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## **INDC International Nuclear Data Committee**

# **18<sup>th</sup> Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion**

### **Summary Report of an IAEA Technical Meeting**

IAEA Headquarters, Vienna, Austria

26–27 April 2012

Report prepared by

B. J. Braams

IAEA Nuclear Data Section

December 2013

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December 2013

# 18th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

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### **Abstract**

The 18<sup>th</sup> meeting of the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) was held on 26–27 April 2012 at IAEA Headquarters in Vienna, Austria. Activities of the Atomic and Molecular Data Unit for the period 2010–2012 were reviewed and recommendations were made for continuing activities in 2012–2013 and for new projects in the 2014–2015 budget cycle. The proceedings, conclusions and recommendations of the Subcommittee meeting are briefly described in this report. Specific recommendations of the Subcommittee from this meeting, as well as the report on the activities of the IAEA Atomic and Molecular Data Unit for the period May 2010 – April 2012, are also included.

December 2013



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## Executive Summary and Recommendations

Prepared by R. Guirlet with B. J. Braams.

The subcommittee heard presentations by the Atomic and Molecular Data Unit staff on activities during the preceding 2 years and discussed priorities for development and dissemination of atomic, molecular and plasma-material interaction (A+M+PMI) data and for specific activities of the unit.

Worldwide, work on atomic and molecular data for fusion is under pressure. The subcommittee affirms the importance of evaluated and internationally recommended data for atomic, molecular and plasma-material interaction processes. ITER is the most important customer for recommended standard data. It is an important role for the unit to try to strengthen the international Data Centres Network and support the individual data centres. The unit should also use its influence to build up (again) a network of data evaluators and encourage data evaluations, both in connection with CRPs and in other activities.

Detailed recommendations are provided in Section 3 of the report. The following are highlighted.

### *ALADDIN and other numerical datasets*

With respect to ALADDIN and other numerical datasets the subcommittee affirms that the Unit should work with Data Centre Network partners and others to realize the original ambition of ALADDIN to serve as an internationally recommended standard library of A+M+PMI data for fusion. For atomic and molecular data emphasis should shift from production of new data to evaluation of existing data. For plasma-material interaction processes there is still much need for new data, especially for fusion-relevant mixed materials.

### *AMBDAS bibliographical database*

The IFRC subcommittee agrees that AMBDAS remains valuable because of the ease with which one can search on specific processes. It is important to reinvigorate the provision of collisional and plasma-material interaction data in AMBDAS.

### *Knowledge Base*

The wiki-style Knowledge Base can be valuable for dialog and qualitative information that doesn't fit well into the numerical databases. In the spirit of wikis and in order not to overwhelm Unit resources it will be necessary to find colleagues willing to contribute to the Knowledge Base.

### *Development of XSAMS*

The subcommittee is very pleased with the adoption of XSAMS by the Virtual Atomic and Molecular Data Centre. The Unit should continue to support XSAMS activities, but with priority for adoption of XSAMS by the fusion community rather than for extensions to the Schema.

### *GENIE Search Engine*

GENIE remains valuable, but the Unit should let its extension to other databases depend on the development of the XSAMS-based portal.

### *Data Centre Network*

The subcommittee emphasized ITER's need for standard and recommended data as a focal point for the work of the DCN. Quality control of data and the provision of recommended data remain the most important issues for the network. A network of data evaluators should be developed in close connection with the Data Centre Network.

### *Code Centre Network*

The subcommittee agrees that CCN should emphasize documentation of codes for the benefit of fusion plasma researchers. Sharing of codes is not encouraged for its own sake; in many cases users are better served by the provision of data produced by experts than by easy availability of a code. A suitable focussed topic for the next meeting of the CCN would be the evaluation of accuracy and uncertainty in theoretical atomic collision data. Another CCN meeting could focus on codes for plasma-material interaction.

### *Coordinated Research Projects*

The subcommittee affirms the importance of the topics of the Light Elements CRP and the Tungsten in Plasma CRP and recommends to continue both these CRPs to a 3rd RCM. The subcommittee considers that the development of a database for collisional and spectroscopic properties of BeH and BeH<sub>2</sub> can be a good topic for a consultancy or consultants meeting in parallel or as a follow-up to the light elements CRP. Being focussed on a single element the Tungsten in Plasma CRP really should lead to evaluated and recommended data for the principal collision processes of tungsten ions in plasma.

The subcommittee emphasizes that the new Hydrogen and Helium CRP should produce a comprehensive recommended standard database of isotope-resolved data for plasma modelling. The subcommittee is pleased with the approval of the beryllium CRP, which will have its first RCM later in 2012. The subcommittee also reiterates its support for a CRP on irradiated tungsten as the highest priority.

Priorities were discussed for a new CRP or CRPs to start in the 2014-2015 biennium. One possibility is a broad CRP on charge exchange, including cross sections and spectroscopic features related to diagnostic and heating neutral beams, although this topic may be more suitable for an incidental Technical Meeting or perhaps a Trieste Workshop. Another possible topic for a new CRP is the plasma material interaction properties of steel, which is once again being considered as plasma-facing material for a DEMO or a reactor.

### *Publications*

The subcommittee is very pleased with the plans developed in cooperation with the IAEA Publications division to produce future instances of Atomic and Plasma-Material Interaction Data for Fusion (APID) as volumes in the IOP open access Journal of Physics Conference Series. The subcommittee also recommends to pursue the publication route of a joint survey article in a major journal, as was done following the Tritium Inventory CRP. This would be in addition to the preparation of the APID/JPCS collection of articles.

### *Other meetings and workshops*

The subcommittee reinforces its support for holding another broad Technical Meeting in 2013 covering atomic, molecular and plasma-material interaction processes and data and materials properties data inasmuch as they are relevant for plasma-material interaction. The subcommittee suggests an effort to make it a joint ITER-IAEA meeting.

The subcommittee views the two recent Code Comparison Workshops as a worthwhile outreach activity at relatively low cost for the Unit. The subcommittee supports the interest of the Unit to cooperate in future similar code comparison workshops.

The subcommittee encourages the Unit to seek to continue the joint IAEA-ICTP workshops with a next instance in 2014 or 2015. It is noted that the ICTP is also an excellent venue for advanced workshops.

### *Conclusions*

In addition to all the specific recommendations there is the broad recommendation to the Unit to use its influence and its meetings to strengthen the community that is involved in data production and data evaluation for atomic, molecular and plasma-material interaction processes. We all recognize that these activities are not the most favoured in basic science, but they are very important for the development of fusion energy. The international Data Centres Network, broadly defined, needs the support and visibility that is brought by the A+M Data Unit of the IAEA.

## 1. Introduction

The International Fusion Research Council (IFRC) Subcommittee on Atomic and Molecular Data advises the Agency about the work of the Agency in the area of atomic, molecular and plasma-material interaction data for fusion, so about the work of the Atomic and Molecular Data Unit. The subcommittee meets in the spring of the even years; a time that is most suitable for input into the initial budget plans for the next biennium. The present report concerns the meeting of the IFRC subcommittee that took place on 26–27 April 2012 at IAEA Headquarters in Vienna.

The meeting proceedings are provided in Section 2 and the discussion and conclusions are summarized in Section 3. The list of participants is in Appendix 1 and the meeting agenda is given in Appendix 2. Activities of the Unit during April 2010 – March 2012 are summarized in Appendix 3.

## 2. Meeting Proceedings

### R. A. Forrest, R. Kamendje, B. J. Braams: Opening

The meeting was opened by Nuclear Data Section (NDS) Head Robin Forrest who welcomed the IFRC subcommittee members to Vienna and provided a short overview of work in the NDS relevant to Fusion. This meeting will review the work of the Atomic and Molecular (A+M) Data Unit, but some of the nuclear data work in the Section is also relevant to Fusion. In particular the NDS is responsible for the Fusion Evaluated Nuclear Data Library (FENDL), which provides evaluated cross-section and activation data for neutron-, proton- and deuteron-induced reactions. In order to meet the modelling needs for the proposed International Fusion Materials Irradiation Facility (IFMIF), which will have a charged particle and neutron energy range much beyond the 14 MeV of D-T fusion neutrons, the most recent FENDL-3 release of the library extends the energy range up to a typical energy of 150 MeV for General Purpose and 60 MeV for Activation files. Also more emphasis is given to covariance data for fusion technology studies. Dr Forrest stressed that the guidance that is provided by the subcommittee is very important to the Section; it affects both the activities in the present (2012-2013) fiscal biennium and the budget planning for the next (2014-2015) biennium.

Atomic and Molecular Data Unit (AMDU) Head Bas Braams extended his welcome and asked the IFRC subcommittee members to briefly introduce themselves. We have two members that were not at the meeting in 2010: Dr K.-D. Zastrow leads the Core Spectroscopy Group at JET and Dr J. Reader is Director of the Atomic Spectroscopy Group at NIST. The full list of meeting participants and their affiliations is provided in Appendix 1. Bas Braams requested members to discuss among themselves about a Chair for the subcommittee to be elected after the lunch break; this was done and Dr R. Guirlet of CEA, France, was nominated and elected by acclamation.

The subcommittee then heard a brief review by Dr Richard Kamendje of Fusion activities in the Physics Section. The best known projects are the biennial Fusion Energy Conference and the Nuclear Fusion journal, but the Physics Section organizes a broad range of technical and topical meetings, workshops, and coordinated research projects in the areas of magnetic fusion, inertial fusion and plasma physics. Recent Technical Meetings include meetings on steady-state operation, ECRH physics and technology, theory of plasma instabilities, and energetic particles. A new activity is the Fusion DEMO workshop to be held at UCLA in October 2012. Dr Kamendje emphasized the wish of the Physics Section to build up work on Fusion Technology. CRPs are being held on small tokamak research, compact fusion neutron sources and materials under intense heat pulses. Joint meetings are organized with ITER: a workshop at ICTP and a TM in Monaco. One special project is the production of a post-graduate level tutorial book on Fusion Physics; 1100+ pages due out later in 2012.

The opening presentations gave rise to discussion about the interaction between the Nuclear Data Section and the Physics Section in the area of fusion energy research. In particular there are several pairs of closely related CRPs. The A+M Data Unit has a CRP on beryllium plasma-facing materials and the Physics Section has one on materials under intense heat pulses. The A+M Data Unit is planning a CRP

on plasma-wall interaction with irradiated tungsten and the Physics Section has one on fusion neutron sources, and the DEMO workshop. In the discussion it was emphasized that the two Sections coordinate their work and avoid overlap. Our beryllium CRP is specifically concerned with erosion and tritium retention behaviour under routine plasma exposure, avoiding the intense heat load (ELM exposure) damage issues. Our planned CRP on irradiated tungsten is devoted to plasma-material interaction and tritium retention whereas the Physics Section activities on irradiated materials are concerned with behaviour of the structural materials.

## **B. J. Braams: General Report on A+M Data Unit Activities**

The Unit head Bas Braams presented an overview of Unit activities and actions in the context of advice given by the IFRC subcommittee at their 17th meeting, 27-28 April 2010. The overview is reproduced here in the format:

### ***Advice from the IFRC Subcommittee meeting of 27-28 April 2010.***

Actions by the Atomic and Molecular Data Unit in the period to April 2012.

***ALADDIN and other numerical data sets: quality control and the provision of unique recommended data are issues of ongoing concern.***

This has developed into an overarching concern for the Unit. Actions include:

- Data evaluation was central topic at DCN meeting in Sep 2011.
- CM on data evaluation at NIFS, 7-9 Feb 2012; developed roadmap and organizational guide for development of standard library.
- Preparing a Cooperating Centre agreement with NFRI focussed on infrastructure and activities for data evaluation.
- CM on data evaluation at IAEA, 20-22 June 2012; to advise about Unit activities next several years.
- Larger TM to be held at NFRI, 4-7 Sep 2012; data evaluation for fusion.
- Maybe TM at ICPEAC in July 2013.

***The Unit should continue its role of coordinating the Data Centre Network activities through the biennial DCN meetings. Quality control of data and the provision of recommended data remain most important issues.***

The 21st Meeting of the DCN was held 7-9 Sep 2011: NIST and CFADC (USA), CRAAMD (China), NFRI and KAERI (Korea), NIFS and JAEA (Japan), FZ Juelich (Germany), Kurchatov (Russia), ADAS (UK) and IAEA; VAMDC (EU) as guest.

Meeting conclusions:

- Continued support for XSAMS; a general desire to make it available as an output format.
- IAEA will continue to coordinate bibliographical database (AMBDAS). New collaboration with NFRI was initiated here.
- Data evaluation very much encouraged; plans were developed here for sequence of meetings.

***Possible actions for the numerical data libraries:***

- ***Have CM/TM or consultant visits to evaluate data, or at least to identify datasets that are ripe for evaluation.***
- ***Focussed question for CM: What should be done to upgrade APID 7A/7B on erosion?***

Consultancy by W. Eckstein in Sep 2010 to update reflection and penetration data in ALADDIN.

TM in Dec 2011 on “Improving the Database for Physical and Chemical Sputtering”: J. W. Davis, R. Doerner, A. Ito, P. Krstic, K. Nordlund, K. Ohya, R. Schneider. Expecting new data from K. Nordlund, R. Schneider.

TM in Dec 2011 on “Ab Initio-Based Methods for Plasma-Material Interaction in Fusion Devices”

***AMBDAS is in recent years based exclusively on compilations done at NIST for spectroscopic data and at CFADC (Oak Ridge) for collisional data. The subcommittee wishes to stress the unique and very valuable role of the CFADC in maintaining and updating these bibliographical data.***

Point of discussion at the DCN meeting in Sep 2011. CFADC has closed; existing CFADC databases to be maintained at Auburn. Resumption of bibliographical work there is very uncertain.

DCN meeting urges continued upkeep of AMBDAS. NFRI Data Center for Plasma Properties has bibliographical database. In the Collaborating Center agreement it is agreed that a conversion tool will be developed (different codes are used) and the NFRI bibliographical data will be integrated into AMBDAS.

***The Bulletin appears most useful in electronic form, searchable through AMBDAS with full-text links through the DOI. Still, the subcommittee endorses continued publication of the paper bulletin for the next few years.***

AMBDAS has been upgraded with new spectroscopic data, but no new collisional data since 2009. We intend to produce the next issue of the Bulletin after we obtain the NFRI dataset. Target date for publication is Q1 2013.

***GENIE provides a valuable interface to multiple datasets. It should be maintained and possibly expanded to access additional databases.***

GENIE was expanded to access also Open-ADAS and Spectr-W3; this was done through a consultancy by D. Humbert.

We support GENIE and its reach could be expanded further, but have no near-term plans for that. At this time we would rather see XSAMS take hold for data exchange.

***The new Knowledge Base can serve for dialog about data, data needs and data quality and to provide background scientific information on methods and context of data. In order not to overwhelm Unit staff it will be necessary to find people to contribute to the Knowledge Base.***

The Knowledge Base quickly became one of the most visited areas on our web pages. On the other hand, we did not succeed to attract other authors. It has been a low-key activity for us since Apr 2010.

***With regard to Code Centre Network: Several suggestions:***

- ***Documentation should clarify weaknesses, appropriate use, etc.***
- ***PMI codes are also appropriate for CCN, e.g., TRIM-SP.***
- ***The interface at the Agency should allow to execute a code or it should point to an official code home; it should not be a repository for downloading a code.***
- ***The Code Center Network should encourage code comparison efforts.***

The CCN meeting was held 27-28 Sep 2010 back to back with a CM on “Data Needs for Plasma Modelling”; it brought code developers together with data users and this was much appreciated. Participants emphasized the need for quality assessment of calculations. Generally we de-emphasize in the CCN the sharing of the codes and we emphasize more the sharing of high quality code results.

Future CCN meetings may have a focus on a specific class of codes.

We are thinking now about CCN in November 2012.

***For the recently concluded CRPs the final APID reports need to be published without undue delay.***

This has been difficult. APID volumes 15 (tritium inventory) and 16 (A+M data for plasma modelling) are with Publishing in the final stage of copy-editing. These volumes are also available on the Unit web pages. APID volume 17 (heavy element impurities) is still within the Unit.

***The subcommittee recommends that the ongoing CRPs on surface composition dynamics and on characterization of dust both be continued to a 3rd RCM.***

The 3rd RCM of the CRP on surface composition dynamics was held 13-15 September 2010. This CRP needs urgently to be brought to a proper close. There is not yet a meeting report of the 3rd RCM and there is not a final report of the CRP.

The 3rd RCM of the CRP on characterization of dust was held 30 Nov – 02 Dec 2011. It is agreed to produce a journal article in FST with C. H. Skinner as lead author and to produce APID Vol 18. Infrastructure for a dust database has been developed at IPP Garching; it intended that the database will be hosted at IAEA in due time. We expect another CM in Q3 or Q4 2012 about the dust database and then conclude this CRP.

***Concerning future CRPs the subcommittee recommends:***

- ***2011-2015: Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma. There should be a CM/TM later in 2010 to identify the most pressing gaps in the data and potential participants in the CRP.***
- ***2012-2016: Erosion and tritium retention for beryllium plasma-facing materials. There should be a CM/TM in 2011 to define this CRP further.***
- ***2013-2017: Plasma-wall interaction of irradiated tungsten and tungsten alloys in fusion devices. (Details to be reviewed at the subcommittee meeting in 2012.)***
- ***(if budget allows it): Data for processes of hydrocarbon ions in fusion plasma.***

A CM on “data needs for plasma modelling” (Sep 2010 back-to-back with CCN) and a session at the “dissociative recombination 2010” conference were helpful to prepare the proposal for a CRP on “Atomic and molecular data for state-resolved modelling of hydrogen and helium and their isotopes in fusion plasma”. The CRP was approved by CCRA and held its first RCM 10-12 August 2011; the second RCM is planned for Q1 2013.

A CM on “Erosion and tritium retention for beryllium plasma-facing materials” was held 30-31 May 2011 with S. Brezinsek, D. Kato, R. Doerner and W. Jacob to develop the proposal for such a CRP. The CRP was approved by CCRA in August 2011. The first RCM is planned for 26-28 Sep 2012. (It is a bit late in the year in order to keep a distance to PSI.)

A CRP on “Plasma-wall interaction of irradiated tungsten and tungsten alloys in fusion devices” is in the Programme and Budget to start in 2013, but we have not yet prepared the detailed proposal. We look forward to discussion here; also we will use PSI in Aachen, 21-25 May, and the hydrogen workshop in Schloss Ringberg, 29-31 May, to gather information.

It was not possible to start a further CRP in 2012-2013. We appreciate the judgement of the IFRC subcommittee in 2010 that a CRP on hydrocarbon molecules should have lower priority than those on beryllium and on tungsten. ITER has all but abandoned carbon-based walls and a CRP on hydrocarbons would not be a priority now.

***The review and publications procedures of APID need to be streamlined. It is very desirable that APID be published electronically in addition to paper; and past issues should be electronically accessible if IAEA publications policy allows it.***

We undertake to streamline the process for APID 18 (erosion and dust). There is an option for electronic publication in the open access IOP Journal of Physics Conference Series (JPCS), in addition to the Greenbook hardcopy.

***Alternative publication routes should be pursued, as exemplified by the joint focussed review article following the Tritium Inventory CRP. Consider also the possibility for summaries in Nuclear Fusion.***

For the dust CRP we expect again a comprehensive article in FST, and we must review still how to publicize the associated database. Next after that is the Light Elements CRP.

***Occasional AMDU Newsletter would be valuable.***

We have not produced an AMDU newsletter, but the latest issue of the NDS newsletter has a special feature on the work of AMDU. We will keep in mind the suggestion for a separate AMDU Newsletter.

***Try to hold another ICTP workshop in 2012, or earlier if the budget allows it. It is suggested to track the participants to estimate better the impact.***

A Joint ICTP-IAEA Workshop on Fusion Plasma Modelling Using Atomic and Molecular Data was held in Trieste 23-27 Jan 2012. Advice from participants in previous meetings was used.

Ten lecturers presented tutorials and reviews on topics in fusion plasma modelling and atomic, molecular and plasma-material interaction processes.

There were 20 participants, generally early-career researchers in the area of A+M+PMI processes and also plasma modellers.

We aim for another ICTP workshop in 2014. It could be similar to the present one, but could also be an advanced workshop on a more specialized topic.

***The subcommittee strongly supports the proposal for the Unit to be the local host for the NLTE-7 code comparison workshop in 2011.***

NLTE-7 was held 5-9 Dec 2011 in Vienna with our cooperation. More than 25 participants submitted results from 19 codes for more than 50 test cases in the workshop. A meeting report will be prepared for journal publication and the publication of detailed comparisons of specific cases will be considered by participating code developers and case coordinators.

Following the same model the Spectral Line Shapes in Plasmas code comparison workshop was held in Vienna 2-5 April 2012 organized by the Weizmann Institute of Science in cooperation with us. There were 22 participants including the organizers.

***The subcommittee supports the Unit's cooperation in a Technical Meeting on ITER materials in connection with the Monaco Fusion Energy Days.***

The First Joint IAEA-ITER Technical Meeting on Analysis of ITER Materials and Technologies was held 23-25 Nov 2010 in association with the Monaco Fusion Energy Days. R. Kamendje of the Physics Section was the principal organizer and we had a supporting role. Selected papers have been published in FST.

***International meetings: highest priority to ICAMDATA, ICPEAC and PSI. Other valuable meetings include EGAS/ECAMP, the ADAS meetings, European Fusion Task Force meetings, EFDA events, APiP, IAEA FEC and others.***

International meetings attended:

- EFDA SEWGs on dust and tritium removal, 8–11 Jun 2010, Garching (BJB)
- 8th IC on Dissociative Recombination, 16-20 Aug 2010, Tahoe City (BJB)
- 7th ICAMDATA, 21-24 Sep 2010, Vilnius, Lithuania (BJB + HKC)
- ADAS Workshop, 3-6 Oct 2010, Armagh, UK (BJB)
- 14th IC on RPHDM, 4-8 Oct 2010, Marbella, Spain (HKC)
- Annual Meeting of EU PWI TF, 3-5 Nov 2010, Vienna (BJB + HKC)
- EFDA SEWGs of PWI TF, 31 Jan – 2 Feb 2011, Tervaniemi, Finland (HKC)
- Annual meeting of the VAMDC, 28-31 Mar 2011, Cambridge, UK (BJB)
- 13th International Workshop on PFMC, 9-13 May 2011, Rosenheim (BJB)
- 6th International Workshop on Warm Dense Matter, 05-09 June, Pacific Grove, CA (HKC)
- 17th APiP, 19-22 Jul 2011, Belfast, UK (BJB)
- 7th IC on Inertial Fusion Sciences and Applications, 12-16 Sep 2011, Bordeaux Lac (HKC)

- ADAS Workshop, 6-8 Oct 2011, Auburn (BJB)
- Annual Meeting of EU PWI TF, 28-29 Nov 2011, Bratislava (HKC)

*The subcommittee notes that there does not exist a true Fusion Atomic Data meeting on par with PSI as the Fusion PMI meeting. This is a role for the infrequent large A+M data meeting last organized in Juelich in 2002.*

The intended larger Technical Meeting on A+M+PMI data for fusion is included in the Programme and Budget for 2013. We have not developed concrete plans yet.

*The subcommittee echoes its earlier Advice for the Unit to maintain a strong role in coordination of development of XSAMS and in encouraging its implementation, but not to take a leading role due to limited Unit resources.*

XSAMS received a strong boost due to its adoption by VAMDC, through which it has been implemented on about 25 databases mainly for astrophysical applications. XSAMS version 1.0 was adopted in Feb 2012. XSAMS has not yet been adopted by the user community.

*The subcommittee recommends to look at possible coordination of XSAMS development and implementation with work by the Integrated Tokamak Modelling task-force.*

We have paid attention to the ITM work (advice from D. P. Coster). Their standardization is concerned with code interfaces.

*The subcommittee took note of the move of the graphite properties database project to NE. The Unit can be open to a future extra budgetary project if the occasion arises.*

We remain open to such a project, but nothing has come up.

#### ***Additional activities not following any specific recommendation***

Collaborating Centre agreement with NFRI (Korea)

- Focussed on the work of their Data Centre for Plasma Properties
- Support data evaluation and the development of standard libraries
- Expected duration is 2012-2016; expected start in Sep 2012
- Intern and SSA agreement for Summer 2012
- Code results for atomic data
- Light elements and tungsten

## **H.-K. Chung: Review of Data Centre Network, Databases and Data Evaluation**

Atomic physicist Hyun-Kyung Chung described the activities since April 2010 that concern the Unit's web pages, bibliographical and numerical databases, coordination of the International Data Centre Network (DCN) and work on atomic and molecular data evaluation. Please see Appendix 3, Section 1, for a detailed summary of the presentation.

The presentation gave rise to an extended discussion on data evaluation. Dr R. Janev recalled the serious data evaluation work that was done before the A+M Data Unit came into existence and during the early years of the Unit. The ORNL Redbooks (C. F. Barnett et al.) constituted an excellent series of evaluations. In Japan much work was led by H. Suzuki and T. Kato and in Belfast there was the work by P. G. Burke and A. E. Kingston. The early work by the A+M Data Unit at IAEA was well recognized through its publication as a supplement to Nuclear Fusion. So there was much work on data evaluation for fusion done by the national data centres and also by CRPs of the Agency; more so during the 1970s and 1980s than now. One critical issue is the need for raw data and another is the interest of subject matter experts to carry out evaluations. Dr Janev urges the Unit to retain two roles: the

production of new data (do not abandon that task) and data evaluation. He notes that data evaluation is an ongoing task and one needs to re-evaluate data that were previously evaluated.

On the subject of data production and data evaluation Dr J. Roth turned to plasma-material interaction processes and reviewed the work of the Garching data centre. Early work there was devoted to measurement of elementary data for (primarily) sputtering, reflection and trapping. Present work is much more complicated as it studies the dependence of particle-surface and plasma-material interaction processes on surface treatment, temperature, flux and fluency and other factors. This new kind of PMI studies is not so suitable for simple tables; almost each effort is a journal publication, and the effort needs the visibility of a journal publication.

In further discussion it is emphasized that a lot of new data is still needed in the area of plasma-material interaction and the data must be understood in a manner that allows extrapolation to fusion reactor conditions. One must study mixed materials, damaged materials (irradiation; melting and resolidification) and effects of material microstructure. Expert advice from the fusion materials community is essential in order to know what PMI data are needed. Atomic and molecular data is much better understood. As example of new data needs Dr G. Mazzitelli mentions that EFDA is now interested in uncoated Eurofer steel and the plasma-material interaction properties are not known.

The discussion turned to publication issues for data evaluations and the need to provide incentives to do the work. Data evaluation does not appear to be attractive to young researchers. We emphasize that the A+M Data Unit actively seeks new people, for example through the IAEA-NFRI meeting later in 2012. Possible publication venues include Nuclear Fusion (NF), Fusion Science and Technology (FST), Journal of Physical and Chemical Reference Data (JPCRD), Atomic Data and Nuclear Data Tables (ADNDT) and the European Journal of Physics D (EPJD). There was some data review articles in NF and NF Supplements were used when C. Bobeldijk was editor, but then the supplement series was abolished. FST is well recognized for plasma-material interaction was used for the tritium article led by C. Skinner. (This article was really a review of work done during a CRP, not a review or data evaluation of tritium retention more broadly.) JPCRD and ADNDT are specialized in data, but have a lower impact factor. EPJD should be considered more often for atomic and molecular data.

Dr J. Reader reviewed the ongoing experience in the NIST Atomic Spectra Group with evaluations. The talk by H.-K. Chung shows the flowchart. The data are compiled at NIST and the Atomic Spectra Group has put a lot of effort into the infrastructure for managing the data compilations. Dr Reader emphasizes that whatever publication mechanism is chosen, it must be on-line. He strongly recommends against a book format.

After this discussion on data evaluation and the provision of recommended data it is clear that data evaluation work must be encouraged, but much more strongly so for A+M data than for PMI data. For plasma-material interaction the focus should still be on the production of new data for more complicated situations. For A+M processes there is need for ongoing evaluations and the Unit should seek the most appropriate mechanism or mechanisms. In general evaluation of data should be among the tasks of a CRP, but this is a heavy mechanism and data evaluation cannot be limited to CRPs. ITER is the most important customer for evaluated and recommended data and it would be very helpful to have their support, including funding for specific evaluations.

Relatively little was discussed about the database management aspects. The loss of the Controlled Fusion Atomic Data Center is unfortunate; in addition to their experimental programme they contributed the collisional and plasma-material interaction part of the AMBDAS bibliographical database. There was general agreement that this work should continue and Dr Reader emphasized that with a good organization a bibliographical database can be kept up-to-date with rather little effort; the NIST spectroscopic database is up-to-date at the level of just a few weeks. It is much more difficult to maintain numerical databases.

The ALADDIN interface for numerical data was discussed and it is agreed that it is not attractive to newcomers and needs to be revisited. This would be done in connection with the ongoing development of the XML Schema for Atomics, Molecules and Solids (XSAMS) as a data exchange mechanism.

## **H.-K. Chung: Code Centre Network and Code Comparison Workshops**

As for the data activities, please refer to Appendix 3 (Section 2) for a detailed summary of the work of the unit on the code centre network and code comparison workshops. This topic, too, gave rise to animated discussion. Dr Janev enquired about the relevance of the NLTE and SLSP code comparison workshops. The Unit emphasizes the outreach aspect of these meetings (outreach to the theoretical AMO physics community); we want computational atomic and molecular physicists to be engaged with our work and with fusion. Drs Mazzitelli and Zastrow emphasized the interest in spectral line shape studies for fusion diagnostics.

There was general agreement about the need to concentrate on the production of high quality data in connection with activities of the Code Centre Network; we don't view the dissemination of codes as the primary activity of the network. Dr Janev recommends that the Code Centre Network members be asked to produce specific data for fusion.

## **B. J. Braams: Review of Coordinated Research Projects**

Please refer to Appendix 3, Section 3 for an overview of recent, ongoing and new CRPs. The latest one is on "Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials" and it is to have its initial meeting later in 2012. The second new CRP in the Programme and Budget for 2012-2013 is on "Plasma-material Interaction for Irradiated Tungsten and Tungsten Alloys"; a detailed proposal should go to the Committee on Coordinated Research Activities near the end of 2012 for the CRP to start some time in 2013.

In the discussion about ongoing CRPs it was emphasized again that the CRPs should lead to evaluated and recommended data; this applies to the CRPs on light elements, on hydrogen and helium in edge plasma, and on tungsten in plasma. The light elements CRP includes work on beryllium hydrides and Dr Janev recommends that there should be a consultancy or consultants meeting in parallel with the CRP or after it to provide recommendations for data for these molecules. In the discussion there was no controversy about the plans for the CRP on irradiated tungsten; this remains a very high priority for the fusion programme. The focus of that CRP should be on tritium deposition, migration and retention.

The main topic for discussion was that of new CRPs to start in the 2014-2015 biennium. In the area of atomic and molecular processes the option of a broad CRP on charge exchange was raised, including cross sections and spectroscopic features related to diagnostic and heating neutral beams. This topic could also be suitable for one or several Technical Meetings or workshops and it probably needs a Consultants Meeting to discuss the options, especially if a CRP is to be proposed. In the area of plasma-material interaction the highest priority would be for a CRP on plasma material interaction properties of some kind of low-activation or reduced-activation steel, which is once again being considered as plasma-facing material for a DEMO or a reactor.

## **S. LeMasurier: Publications**

Please see Appendix 3, Section 4, for a summary of the presentation by Ms LeMasurier of the Publications Section on options for the future of the Atomic and Plasma-Material Interaction Data for Fusion (APID) series. Ms LeMasurier and the Unit consider the present situation with APID not acceptable. The recommendation is made to adopt an open access publications model for the final report of our CRPs, and specifically to use the IOP Journal of Physics: Conference Series (JPCS).

In the discussion the tritium review article in Fusion Science and Technology was brought up again as an attractive model for a publication following a CRP. However, there is a need for final reports by participants and it was agreed that for this purpose the present APID is not suitable and the proposed JPCS mechanism is attractive.

## **B. J. Braams: Other Activities of the Unit**

Please see Appendix 3, Section 5, for a summary of other activities including the ongoing work on the XML Schema for Atoms, Molecules and Solids (XSAMS) and various meetings and workshops organized by the unit.

This presentation was primarily an occasion to discuss future meetings organized by the Unit and especially a large meeting on atomic, molecular and plasma-material interaction data such as was most recently organized in Jülich (2002) and before that in Cadarache (1992), Fontenay-aux-Roses (1980) and Culham (1976). It is attractive to follow precedent and hold it outside the IAEA, so one needs a local organizer. The previous such meetings have been important to bring A+M+PMI data work to the fusion community; for many fusion researchers this meeting has been a memorable event. One may try to attach the next big meeting to another event, maybe APiP, but the meeting can also stand on its own. ITER should play an important role and it is recommended to seek to make it an IAEA-ITER joint meeting. However, the meeting should also be concerned with data needs for current experiments.

## **All: Concluding Discussion**

In conclusion the subcommittee revisited the most important topics raised earlier during the meeting. The conclusions were reviewed and these are provided in Section 3. The discussion also reiterated that atomic and molecular data work for fusion is under pressure and it is important for the Unit to try to strengthen the Data Centres Network and support the individual data centres. ITER is the most important customer for recommended standard data. The Unit should also use its influence to try to build up (again) a network of data evaluators and encourage data evaluations; these should take place as a follow-up to a CRP and in other activities.

## **3. Recommendations and Conclusions**

### **ALADDIN and other numerical datasets**

The ALADDIN database was created with the ambition that it would be the internationally recommended standard library of atomic, molecular and plasma-material interaction (A+M+PMI) data for fusion. In fact it has developed as a record of data production done in association with IAEA. The data are generally of high quality at the time of compilation, but ALADDIN is not the recognized international standard (evaluated and recommended) library.

The subcommittee recommends that ALADDIN should be maintained as a record of work done in collaboration with IAEA. The Unit should work with the Data Centre Network partners and others to realize the original ambition of ALADDIN and develop an internationally recommended standard library of A+M+PMI data for fusion. The Roadmap that was laid out at the Consultants Meeting at NIFS in Feb 2012 provides good guidance for the development of the standard library.

The main areas of activity of the A+M Data Unit are atomic collision data, molecular collision data and plasma-surface interaction data. In addition material structure data is an area of interest in connection with problems of tritium retention. At this time the data evaluation activities should be concentrated primarily on atomic and molecular data. It is appropriate for the Unit to redirect effort from the production of new data for A+M collision processes to the evaluation of existing data. This is appropriate effort within a CRP and also for technical meetings and consultancies.

For plasma-material interaction data and material structure data there is a strong need still for the production of original data relevant for fusion energy. In the area of PMI data the main issue is to improve basic data for sputtering and reflection for mixed materials, especially Be-C-W. Consultancy visits or small CM/TM are a good mechanism for this.

## **AMBDAS bibliographical database**

The easy availability of bibliographical search through Google Scholar, Elsevier Scopus and ISI Web Of Knowledge has changed the nature of bibliographical search and it is appropriate to reassess the role of our AMBDAS. This topic was discussed at the Data Centres Network meeting in September 2011 and the IFRC subcommittee agrees with the assessment of the DCN that AMBDAS remains valuable because of the ease with which one can search on specific processes. For spectroscopic data the Unit is fortunate to be able to rely on compilations done at NIST, but for collision data and for PMI data a new source is needed following the closing of the CFADC at Oak Ridge. If this can be done through collaboration with NFRI then that is much appreciated; else one should try to organize it as a distributed community effort.

The Bulletin appears most useful in electronic form, searchable through AMBDAS with full-text links through the DOI. However, the subcommittee endorses continued publication of the paper bulletin for the next few years. It is noted that the printed distribution was much reduced recently, from about 800 to about 200.

## **Knowledge Base**

The subcommittee appreciates the work that was done since early 2010 on the development of the Unit's wiki-style Knowledge Base on atomic, molecular and plasma-material interaction data for fusion. The Knowledge Base can be valuable for dialog about data, data needs and data quality and it can provide background scientific information on methods and context of data; information that doesn't fit well into the numerical databases. In the spirit of wikis and in order not to overwhelm Unit resources it will be necessary to find colleagues willing to contribute to the Knowledge Base. Perhaps it will be possible to find students (graduate students connected to our work) willing to contribute.

## **Development of XSAMS**

The subcommittee is very pleased with the adoption of XSAMS by the Virtual Atomic and Molecular Data Centre, which happened in 2010, and with the recent community agreement on the content of XSAMS version 1.0. The subcommittee recommends to the A+M Data Unit to encourage wider use of XSAMS in the fusion plasma community for exchange of A+M data.

Over the next two years the XSAMS schema itself is expected to be in "maintenance mode" as attention is focussed on the portals and other user-oriented infrastructure. The subcommittee agrees with this allocation of resources. The Unit should give priority to supporting the implementation of XSAMS as it exists rather than to extension of the schema. As in previous years the subcommittee recommends that the Unit support XSAMS activities but not take a leading role due to limited Unit resources.

## **GENIE Search Engine**

GENIE has provided for the past 8 or 9 years a valuable interface to multiple datasets. It may become superseded now by a new portal based on XSAMS. In the meantime, however, GENIE should be maintained and possibly expanded to access additional databases for atomic collisions (e.g. DREAM, DESIRE). The subcommittee recommends that the Unit consider such expansion of GENIE, but let it depend on the development of the XSAMS-based portal for these and other databases.

## **Data Centre Network**

The coordination of the DCN was one of the original tasks of the A+M Data Unit and the Unit should continue its role of coordinating the data centre network activities through the biennial DCN meetings. The Unit and the DCN share an important role to support the work at national data centres. The subcommittee emphasized ITER's need for standard and recommended data as a focal point for the work of the DCN. Quality control of data and the provision of recommended data remain the most important issues for the network.

A network of data evaluators should be developed in close connection with the Data Centre Network.

## Code Centre Network

The code centre network was created in 2005 as a flexible group. The 3rd meeting was held in 2010 with additional participants from the PMI area and from plasma modelling. The subcommittee recommends a continued expansion of the code centre network in the area of plasma-material interaction codes.

Such an expansion implies that meetings of the CCN will not be meetings of the whole. Instead, the CCN will serve as an umbrella for smaller meetings focussed on specific classes of codes that may be used to produce A+M+PMI data that are relevant for fusion.

A suitable focussed topic for the next meeting of the CCN would be the evaluation of accuracy and uncertainty in theoretical atomic collision data. Another CCN meeting could focus on codes for plasma-material interaction.

The subcommittee agrees with other policies that were agreed at the CCN meeting in 2010. The shared objective of the CCN participants is to document codes for the benefit of fusion plasma researchers, but the CCN or the IAEA should not have the responsibility to distribute these codes. In addition, sharing of codes is not encouraged for its own sake; in many cases users are better served by the provision of data produced by experts than by easy availability of a code.

## Coordinated Research Projects

The Light Elements CRP had its second RCM in May 2011 and the Tungsten in Plasma CRP is scheduled to have its 2nd RCM in August 2012. The subcommittee considers that the topics of these CRPs remain of high importance for fusion and recommends to continue both these CRPs to a 3rd RCM.

The Light Elements CRP would have its 3rd RCM in early 2013. One prominent and highly relevant topic that is being addressed within this CRP is the development and assessment of data for processes of beryllium hydrides BeH and BeH<sub>2</sub>, which are produced at walls and for which very little data exists. The subcommittee considers that the development of a database for collisional and spectroscopic properties of BeH and BeH<sub>2</sub> can be a good topic for a consultancy or consultants meeting in parallel or as a follow-up to the light elements CRP.

Being focussed on a single element the Tungsten in Plasma CRP should really should lead to evaluated and recommended data for the principal collision processes of tungsten ions in plasma.

The new Hydrogen and Helium CRP had its 1st RCM in August 2011 with the 2nd RCM expected in early 2013; therefore the question of continuation to a 3rd RCM is not yet asked. The subcommittee emphasizes that this CRP should produce a comprehensive recommended standard database of isotope-resolved data for plasma modelling.

At its meeting in 2010 the subcommittee recommended two CRPs to start in the 2012-2013 biennium: the first on “data for erosion and tritium retention in beryllium plasma-facing materials” and the second on “plasma-wall interaction with irradiated tungsten and tungsten alloys”. (Both are working titles only.) The subcommittee is pleased with the approval of the beryllium CRP, which will have its first RCM later in 2012. The subcommittee also reiterates its support for a CRP on irradiated tungsten as the highest priority. The focus of that CRP should be on tritium deposition, migration and retention.

Several candidate topics were discussed for a CRP or CRPs to start in the 2014-2015 biennium, for which a preliminary budget proposal is due in August 2012. One possibility is a broad CRP on charge exchange, including cross sections and spectroscopic features related to diagnostic and heating neutral beams. It needs further thought if this topic is perhaps more suitable for an incidental Technical Meeting or perhaps a Trieste Workshop. Another possible topic for a new CRP is the plasma material interaction properties of steel, which is once again being considered as plasma-facing material for a DEMO or a reactor.

## Publications

The subcommittee is very pleased with the plans developed in cooperation with the IAEA Publications division to produce future instances of Atomic and Plasma-Material Interaction Data for Fusion (APID)

as volumes in the IOP open access Journal of Physics Conference Series. The subcommittee envisages that by doing so the refereeing procedures will be strengthened, the stature of the individual contributions will be enhanced, the output will be more visible and the publication procedure will be streamlined. The subcommittee considers that it is still desirable to produce a limited hard copy print run, but the primary publication should be the on-line instance of JPCS.

The subcommittee also recommends to pursue the publication route of a joint survey article in a major journal, as was done following the Tritium Inventory CRP. This would be in addition to the preparation of the APID/JPCS collection of articles.

The subcommittee recommends occasional publication of an AMDU Newsletter similar to the Nuclear Data Section newsletter.

## **Other meetings and workshops**

The subcommittee discussed plans for a larger Technical Meeting on atomic, molecular and plasma-material interaction data for fusion such as was previously held in Jülich () and in Cadarache (12-16 October 1992). Both these meetings were viewed very positively and at their meeting in 2010 the subcommittee had already recommended that the Unit plan to organize again such a meeting in the 2012-2013 biennium. The meeting is included in the preliminary budget for 2013.

The subcommittee reinforces its support for organizing such a meeting in 2013. The meeting should be broad and cover atomic, molecular and plasma-material interaction processes and data, and materials properties data inasmuch as they are relevant for plasma-material interaction. The subcommittee suggests an effort to make it a joint ITER-IAEA meeting, which would then probably imply a return to Cadarache. In any case it should be clear that the needs of ITER for A+M+PMI data have a very important role in the meeting.

The subcommittee views the two recent Code Comparison Workshops as a worthwhile outreach activity at relatively low cost for the Unit. It is understood that in both cases the IAEA support was incidental and is not a precedent for future instances of the same series. The non-local thermodynamic equilibrium (NLTE) workshop series is well established and the next instance is not expected to be in Vienna. The spectral line shapes in plasma (SLPS) workshop was the first of its kind and if it repeated in 2 or 3 years then our contribution in 2012 will have been a useful seed.

The subcommittee supports the interest of the Unit to cooperate in future similar code comparison workshops. A possible topic would be codes for particle-surface interaction, for which one would specify model problems that can be treated using methods ranging from the binary collision approximation to ab initio-based molecular dynamics. Another possible topical area would be some well specified plasma modelling cases that rely strongly on A+M+PMI data.

Joint IAEA-ICTP workshops in Trieste on A+M+PMI data for plasma modelling have now been held in 2003, 2006, 2009 and 2012 and the subcommittee encourages the Unit to seek to continue this series of introductory workshops with a next instance in 2014 or 2015. It is noted that the ICTP is also an excellent venue for advanced workshops. Any workshop needs to be agreed between IAEA and ICTP and the Unit should discuss with ICTP what proposals have the best chance of success.

The subcommittee appreciates the Unit's involvement in a planned Technical Meeting on Materials and Technologies for ITER; at IPR in India, Dec 2012 (following an earlier such meeting in Monaco, Nov 2010).

Smaller TM/CM are organized as the need arises. One topic suitable for such an experts' meeting is that of spectroscopy for measurement of erosion, especially for beryllium surfaces.

## **Unit participation in other meetings**

It is important for Unit staff to participate in international scientific meetings in order to present the work of the Unit and that of its partners on database development and data evaluation, attract new researchers into the field, discuss data needs and generally be informed about relevant work. The choice of meetings will be determined by geography and schedule; the most important ones appear to be ICAMDATA, ICPEAC and APiP for atomic and molecular data and PSI and PFMC for plasma mate-

rial interaction data, but many other meetings and workshops are appropriate venues at times. In this “other” category we note EGAS/ECAMP, the ADAS meetings, EFDA task force meetings, meetings on warm or hot dense matter and meetings devoted to fusion plasma modelling.

### **Other activities**

Since a few years the Department of Nuclear Applications has a programme on Collaborating Centres; a four-year agreement between the IAEA and another party for work of interest to the Agency. The subcommittee noted with appreciation the expected Collaborating Centre agreement with the Korea National Fusion Research Institute for their work on data evaluation and database development for A+M processes for fusion.

### **Conclusions**

In addition to all the specific recommendations there is the broad recommendation to the Unit to use its influence and its meetings to strengthen the community that is involved in data production and data evaluation for atomic, molecular and plasma-material interaction processes. We all recognize that these activities are not the most favoured in basic science, but they are very important for the development of fusion energy. The international Data Centres Network, broadly defined, needs the support and visibility that is brought by the A+M Data Unit of the IAEA.

## Appendix 1: List of Participants

**Dr James W. Davis**, University of Toronto, Institute for Aerospace Studies, Toronto, Canada.

**Dr Rémy Guirlet**, Association EURATOM-CEA, Département de Recherches sur la Fusion Contrôlée, Centre d'Etudes Nucleaires de Cadarache, Saint-Paul-lez-Durance, France.

**Dr Ratko K. Janev**, Macedonian Academy of Sciences, Skopje, Macedonia.

**Dr Yury V. Martynenko**, National Research Centre "Kurchatov Institute", Moscow, Russian Federation.

**Dr Igor V. Mazul**, D. V. Efremov Scientific Research Institute of Electrophysical Apparatus (NII-EFA), St Petersburg, Russian Federation.

**Dr Giuseppe Mazzitelli**, Associazione EURATOM-ENEA, Frascati Fusion Research Centre, Frascati, Rome, Italy.

**Dr Tomohide Nakano**, Japan Atomic Energy Agency (JAEA), Tokamak Experimental Group, Naka Fusion Institute, Naka Ibaraki, Japan.

**Dr Joseph Reader**, National Institute of Standards and Technology (NIST), Atomic Spectroscopy Group, Gaithersburg, MD, United States of America.

**Dr Joachim Roth**, Max Planck Institute for Plasma Physics (IPP), Garching, Germany.

**Dr Klaus-Dieter Zastrow**, EURATOM/CCFE Fusion Association, Culham Science Centre, Abingdon, Oxfordshire, United Kingdom.

**Dr Bastiaan J. Braams**, International Atomic Energy Agency, Atomic and Molecular Data Unit, Vienna International Centre, P.O. Box 100, A-1400 Vienna, Austria.

**Dr Hyun-Kyung Chung**, International Atomic Energy Agency, Atomic & Molecular Data Unit, Vienna International Centre, P.O. Box 100, A-1400 Vienna, Austria.

## Appendix 2: Agenda

**Thursday 26 April 2012**

**Meeting Room: A0531**

- 09:30 – 10:10 Welcome (R. Forrest, R. Kamendje, B. Braams, H.-K. Chung)
- 10:10 – 11:10 General report on activities, B. Braams
- 11:10 – 11:30 Break
- 11:30 – 12:30 Review of DCN, databases and the CM on data evaluation, H.-K. Chung
- 12:30 – 14:00 Lunch
- 14:00 – 15:30 Discussion: Data evaluation, establishment of standard library, related future meetings including a possible large A+M+PSI data meeting in 2013
- 15:30 – 16:00 Break
- 16:00 – 16:30 Code Centre Network and Code Comparison Workshops, H.-K. Chung
- 16:30 – 17:30 Discussion: Code library, code comparison, related activities
- 19:00 – Social dinner

**Friday 27 April**

**Meeting Room: A0531**

- 09:00 – 09:45 Review of CRPs, B. Braams
- 09:45 – 10:30 Discussion, plans for future CRPs
- 10:30 – 11:00 Break
- 11:00 – 11:30 Publications, S. Le Masurier and B. Braams
- 11:30 – 12:30 Other activities (XSAMS, other meetings, ICTP workshop), B. Braams
- 12:30 – 14:00 Lunch
- 14:00 – 15:30 Recommendations for any new projects, priorities for Unit activities, Subcommittee members
- 15:30 – 16:00 Break
- 16:00 – 17:30 Membership issues, other business, meeting conclusions, Subcommittee members

## Appendix 3: Activities of the Unit, April 2010 – March 2012

### A3.1. Data Centre Network, Databases and Data Evaluation

#### Web home and web access statistics

The web services and the databases of the A+M Data Unit are reached through the web address <http://www-amdis.iaea.org/>; it is organized in a manner similar to the Section's Nuclear Data Services page at <http://www-nds.iaea.org/>. At present (April 2012) both web pages are maintained on the same server, which since 2009 is a 64-bit Compaq with 2 quad-core Intel Xeon processors, 16 GB memory and 584 GB hard disk with RAID5. The system runs Redhat Enterprise Linux. A server migration is planned for later in 2012 and after that migration the A+M Data Unit will have its own server separate from the one that hosts the Nuclear Data Services web pages.

Access statistics display a steady growth since 2004 through today. In 2011 the most visited sections of our web pages are the ALADDIN numerical database, the hydrogen molecule data collection of U. Fantz and D. Wunderlich (2004), our general activity pages (publications, meetings, CRPs), and the new FLYCHK pages, all with 20K-40K accesses over the year. The GENIE search engine has about 8000 accesses and the AMBDAS bibliographical database about 3000. Since July 2011 we also obtain statistics from Google Analytics; these are resolved with respect to nature of the visit, unique visitors, new or returning visitors, visit duration and other parameters. According to Google Analytics the recent most visited pages below the main page belong to ALADDIN, GENIE, AMBDAS and FLYCHK in that order. It is seen that 44% of the visitors come via a search, 26% arrive by following a referral link (mainly from the www-nds page) and 30% are direct visitors.

#### ALADDIN numerical database

The full source list is here: <http://www-amdis.iaea.org/ALADDIN/datalist.php>. Evaluated or newly compiled data were added during the years 1980-2006. Recent new data from our CRPs include about 17600 entries for A+M data (half of them one dataset on radiative recombination) and about 6200 entries for Surface data. A consultancy by W. Eckstein provided an update of reflection and penetration data. New data were also obtained through a Technical Meeting on "Improving the Database for Physical and Chemical Sputtering".

We believe that ALADDIN is useful as a record of work done under the umbrella or near the umbrella of the A+M Data Unit, but the database is not serving as the trusted best supplier of A+M+PMI data for fusion. In future work we need to pay fresh attention to a review of the data quality and to new data compilations and evaluations. Also the interface can be improved.

#### AMBDAS bibliographical database

AMBDAS provides bibliographical data for articles on atomic, molecular and plasma-material interaction processes relevant to fusion. A selection criterion for including a reference in AMBDAS is that the article provides numerical data (in tabulated or graphical form) for a specific process. The AMBDAS content in the area of spectroscopy is obtained from National Institute of Standards and Technology (NIST) and follows their Atomic Spectra Database (ASD). For collision processes (A+M+PMI) we have not had new data since 2010 and the collision data in AMBDAS have not been updated. We wish to work with the DCN and specifically with the data centre at NFRI to renew the collisional component of AMBDAS. We also expect to work with NFRI to add numerical data available for the bibliographic records.

#### Database on dust particles in fusion devices

In connection with the CRP on Dust a pilot database on properties of dust particles was developed at IPP Garching (V. Rohde et al.). Parameters in the database characterize the shape, surface morphology and element composition of the particles and also their origin and the nature of the plasma campaign. At present this database operates at IPP, but it is intended to make it accessible to fusion users anywhere through our IAEA web site. Some more work is needed to agree on reproducible ways to do the image analysis for the classification and on management issues.

## **Knowledge base**

The wiki-style knowledge base at <http://www-amdis.iaea.org/w> was mainly developed in early 2010, but maintained through the present. The content comes largely from our INDC reports, APID volumes and presentations at meetings. Technical content is organized under main headings Data Needs, Data Sources, Data Exchange, Special Topics and (general) Fusion Research. The knowledge base is meant to serve fusion researchers who need information about A+M+PMI data and data producers who need to know more about applications and interests. These wiki pages are easily found in web search and they increase the visibility of our work. Development of the pages has remained entirely within the unit.

## **General database search engine GENIE**

GENIE, <http://www-amdis.iaea.org/GENIE/> provides a common query interface to 9 databases for radiative properties and 6 databases for electron impact cross sections or rate coefficients. Recent additions are the Spectr-W3 database for spectroscopy and Open-ADAS and Spectr-W3 for collisional data. The role of GENIE is being taken over at a more ambitious level by the Virtual Atomic and Molecular Data Centre (VAMDC), which provides not only a common query interface but also a common response format, plus discovery services and further tools. However, we think it valuable to maintain GENIE as a lightweight mechanism for convenient access to the included databases.

## **Data Centre Network**

The Data Centre Network (DCN) brings together data centres that have programmes on collection, dissemination, critical assessment and generation of data for atomic and molecular (A+M) processes, particle surface interaction (PSI) and plasma-material interaction (PMI) processes for fusion and other applications. Bulk material properties are included in the domain to the extent that they influence plasma-material interaction properties. Present and proposed new members are CFADC at Oak Ridge, the Chinese collaboration CRAAMD, the IAEA A+M Data Unit, data groups at JAEA, KAERI and Kurchatov, the Atomic and Molecular Processes Section at NIFS, the Atomic Spectra Group at NIST, the ADAS project, the Data Center for Plasma Properties at NFRI and the EIRENE group at FZ Jülich. Past members include the data group at ENEA, GAPHYOR in France and the “TRIM” effort at IPP Garching.

The 21st meeting of the DCN was held in September 2011. The meeting serves for general information exchange about activities by the centres and for discussion and planning. There were invited presentations and discussion on XSAMS, on the VAMDC project, and on coordinated activities for nuclear data evaluation.

In view of the success of VAMDC project, DCN agreed to start implementation of XSAMS for some data sets for fusion. Maintenance of bibliographical data for fusion is an area of concern for DCN, and members support continued compilation of such bibliographical data. DCN meeting participants are committed to data evaluation activities and they wish to collaborate on the collection and compilation of data sets and the development of guidelines for uncertainty assessment and evaluation.

At previous DCN meetings considerable time was spent on reassessing a list of priorities for compilation and evaluation of atomic, molecular and plasma-material interaction data for fusion. At this meeting DCN members decided that more input from the fusion plasma data user community is needed. The DCN and A+M data Unit will try to assemble this information. The review of the data priorities list is deferred to later meetings.

## **Meetings on data evaluation**

The A+M Data Unit is strongly encouraging new activities on data evaluation, with emphasis on data for atomic and molecular collision processes. A first Consultancy Meeting (CM) on Data Evaluation was held at NIFS in February 2012. A subsequent CM is scheduled for June 2012 and a larger Technical Meeting is to be held in Korea in September 2012 jointly organized with NFRI.

The meeting at NIFS, hosted by I. Murakami, brought together 14 participants from Korea, Japan and China to review current data evaluation activities and data evaluation methods and to make recommendations about the creation of a data evaluator's network and about a long-term project to develop an international standard data library for fusion relevant A+M+PMI data. At the meeting the modern

Uncertainty Approach towards measurement and evaluation was emphasized. This approach is laid out in documents VIM (Vocabulaire International de Métrologie, 2007) and GUM (Guide to the expression of Uncertainty in Measurement, 2008) and is adopted by the International Standards Organization (ISO) and many other international organizations including IAEA.

At the meeting at NIFS it was discussed how to develop a Data Evaluators Network (or a community of evaluators). Data Centres of the DCN should be in the network and may have an editorial or coordinating role. The network should actively involve senior experts (including retired scientists, who are often still active in evaluation) and younger scientists. The expected tasks of such a network would include:

- develop guidelines for evaluation of AM/PSI data;
- evaluate data according to the guidelines and update older evaluations;
- document evaluations for publication in technical journals;
- document expertise to train young generation;
- hold meetings to recruit and train new evaluators and expand the community;
- identify urgent data needs;
- review the status of evaluated data for fusion relevant applications;
- participate in editorial board meeting to recommend data for the standard library.

The meeting emphasized the importance of organizing data evaluations as a collaborative activity. The long term goal is an internationally agreed standard data library for A+M+PMI data for fusion applications. A roadmap towards this goal was sketched out as follows.

- Phase 1: Establishment of infrastructure for evaluated data library
  - IAEA A+M Unit: Development of databases to host the standard data library
  - Data Centres: Compilation of relevant data for evaluation
  - Data Centres and Evaluators: Establishment of data evaluators' network
  - Data Evaluators: Guidelines of evaluation methods
  - Data Producers: Guidelines of uncertainty estimates.
  - Data Users: Priority list of critical data needs
- Phase 2: Establishment of evaluated data library
  - IAEA: Establishment / maintenance of databases to host the evaluated data library
  - Data Centres: Coordination of data evaluators' network activities
  - Data Evaluators: Evaluation of data sets
  - Data Producers: Guidelines of scaling laws / fit expressions
  - Data Users: Development of data format compatible to applications
- Phase 3: Establishment and maintenance of standard data library
  - IAEA: Establishment / maintenance of databases to host the standard data library
  - Data Evaluators and Data Centres: Coordination of Technical Committees
  - Data Producers: Feedback on data sets (production of missing data, data improvement)
  - Data Users: Feedback on data sets

At the time of the IFRC subcommittee meeting (April 2012) this is all in an early stage. The next major event is the Joint IAEA-NFRI Technical Meeting on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion, to be held 4-7 September 2012 in Daejeon, Republic of Korea, in conjunction with the 8th International Symposium on Standard Reference Data (sponsored by the Korea Research Institute of Standards and Science, KRISS).

## A3.2. Code Centre Network and Code Comparison Workshops

### Code Centre Network

The International Code Centre Network of developers of atomic and molecular physics codes was originally established to help fusion scientists by making codes and their documentation available on-line and through a web interface. Participants in the network (codes, institute and responsible person) are:

- CCC & RCCC, Curtin University, Australia, I. Bray;
- CR Model, Kitasato University, Japan, F. Koike;
- MELDF\*-TCAM, QUAN, EIKON, CTMC, Universidad Autónoma de Madrid, Spain, I. Rabadan;
- CDW and VPN, University P. & M. Curie, France, Alain Dubois; Centro Atómico Bariloche, CNEA, Argentina, P.D. Fainstein;
- Molecular cross Sections, SI calculations, University of Bari, