Computational Atomic and Molecular Physics for Transport Modeling of Fusion Plasmas

M S Pindzola[1], F J Robicheaux[1], J P Colgan[1], S D Loch[1], J Ludlow[1], D R Schultz[2], T Minami[2], J T Hogan[2], D C Griffin[3], C P Ballance[3], T Evans[4], N R Badnell[5], H P Summers[5], A D Whiteford[5], B M McLaughlin[6], P G Burke[6] and K A Berrington[7]

[1]Dept of Physics, Auburn University, Auburn, AL [2]Physics Division, Oak Ridge National Laboratory, TN
[3]Dept of Physics, Rollins College, FL [4]DIII-D, General Atomics, CA [5]Dept of Physics, Univ. of Strathclyde
[6]School of Mathematics & Physics, Queen's University of Belfast [7]Dept of Mathematics, Sheffield Hallam University

ITER relevant modelling efforts

Numerous issues are now pertinent in the run up to ITER operation. A DoE Scientific Discovery through Advanced Computing (SciDAC) program has brought together a US-UK collaboration to implement state-of-the-art atomic collision codes on the next generation of terascale computing facilities, to assist in answering questions such as

- The final choice for plasma-facing materials, in particular the possible use of
  - Be, C, and W components for the first wall
- Relevance of innovations on operational regimes
- Study of ELM transient in standard ITER operation

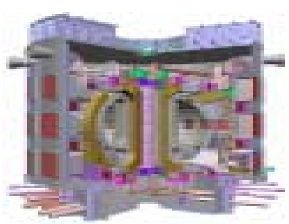

Figure 1. Schematic of ITER

Plasma transport codes (such as SOLPS, SANCO) provide an insight into the transport of plasma impurities, the radiated power loss from various plasma impurity mixtures, and the behaviour of ELM and transport barriers. These codes require good atomic data for

- effective ionization and recombinations rate coefficients to track the ionization balance, and hence the plasma transport of impurity species
- emissivity coefficients to predict radiated power losses, and to compare with spectral observations.

Collisional-Radiative Modeling using ADAS

A modeling suite of codes called ADAS (Atomic Data and Analysis Structure) processes fundamental atomic data into a form useful for such transport codes, which are then used at facilities such as JET, ASDEX-Upgrade, DIII-D, JT-60, Tore-Supra and Alcator C-Mod.

- Solution to collisional-radiative equations to get the emitting populations requires:
  - Atomic structure for energies, radiative rate coefficients
  - Collisional electron excitation, ionization and recombination rate coefficients
  - Collisional charge transfer recombination with neutral beam species

Various coefficients are produced from the ADAS codes, which can be transparently used in transport codes, namely:

- Generalised collisional-radiative coefficients
- Radiated power loss coefficients
- Photon emissivity coefficients

We have completed calculations for the following systems

- He, Li and Be

However, the accuracy of the coefficients which are passed to the transport codes is directly related to the atomic data which is used to generate them. Thus, much work has been done on generating highly accurate atomic data for key fusions species. These calculations are pushing the limits of current large scale computational resources, and are opening up new frontiers in atomic collision theory. We present some of these calculations in the following sections.

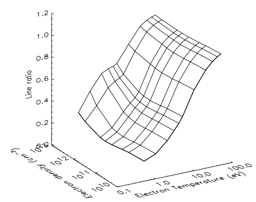

Figure 1. He (1s4s $^1S \rightarrow$ 1s2p ^1P) / (1s4s $^3S \rightarrow$ 1s2p ^3P) line ratio as evaluated by ADAS, for use as a plasma electron temperature diagnostic, under joint investigation with Troy State University. The theoretical line ratio uses new RMPS calculations, and represents a significant increase in data quality over existing data.

AM Calculations: Time dependent Semi-Classical

- Electron modeled as moving in the field of two moving Coulomb fields
- Especially useful for charge transfer cross sections, of relevance for fusion studies
- Applications such as p+H, p+Li, α + H, Be^{4+}+H, p+H_2^+

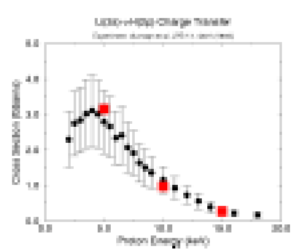

Figure 8. State-selective charge transfer cross section of protons on ground state lithium

AM Calculations: Time independent R-Matrix

- Developed in the UK by P.G. Burke and co-workers, the method can be used to generate electron collisional excitation, ionization and recombination cross sections.
- All eigenvalues and eigenvectors of 50,000 x 50,000 matrices are required. Thousands of energies are needed to map out the Feshbach resonances sections. This can only be achieved on modern massively parallel computers.

