>
<td>0.021</td>
<td>0.015</td>
</tr>
<tr>
<td>Xe$^{3+}$, I$^{3+}$</td>
<td>0.004</td>
<td>0.003</td>
</tr>
</tbody>
</table>
XENON VS IODINE

- Similar result between Xe vs. I
Estimate of Iodine Flux on Surface

- Fluxes decrease away from the thruster in general
- Higher flux on outer edge of the front surface of s/c body and solar array
- Highest total iodine flux on the solar array: $4.5 \times 10^{16} \text{ m}^{-2} \text{s}^{-1}$
- Deposition per unit area: 0.34 mg/cm$^2$ over the entire thruster operation duration assuming 100% deposits

Neutral Number Flux ($\text{m}^{-2}\text{s}^{-1}$)  Ion Number Flux ($\text{m}^{-2}\text{s}^{-1}$)
• Verified the model using Xe data
• Simulated iodine plume with the mass flow rates based on experimental data
• Deposition per unit area: 0.34 mg/cm² over the entire thruster operation duration assuming 100% deposits
• In reality, only some portion of iodine colliding with the surface may chemically react with the surface
• How many particles actually react to or reflect off the surface will depend on the surface properties of the solar panel
• For more physically accurate simulation of iodine plasma plume, one needs to model the detailed reactions, especially the dissociative ionization
ACKNOWLEDGEMENT

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