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Summary Report of a Consultancy Meeting in preparation of a Coordinated Research Project on Atomic Data for Injected Impurities in Fusion Plasmas

7 – 8 June 2022
IAEA Headquarters, Vienna Austria and virtual

C. Hill

June 2022

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Introduction

Impurity ions are deliberately seeded into fusion plasmas for a variety of purposes. From the earliest days of magnetic-confinement fusion energy research, the spectra of light impurity ions, such as those of helium, lithium and carbon were used as a diagnostic tool to determine plasma properties. With the advent of very large scale experimental devices such as ITER, impurity injection is increasingly being used to redistribute the power transported from the plasma core to the reactor wall in order to reduce the heat load on, and hence damage to, the plasma-facing reactor wall components. Furthermore, impurities such as nitrogen, neon and argon and have been used in such devices to improve plasma control by diminishing the amplitude of edge-localized modes (ELMs), plasma disruptions and other transient events that inhibit confinement and have the potential to cause serious damage to wall components.

In order to interpret and predict the behaviour and properties of impurities in fusion plasma, a significant amount of modelling, involving data on the collisional-radiative characteristics of the impurities and their environment is required. For a few species, high-quality data is available, but in many cases the currently-available data is incomplete, missing, or of uncertain quality.

The Consultancy Meeting reported here met, in hybrid form, at IAEA Headquarters in Vienna, Austria and online using the Webex videoconferencing software to discuss the scope, participation and expected outcome and impact of Coordinate Research Project (CRP) F43026: *Atomic Data for Injected Impurities in Fusion Plasmas*. This project will run for approximately five years from late 2022. 14 participants from five Member States were involved in the meeting, with research presentations from eight of them.

Discussion Summary

The meeting considered the data needs of plasma models that incorporate interactions with deliberately injected impurities, the application of such models, and the specific species, processes and energy ranges for which the currently available data are deficient.

The discussion outcomes can be summarised as the answers to a handful of main questions:

1. What categories of data are needed for modelling the atomic and molecular physics of injected impurities?

Cross sections (possibly differential cross sections), and in particular for state-resolved processes

Rate coefficients (also state-resolved, where possible)

Spectral data: Line strengths / Einstein *A* coefficients; wavelengths. It was noted that no particular data are currently required by modelling codes regarding the Zeeman and Stark effects and that these are adequately parameterised from well-known physics considerations.

It was also noted that the uncertainties associated with existing data are often not well characterised and that particular effort should be expended, where possible, to promote the appropriate assessment of uncertainties in data produced or evaluated during the CRP.

2. Are impurities for both power mitigation and for plasma diagnostics in scope?

Yes, for a limited number of injected species of broad interest; argon should certainly be considered for its proposed use in disruption mitigation.

3. Which species should (and should not) be considered within the scope of the CRP?

a. Tungsten in plasma is not in scope; in particular, W as a catalyst for NHx formation should be considered as part of the forthcoming CRP F43027: *Molecules in Edge Plasmas;*

b. The following species should be considered, in order of priority:

Ar, N, Ne, (Kr), (Xe)

(the first three in all ionisation states, the last two in those ionisation states present for T_i > 500 eV);

c. Lithium, particularly in its interactions with $H_2(v)$ and its isotopologues, and isotopes of H and H^+ may be considered, but with lower priority than the above species and may be better served by CRP F43024: *Atomic Data for Vapour Shielding in Fusion Devices*. Similarly for tin;

d. Boron and related species (BN, BC) may also be considered, with lower priority, depending on the need for modelling the effects of its ions in edge plasmas.

4. Which processes involving these species are of greatest importance?

In order of priority:

a. Charge exchange (HCX) with H^0 across the energy ranges for which the relevant ions exist;

b. Electron impact excitation (EEX), above threshold;

c. Dielectronic recombination (ERD), for Ar and Ne, and state-resolved;

d. Spectra: line strengths and wavelengths;

e. (With lower priority) collisions with He^{2+} (alpha particles), for energies > 100 keV.

5. What is the current status of collisional and spectroscopic data for species of interest to the CRP?

Rather patchy, particularly with respect to charge exchange and dielectronic recombination. There should be a literature search and critical assessment of existing data sets with a view to establishing where reliable data are required, either because no data exist or because the existing data are based on approximate scaling relations rather than explicit calculated or measured cross sections.

The thesis of Matthew Bluteau may form a starting point for argon: *Fundamental atomic data and prototype techniques for a generalised collisional-radiative model of medium-weight elements in fusion and astrophysical plasma* (https://stax.strath.ac.uk/concern/theses/t435gd05c?locale=en)

6. Which experiments would benefit from better modelling of injected impurities and which species are used in these experiments?

Tokamaks and Stellerators
ITER, France (**Ne**, **Ar**, **Xe**, **N**)
ASDEX-U, IPP Garching, Germany (**Ar, Ne**, **N**)
LHD, NIFS, Toki, Japan (**B**, **Ar**, **Ne**, **N**, (C))
EAST, Hefei Institutes of Physical Science, Hefei, China (**Ar**, **Ne**)
JET, UKAEA, Culham, UK (**N**, **Ne**)
DIII-D, General Atomics, San Diego, CA, United States of America (**Ne**, **N**)
KSTAR, Korea Institute of Fusion Energy, Daejeon, South Korea (**N**, **Kr**, …)
JT-60SA, JAEA, Japan

MAST-U, UKAEA, Culham, UK(**N**)
COMPASS-U, IPP.CR, Prague, Czechia (**W**, **Ne**, **Ar**)

Linear plasma devices
Magnum-PSI, DIFFER, Netherlands
GyM (Medium Flux Linear Plasma Device), Milan, Italy
Pilot-PSI, DIFFER, Netherlands

7. How are data incorporated into models like SOLPS-ITER and how can integration of new data be facilitated?

Basically, in ADAS format; ITER uses the AMNS (Atomic, Molecular, Nuclear, and Surface) library to interface with its Integrated Modelling and Analysis Suite (IMAS) software. The CRP should consider the development of an Application Programming Interface (API) that AMNS can use to access ALADDIN(2) and CollisionDB data sets in the same way that it accesses ADAS and the databases of data originally compiled by Janev that are curated by Forschungszentrum Jülich (FZJ), Germany.

The development of an entire data pipeline, from the aggregation of state-resolved data through to CR modelling is, however, outside the scope of this CRP.

Roadmap and Outputs

The CRP will hold three Research Coordination Meetings (RCMs) over the course of about five years, probably in Q4 2022, Q2/3 2024 and Q4 2026.

The principal output will be evaluated and recommended data on **Ar**, **Ne** and **N** for charge-exchange and electron impact excitation processes, to be stored in the ALADDIN(2) database and searchable online and through a suitable API. Additionally, state-selective dielectronic recombination cross sections and spectral data on these species will be collected and assessed where possible.

As with previous CRPs, Code Comparison Workshops may be initiated to compare and benchmark computational methodologies for calculating collisional cross section data; the precise nature of these exercises is dependent on the CRP participants' research interests and expertise, but a comparison of dielectronic recombination cross sections by different theoretical methods would be of particular interest.

Conclusions

After reviewing the current state of atomic and molecular data for modelling injected impurities in magnetic confinement fusion devices, this Consultancy Meeting narrowed to focus of CRP F43026, with the main species of interest being Ne, N and Ar: species in common use or proposed use by a wide variety of fusion experiments. Xe and Kr, important for ITER (and, later, DEMO) diagnostics may also be considered at appropriate energies; Li, Sn (perhaps) and B may also form part of the CRP depending on the participants.

It is clear that it would be valuable to fully audit and aggregate the currently-available data on these species, at least in so far as it relates to HCX and EEX. However, this is likely to be a labour-intensive exercise requiring expert knowledge and it is not clear how or who would be able to undertake this project.

In addition to the usual IAEA channels for promoting new CRPs, potential participants will be contacted between June and August 2022 with a view to soliciting their proposals for a Research Agreement or Research Contract (for developing Member States) to start by Q4 2022 before the first RCM.

All data created or evaluated within the CRP will be deposited in the IAEA's CollisionDB and ALADDIN databases, as appropriate.

Participants

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Agenda

Tuesday, 7 June 2022

15:00 – 15:15	**Christian HILL**, *IAEA, Austria* Meeting opening; background and purposes

Session 1: Participant Presentations

Chair: Christian HILL

15:15 – 15:30	**NAKANO Tomohide**, *National Institutes for Quantum and Radiological Science and Technology (QST), Japan* A+M data needs for injected impurities in fusion research
15:30 – 15:45	**ASHIKAWA Naoko**, *National Institute for Fusion Science, Japan* Injected impurity data needs at NIFS
15:45 – 16:00	**David TSKHAKAYA**, *Institute of Plasma Physics of the Czech Academy of Sciences, Czechia* Needs for impurity collision data for kinetic modelling of the tokamak plasma edge
16:00 – 16:15	**Ralph DUX**, *Max Planck Institute for Plasma Physics, Garching, Germany* Atomic data needed for analysis of plasmas with injected impurities
16:15 – 16:30	**Xavier BONNIN**, *ITER, France* IAEA CRP on atomic and molecular data for injected impurities
16:30 – 16:45	**Mark ZAMMIT**, *Los Alamos National Laboratory, United States of America* LANL capabilities for modelling impurities in fusion plasmas

Wednesday, 8 June 2022

Session 2: Participant Presentations

Chair: Christian HILL

15:00 – 15:15	**Jacob SCHWARTZ**, *Princeton Plasma Physics Laboratory, United States of America* Needs for Li reaction data, especially for Li-wall or Li-divertor concepts
15:15 – 15:30	**Yuri RALCHENKO**, *National Institute of Standards and Technology, United States of America*

	Radiative data for injected impurities: NIST ASD
15:30 – 16:15	Discussion: CRP scope, species of interest, data priorities; potential code comparison and benchmarking activities
16:15 – 16:45	Discussion: data curation and dissemination; facilitation of the integration of data into modelling codes.
16:45 – 17:15	Discussion: potential CRP participants; project timetable and roadmap.

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