Transformation of fundamental atomic data for use in interpreting diagnostics and plasma modelling

Martin O’Mullane
Hugh Summers, Nigel Badnell, Simon Preval, Stuart Henderson, Matthew Bluteau, Ephrem Delabie, Alessandra Giunta and many ADAS contributors
Outline

- Lithium - example of how fundamental data relates to the ‘atomic data’ used in magnetic confined fusion modelling.
- ADAS - atomic models and database to store both fundamental and effective atomic data.
- Tungsten.
- Perspectives from marshalling and data provision.
Fundamental vs. derived data - ionization of Li$^0$

**FIG. 2.** Total electron-impact ionization cross section for electron scattering from lithium. Solid squares: time-dependent close-coupling method, solid line: distorted-wave method, dashed line: convergent close-coupling method [2], solid diamonds with error bars: experiment [10]. (1.0 Mb $= 1.0 \times 10^{-18}$ cm$^2$.)


ADAS effective rate for Li$^0 + e$ ionization.

A derived coefficient dependent on the local electron temperature and density.
The collisional-radiative model is a good description of a finite density plasma.

**Figure 8.** Ionization rate of sputtered lithium atoms as a function of electron temperature under PF plasma bombardment in H-mode plasma. Figure shows how the ADAS collisional–radiative model must be used to explain experimental data from Li–DiMES in PF plasma.

Finite density environment
collisonal-radiative picture for ionisation and recombination

Reactions:

At higher densities, collisional excitation and de-excitation between excited levels compete with spontaneous emission.

\[ \mathcal{A}^{+z}(i) + e \rightleftharpoons \mathcal{A}^{+z}(j) + e \]

Indirect pathways lead to line emission and ionisation may occur in a stepwise manner.

Three-body recombination must be added to the reactions which pairs with collisional ionisation from excited states

\[ \mathcal{A}^{+z}(i) + e \rightleftharpoons \mathcal{A}^{+z+1}(g) + e + e \]

Not all recombinations lead to growth of the ground population of the recombined ion.
Finite density environment
generalized collisional-radiative approach - projection of high-n levels

• For light/medium weight elements there is a truncation problem since the true atom with its infinite number of Rydberg states.

• Dielectronic recombination populates high lying states.

• Setup a bundle-n collisional-radiative matrix for the whole system. Use the inverse sub-matrix propagator for the \( \text{ry} \) n-shells to project onto the \( \text{ry}_{ls} \) n-shells.

• Eliminate the direct couplings and expand statistically over the \( \text{ry}_{ls} \) nS-shell substructure and add to the more exact collisional-radiative matrix for \( \text{ry} \).
**Timescales for transport and atomic processes**

- **Emission** \( n_e X \approx 10^{20} \, \text{m}^{-3} \times 10^{-12} \, \text{m}^3/\text{s} \approx 10^8/\text{sec} \)
- **Ionisation** \( n_e S \approx 10^{20} \, \text{m}^{-3} \times 10^{-14} \, \text{m}^3/\text{s} \approx 10^6/\text{sec} \)
- **Diffusion** \( \frac{D}{(0.1 \, \text{a})^2} \approx 1 \, \text{m}^2/\text{sec} / 0.01 \, \text{m}^2 \approx 100/\text{sec} \)
- **Convection** \( v/(0.1 \, \text{a}) \approx 1 \, \text{m/ sec} / 0.1 \, \text{m} \approx 10/\text{sec} \)
- **Recombination** \( n_e \alpha \approx 10^{20} \, \text{cm}^{-3} \times 10^{-20} \, \text{m}^3/\text{s} \approx 1/\text{sec} \)

- **Emission is a local process**
- **Timescale for transport is slower than ionisation but faster than recombination, therefore density profile of individual ionisation stage is determined non-locally**
Spatial Distribution of Ions

Equilibrium (coronal) ionisation balance is not a safe assumption for tokamak plasmas.

Charge exchange with neutral hydrogen can also be a significant contributor to overall recombination.
Finite density and metastables

- A finite electron density plasma results in ‘effective’ source coefficients.
Finite density and metastables

- A finite electron density plasma results in ‘effective’ source coefficients.

Metastables are followed in time

\[ \frac{d}{dt} N^z_\rho \neq 0 \quad 1 \leq \rho \leq m \]

Ordinary levels are in quasi-static equilibrium with their metastable

\[ \frac{d}{dt} N^z_i = 0 \quad i > m. \]
\[
\frac{dN_{\rho}^{+z}}{dt} = -(N_e S_{CD,\sigma \rightarrow \nu} N_{\sigma}^{+z} + N_e \alpha_{CD,\nu \rightarrow \rho} N_{\nu\nu}^{+z+1} + N_e Q_{CD,\sigma \rightarrow \rho} N_{\sigma}^{+z}) + \ldots
\]

- Be\(^{+4}\) Nucleus 398 eV
- Be\(^{+3}\) 1s\(^2\) \(^1\)S 182 eV
- Be\(^{+2}\) 1s 2s \(^3\)S 146 eV
- Be\(^{+1}\) 1s\(^2\) 2s \(^2\)S 27.5 eV
- Be\(^0\) 1s\(^2\) 2s 2p \(^3\)P 9.32 eV
- Be\(^0\) 1s\(^2\) 2s\(^2\) \(^1\)S 2.73 eV
- Be\(^0\) 1s\(^2\) 2s\(^2\) \(^1\)S 0.00 eV
What we need to model emission from fusion plasmas

If we wish to interpret/predict the emission from plasmas:

• Require atomic and molecular data
• Not necessarily of highest quality - completeness is as important
• Fundamental data mediated via models to be useful for modelling and diagnostic use.
• The derived/effective data must be a parameterization of atomic features with macroscopic plasma quantities (Te, Ti, Ne, B, I etc.).
• Large amounts of data involved.

Necessary tasks:

• Gather/calculate fundamental data.
• Develop appropriate (collisional-radiative) models.
• Store data in a well defined way.
• Assess the quality of the data.
Most data within ADAS is \textit{ab initio}

Rely on the atomic codes being benchmarked against experiment when possible.

**FIG. 2.** Total electron-impact excitation cross sections for the $2s \rightarrow 2p$ and $2s \rightarrow 3s$ transitions in Li. Solid curves, present 14-state $R$-matrix calculation; dashed curves, present 55-state RMPS calculation; open circles, present TDCC calculation; dot-dashed curves, from fits to the CCC calculations given by Schweinzer \textit{et al.} [10]; crosses, CCO calculation of Bray \textit{et al.} [9]; upward triangles, experimental measurements of Williams \textit{et al.} [11]; downward triangles, experimental results of Vušković \textit{et al.} [12].

**FIG. 3.** Total electron-impact excitation cross sections for the $2s \rightarrow 3p$ and $2s \rightarrow 3d$ transitions in Li. Solid curves, present 14-state $R$-matrix calculation; dashed curves, present 55-state RMPS calculation; open circles, present TDCC calculation; dot-dashed curves, from fits to the CCC calculations given by Schweinzer \textit{et al.} [10]; crosses, CCO calculation of Bray \textit{et al.} [9].

\textbf{Li}\textsuperscript{0} excitation cross sections
Scrutiny of individual transitions becomes difficult when the complexity of the ion structure increases.
All ADAS data is stored in a well defined, tightly specified, format - eg. *adf04* format.

<table>
<thead>
<tr>
<th>Element</th>
<th>Ion Charge</th>
<th>Nuclear Charge</th>
<th>Description Field</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>+1</td>
<td>2</td>
<td>196664.7(18)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>249084.0(33)</td>
</tr>
<tr>
<td>1</td>
<td>2S2 2P1</td>
<td>(2)1( 2.5)</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>2S1 2P2</td>
<td>(4)1( 5.5)</td>
<td>42993.5(2)</td>
</tr>
<tr>
<td>3</td>
<td>2S1 2P2</td>
<td>(2)2( 4.5)</td>
<td>74888.8</td>
</tr>
<tr>
<td>65</td>
<td>2P2 3S1</td>
<td>(2)0( 0.5)</td>
<td>306228.0</td>
</tr>
<tr>
<td>66</td>
<td>2P2 3P1</td>
<td>(2)1( 2.5)</td>
<td>317787.7</td>
</tr>
<tr>
<td>67</td>
<td>2P2 3D1</td>
<td>(2)2( 4.5)</td>
<td>329762.3</td>
</tr>
<tr>
<td>-1</td>
<td></td>
<td></td>
<td>24.94 3.14 2.13</td>
</tr>
<tr>
<td>2.0</td>
<td></td>
<td></td>
<td>0.74 0.59 0.48</td>
</tr>
<tr>
<td>7</td>
<td></td>
<td></td>
<td>0.36 0.30 0.26</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
<td>2.00+03 4.00+03</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>8.00+03 2.00+04</td>
</tr>
<tr>
<td>9</td>
<td></td>
<td></td>
<td>4.00+04 8.00+04</td>
</tr>
<tr>
<td>12</td>
<td></td>
<td></td>
<td>2.00+05 4.00+05</td>
</tr>
<tr>
<td>67</td>
<td>6.24+06</td>
<td></td>
<td>1.20-01 1.20-01</td>
</tr>
<tr>
<td>66</td>
<td>3.21+07</td>
<td></td>
<td>1.20-01 1.20-01</td>
</tr>
<tr>
<td>R</td>
<td>+2</td>
<td></td>
<td>1.53-13 1.10-13</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>8.46-14 6.58-14</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>5.08-14 3.71-14</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2.48-14 1.89-14</td>
</tr>
<tr>
<td>R</td>
<td>+2</td>
<td></td>
<td>1.00-30 1.00-30</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.00-30 1.00-30</td>
</tr>
<tr>
<td>H</td>
<td>+1</td>
<td></td>
<td>6.34-13 8.04-13</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>9.10-13 9.87-13</td>
</tr>
<tr>
<td>H</td>
<td>+1</td>
<td></td>
<td>1.03-12 8.27-13</td>
</tr>
<tr>
<td>S</td>
<td>+1</td>
<td></td>
<td>2.35-18 3.05-18</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.60-17 3.31-14</td>
</tr>
<tr>
<td>-1</td>
<td></td>
<td></td>
<td>2.59-09 9.07-09</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>8.96-09 1.11-08</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.50-08 1.88-08</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2.30-08 2.55-08</td>
</tr>
</tbody>
</table>

A free-format comment section at the end details the source and responsible person.
Modelling lithium results in 64 datasets

Driver for adas8#1 adf04
adf34/lithium/li0.dat
adf34/lithium/li1.dat
adf34/lithium/li2.dat

Baseline adf04 to give baseline fill-in and A-values
adf04/copmm#3/ls#li0.dat
adf04/copmm#3/ls#li1.dat
adf04/copmm#3/ls#li2.dat

R-matrix data from Connor Ballance and Don Griffin
adf04/lilike/lilike_cpb02#li0.dat
adf04/helike/helike_cpb02#li1.dat
adf04/hlike/hlike_cpb02#li2.dat

Metastable and excited state resolved ionisation data from S Loch
adf07/szd02#li/szd02#li0.dat
adf07/szd02#li/szd02#li1.dat
adf07/szd02#li/szd02#li2.dat

State resolved radiative recombination from Nigel Badnell
adf48/nrb05#he/nrb05#he_li1ls.dat
adf48/nrb05#h/nrb05#h_li2ls.dat
adf48/nrb05###nrb05##_li3ls.dat

State resolved dielectronic recombination from Nigel Badnell and M Bautista
adf09/nrb00#he/nrb00#he_li2ls12.dat
adf09/nrbmb00#he/mb00#he_li1ls12.dat
adf09/nrbmb00#he/mb00#he_li1ls23.dat

Fully specified adf04 file for processing
adf04/adas3#3/cpb02_ls#li0.dat
adf04/adas3#3/cpb02_ls#li1.dat
adf04/adas3#3/cpb02_n#li2.dat

Mapping high-n to low levels
adf18/a17_p208/exp96#li/exp96#li_li0ls.dat
adf18/a17_p208/exp96#he/exp96#he_li1ls.dat
adf18/a17_p208/exp96#h/exp96#h_li2n.dat

iso-electronic GCR data
adf10/acd96/pj#acd96_li11.dat
adf10/acd96/pj#acd96_li21.dat
adf10/scd96/pj#scd96_li11.dat
adf10/scd96/pj#scd96_li21.dat
adf10/xcd96/pj#xcd96_li12.dat
adf10/xcd96/pj#xcd96_li21.dat
adf10/plt96/pj#plt96_li##.dat
adf10/prb96/pj#prb96_li10.dat
adf10/prb96/pj#prb96_li20.dat

Iso-nuclear source and power - unresolved
adf11/acd96/acd96_li.dat
adf11/scd96/scd96_li.dat
adf11/ecd96/ecd96_li.dat
adf11/ycd96/ycd96_li.dat
adf11/zcd96/zcd96_li.dat
adf11/plt96/plt96_li.dat
adf11/prb96/prb96_li.dat

iso-nuclear source and power - unresolved
adf13/sxb96#li/sxb96#li_pjr#li0.dat
adf13/sxb96#li/sxb96#li_pju#li0.dat
adf13/sxb96#li/sxb96#li_pjr#li1.dat
adf13/sxb96#li/sxb96#li_pju#li1.dat
adf13/sxb96#li/sxb96#li_pjr#li2.dat
adf13/sxb96#li/sxb96#li_pju#li2.dat

Photon emissivity coefficients
adf15/pec96#li/pec96#li_pjr#li0.dat
adf15/pec96#li/pec96#li_pju#li0.dat
adf15/pec96#li/pec96#li_pjr#li1.dat
adf15/pec96#li/pec96#li_pju#li1.dat
adf15/pec96#li/pec96#li_pjr#li2.dat
adf15/pec96#li/pec96#li_pju#li2.dat

In OPEN-ADAS
Lithium - only 3 electrons

• 64 adf datasets
• 43 in OPEN-ADAS: fundamental data (excitation, DR, RR and ionisation)
  derived data (source, power, S/XB and PEC coefficients)
What is ADAS?

• ADAS, as a database delivers:
  ○ extensive fundamental and derived data tuned for plasma modelling and spectroscopic analysis,
  ○ provides ‘baseline’ level data for any element and ion stage.
  ○ atomic data source for many modelling codes and systems,
  ○ makes a significant quantity of data publically available via OPEN-ADAS http://open.adas.ac.uk (with IAEA).

• ADAS, as a computer system, is designed to:
  ○ provide a set of interactive codes which are easy to use,
  ○ provide subroutine libraries for inclusion in other codes,
  ○ allow direct access to diagnostically relevant data.

• ADAS, as a collaborative organisation:
  ○ provides guidance (training courses, visits etc.) on running codes,
  ○ gives recommendation on the best data to use,
  ○ assists in analysis and development of analysis tools and models.

It is structured as a self-funded consortium between most major fusion laboratories and universities. Its historical roots are in JET and is now managed by Strathclyde University but governed by a steering committee of the participating members.
ADAS data and computational overview

There are 55 different ADAS data formats

Some key ADFs and MDFs for general application

ADF01: charge exchange cross sections
ADF04: specific ion data
ADF11: coll.-rad. ionis., recom. and related coefficients.
ADF13: ionisation per photon ratios
ADF15: emissivity coefficients
ADF40: envelope feature photon emiss. coefficients
ADF21: beam stopping coefficients
ADF39: photoionization cross sections

MDF00: fundamental diatomic molecular constants
MDF01: rovibronic models
MDF02: fundamental cross-section data
MDF04: specific molecule data

Interactive user interface
ADAS series (9 series with 85 programs)

The application interface
ADAS Fortran subroutine (~1900), IDL procedure (~1700) and python (~30) routine libraries
Data extraction procedures and subroutines by format: xxdata_<nn>, read_adf<nn>, xxdatm_<nn>, read_mdf<nn>.

Offline-ADAS for large scale production
6 large scale production packages: adas7#1, adas7#3, adas8#1, adas8#2, adas8#3, adas8#4.

Documentation - examples, manual and course material.
OPEN-ADAS: http://open.adas.ac.uk

**About OPEN-ADAS**
OPEN-ADAS is a system to search and disseminate atomic data from the Atomic Data and Analysis Structure (ADAS).

ADAS is a computer program managed by the University of Strathclyde and made up of a consortium of 27 community members.

The OPEN-ADAS system enables new members, with an interest in fields and astrophysics, to download and use ADAS data.

More about OPEN-ADAS

**The OPEN-ADAS data classes**
The data contained within ADAS is strictly organized and preciously formatted. There are over fifty distinct types of data file. The scope of OPEN-ADAS is targeted and limited to the release and organization of general user relevant data from the ADAS databases and the provision of code, instructions and procedures to enable such use. OPEN-ADAS is used to release the released data. These data classes are given below.

- **Fundamental data**
- **Derived data for modelling and diagnostics**

---

**FUNDAMENTAL CLASSES**

- **01** Charge exchange cross sections of re-arranged charge exchange cross sections over a range of systems for a donor metal atom and an acceptor impurity receiver.
- **04** Resolved line specific ions data collection.
- **07** Electron ionisation coefficients.
- **08** Resolved dielectronic recombination coefficients.
- **38** Photonisation autoionisation rate coefficients.
- **39** Photionisation excitation cross sections.
- **48** Resolved line specific ions recombination coefficients.

**DERIVED CLASSES**

- **11** iso-molecular materials.
- **12** Effective (collinear-reductive) coefficients which are required to establish the ionisation state of a dynamic or steady-state plasma.
- **13** Charge exchange effective excitation coefficients.
- **15** Photon autoionisation coefficients.
- **21** Effective beam stopping recombination coefficients.
- **22** Effective beam ionization recombination coefficients.

---

1st Meeting of Experimentalists Network, IAEA, Vienna, 19-21 Nov. 2018
Who thought that tungsten was a good idea?

- Interpret emission from fuel (H, D, T and He) and impurities (Be, Ne, Ni, W).

Although emission from impurities gives information, their presence is not always benign.
W$^{18+}$ dielectronic recombination

Dielectronic recombination rates for tungsten were the most poorly calculated input to the ionization balance.

T Pütterich scaled the ADPAK average ion rates to match AUG measurements. Limited to $2 \text{keV} < T_e < 10 \text{keV}$ ($W^{20+} - W^{55+}$ or Xe-like to K-like) PPCF, v50, 085016 2008

DR rates for ions with open $4f^n$ shell ions are x3 higher than expected, Schippers et al, Phys Rev A 83, 012711, 2011 & Badnell et al, Phys Rev A 85, 052716 2012

ADAS DR Project started in 2016 and is ongoing

$4f^n$ still an issue

- But now constrained from both sides
- It’s the pedestal region for JET (100-1000eV)

Preval et al,
- 73 - 56: PRA 93, 042703 (2016)
- 55 - 38: JPB 50, 105201 (2017)
- 27 - 14: calculations underway
Optimizing the radiated power

- A rule-based algorithm to choose the configurations needed based on the metric of optimizing the total radiated power.
- Data from Cowan with AUTOSTRUCTURE supplementation for spin-changing and higher multipole transition probabilities.

S Henderson et al, PPCF. 59, 055010 (2017)
Optimizing atomic structure

- Wish to move to AUTOSTRUCTURE distorted-wave as a new baseline quality.
- Same driver files for R-matrix.
- Good atomic structure is essential for high quality derived data.
- And is the basis for uncertainty estimation.
- Default results could be better.
- Optimization converges quickly.
- But it needs a ‘good’ target.
Optimizing structure across iso-electronic and iso-nuclear sequences

- AUTOSTRUCTURE uses a Thomas-Fermi potential and individual orbitals can be scaled to improve results along iso-electronic and iso-nuclear sequences.
- Unfortunately data from NIST becomes sparse very quickly.
Optimizing the radiated power

- One outcome is a set of adf04 excitation data in collision strength and effective collision strength forms.
- These can be applied to spectral problems

Mono-energetic ADAS population model, producing a spectral feature, fitted to an EBIT spectrum with ADAS feature-fitting LSQ code.

Goal is to apply (shifted) features to tungsten emission from tokamaks.
Intermediate coupling GCR - prototyped with Argon

- Required ion impact to mix closely-spaced energy levels (stored in adf06 files)
- Increases the number of metastables.
- Raises questions on how to handle/classify these metastables.

Generating derived data targeted at the plasma environment under study is necessary.
Conclusions

• Advancing the quality of atomic data required for fusion is important.
• The quantity and use of data for modelling and diagnostics is such that the *ab initio* codes used to produce these data must be validated by measured data wherever possible.
• The code validation does not necessarily need to be fusion relevant.

• The way atomic data will be used is changing, being embedded into complex analysis chains, some with machine protection implications (and responsibilities).
• Provenance of atomic data is important.
• Provenance goes hand in hand with validation.

• At ITER a measurement requirement (a diagnostic) is characterised and ranked by:
  • needed for machine protection.
  • needed for basic machine control.
  • required for advanced plasma control.
  • required for evaluation and physics studies.

• But all discharges at ITER must be modelled and verified before execution so accurate atomic data is still essential.
Spend more time on atomic data and models!

ADAS
Atomic Data and Analysis Structure

News
About ADAS
Members
Documentation
  • Manual
  • Bulletins
  • Subroutines
  • Publications
  • Notes
  • Theses
ADAS-EU
OPEN-ADAS
Support / Bugs
ADAS Courses
Workshops
  • 2006
  • 2007
  • 2008
  • 2009
  • 2010
  • 2011

ADAS Workshop 2018

The 2018 ADAS Workshop will be held 9–11 December at Physikzentrum Bad Honnef in Germany.

The Institute of Energy and Climate Research (IEK-4) of Forschungszentrum Jülich FZJ are kindly hosting the 2018 meeting. It has been five years since we last held the ADAS workshop in Germany and we are delighted that the venue will be the Physikzentrum in Bad Honnef.

http://adas.ac.uk/