ADAS beam population model – a sensitivity study

Martin O’Mullane
Ephrem Delabie¹, Sam Humphris², Edward Litherland-Smith³
and ADAS contributors

¹ ORNL, ² University of Durham, ³ UKAEA
Dominant atomic process

- Beam stopping is an effective ionisation rate.
- The primary $H^0 + H^+ \rightarrow H^+ + H^+ + e^-$ controls the overall value.
- New work since the Janev compilation of 1993.
- Suggest an increase of $\sim 10\%$ at peak of cross section.

I B Abdurakhmanov et al, J Phys B, 49 (2016) 03LT01
Difference in stopping coefficient

- Only alter the primary $H^0 + H^+ \rightarrow H^+ + H^+ + e^-$ cross section.
- $Te = Tion = 2keV$. Electron and ion density of $6 \times 10^{13}$ cm$^{-3}$.
Difference in stopping coefficient

- Only alter the primary $H^0 + H^+ \rightarrow H^+ + H^+ + e^-$ cross section.
- Simple pencil attenuation calculation – just to explore the atomic physics.
- ITER test case with beam energy of 100keV/amu, $T_e = T_{ion}$ and $N_e = N_{ion}$. 

![Graphs showing temperature and electron density variation along the beam distance.]

*With Abdurakhmanov ionization vs Current ADAS recommendation*
The ADAS beam model is a bundle-n collisional-radiative calculation:

- $n \sim 100$ included with assessed/recommended data for $n=1-5$ levels.
- Impact parameter formulasims for electron and ion excitation and ionisation (Lodge, Percival-Richard, Van Regemorter, Burgess, Vainstein) are used when other data are not available.

- Develop a new ADAS code (adas316) combining the role adas310 and adas312.
- adas316 is instrumented to modify any, or all, $n-n'$ rates or ionization from any $n$.  

Stopping coefficient for D-beam in $2 \times 10^3$ plasma.
Propagation of uncertainty

The ADAS beam model is a bundle-n collisional-radiative calculation:

- CR model driven by atomic cross sections; excitation, de-excitation and ionization
- Plasma ion and electron populations are the drivers.
- Beam stopping and emission are parameterized by beam energy and \( T_e, T_{ion}, N_e \) and \( N_{ion} \).
- Assume a normal distribution for each atomic process and see if we recover sufficiently normal bms and bme coefficients.

- Apply \( sd=0.2 \) for ion impact ionization
- \( sd=0.1 \) for e-impact ionization
- 250 samples for each

Result: bms/un-modified bms mean is 1.0055 with \( sd=0.0619 \)
Propagation of uncertainty – as an error bar

Sample uncertainties in H⁰-impact and e-impact ionization

- Apply $sd=0.2$ for ion impact ionization
- $sd=0.1$ for e-impact ionization

- How close the stopping coefficient matches the value recovered by fitting the spread from the sampled atomic cross sections depends on the number of samples.
- For bms vs. energy 250 was sufficient but $Te (=T_{ion})$ required 450 samples.
- The error bar is the standard deviation from the Gaussian (normal) fit.
- Error bar decreases for increasing energy but remains similar over $Te$. 
Propagation of uncertainty – multiple simultaneous processes

Sample uncertainties in ionization and H⁰-impact excitation

- Apply $sd=0.2$ for ion impact ionization
- $sd=0.1$ for e-impact ionization
- $sd=0.2$ for ion impact excitation for $n=2 \rightarrow 1$, $n=3,4,5 \rightarrow 1$ and $n=3,4,5 \rightarrow 2$
- 250 samples for each
- $bms$ mean, $sd$: 0.992, 0.142
- $n=3$ mean, $sd$: 1.002, 0.038

Slight skew on fits – possible indication of correlation?
Ranking the contribution of atomic processes

The ADAS beam model is a bundle-n collisional-radiative calculation:

- The influence of each atomic process can be ranked.
- Not each processes has the same influence on beam stopping and on beam emission (n=3 population).

<table>
<thead>
<tr>
<th>Normalised Ion Interaction Sensitivities (Beam Stopping Coefficient)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam stopping coefficient</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>n</th>
<th>n'</th>
<th>Ion impact processes</th>
<th>Electron impact processes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>2</td>
<td>0.0003</td>
<td>0.0001</td>
<td>0.0003</td>
</tr>
<tr>
<td>3</td>
<td>0.0009</td>
<td>0.0009</td>
<td>0.0009</td>
</tr>
<tr>
<td>4</td>
<td>0.0027</td>
<td>0.0014</td>
<td>0.0027</td>
</tr>
<tr>
<td>5</td>
<td>0.0141</td>
<td>0.0141</td>
<td>0.0141</td>
</tr>
<tr>
<td>6</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>
Ranking the contribution of atomic processes

The ADAS beam model is a bundle-n collisional-radiative calculation:

- The influence of each atomic process can be ranked.
- Not each processes has the same influence on beam stopping and on beam emission (n=3 population).

Beam emission (n=3 relative population) coefficient

Ion impact processes

Electron impact processes
Goals and next steps

• The workshop came a little early for our investigations.
• A goal for ADAS is to provide an error surface over the parameters of the bms (adf21) and bme (adf22) files.
• Assigning an error to each atomic process is fraught with subjective opinion.
• Correlation effects are ignored for now but any skew in the recovered distributions may be small enough to be neglected.

• How to use the uncertainty estimations is also uncertain – compare using an adf21 + error approach to a sampling population model at each point in the beam attenuation calculation.

• Run simple/toy ADAS beam attenuation model for workshop cases with central ADAS adf21 and with the new ionization data of Abdurakhmanov.
• ‘Benchmark’ the simple ADAS beam attenuation model against the more sophisticated CHEAP algorithm to assess whether it can be used to give a physics insight to beam attenuation behaviour.
• Prepare a list of atomic processes, ranked by importance for bms and bme, to focus future discussions on how to assign uncertainty estimates to the fundamental atomic cross sections.