R-Matrix with pseudo-states calculations are completed for

- He, He^+, Li, Li^+, Li^{2+}
- Be, Be^+, Be^{2+}, Be^{3+}
- B^+, B^{4+}, C^{2+}, C^{3+}, C^{5+}, O^{5+}

Standard *R*-Matrix calculations are completed for

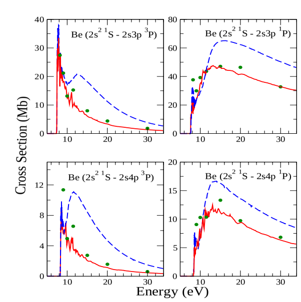

Figure 4. Electron excitation collision strengths for Be, from the recent RMPS calculations. The effects of including pseudo states can be clearly seen.

AM Calculations: Time dependent Close-Coupling

- Treats the three body Coulomb breakup exactly
- Close coupled set of 2D lattice equations
- Calculations are completed for
  - H, He, He^+, Li, Li+, Li^{2+}
  - Be, Be+, Be^{2+}, Be^{3+}
  - B^{2+}, C3+, Mg^+, Al^{2+}, Si^{3+}

Have now started to treat

- four body Coulomb breakup problem
- the three-body two Coulomb center breakup problem

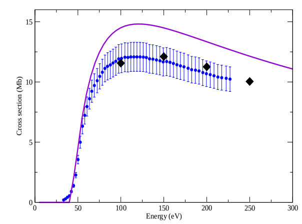

Figure 6. C^{2+} ionization cross section. The experimental results are shown in the blue circles, and have 60% 2s2p ^3P metastable in the beam. The solid line shows the distorted-wave calculation, and the diamonds show the TDCC calculation. This result is the first agreement between theory and experiment for a case with significant metastable fraction in the beam.

AM Calculations: Distorted-wave and Classical Trajectory

The distorted-wave techniques use perturbation theory

- They are accurate for radiative and autoionization rates, and for electron collisions with highly charged ions.
- There are various levels of calculation
  - Intermediate coupled distorted-wave (ICDW)
  - LS coupled distorted-wave (LSDW)
  - Configuration-average distorted-wave (CADW)
  - Classical Trajectory Monte Carlo (CTMC)

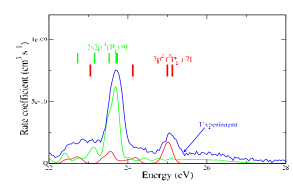

Figure 9. The first observation of trielectronic recombination, as seen in Cl^{13+}

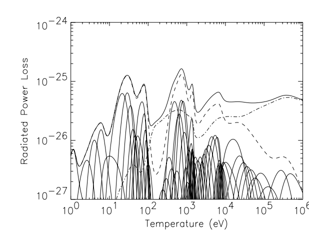

Figure 10. Equilibrium radiated power loss from all ionization stages of tungsten

Applications of our data

Data we have generated is in use at various institutes

- ASDEX-Upgrade : Tungsten ionization data is to be used in heavy species studies
- EFDA-JET : Helium excitation data we generated is in use in He beam studies
- RFX : Krytpon ionization data we made is in use in impurity transport studies
- DIII-D : Lithium effective ionization and recombination data is being used for impurity transport studies

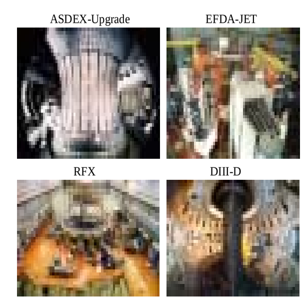

Figure 10. Images of various tokamaks where our data is being used

General science spin-offs

The advancements made as part of the work presented here, has also allowed progress to be made in other scientific areas, providing a valuable benchmarking of the codes. Some of these spin-offs include

- Photoionization of atoms and molecules
- RMPS for (γ, e) atoms and molecules
- TDCC for $(\gamma, 2e)$ on He, Be, Li^+, quantum dots, H_2, $(2\gamma, 2e)$ on He, $(\gamma, 3e)$ on Li
- TDCC for e^+ + H, TDSC for $\bar{p}$+H and BEC in fields, CTMC for e + atoms in ultracold plasmas, γ + atomis in high Rybberg states

Conclusions

- High quality atomic data is being processed into a form useful for plasma transport modeling, wall erosion and ELM experimental studies
- Recent advances in non-perturbative methods allows high quality atomic data to be generated for electron-ion and ion-atom collisions for low Z systems
- DW calculations provide high quality DR data for medium Z systems, and high quality electron ionization and excitation data for species such as tungsten

Fig. 1.—

Fig. 2.—

Fig. 3.—

Fig. 4.—

Fig. 5.—

Fig. 6.—

Fig. 7.—

Fig. 8.—

Fig. 9.—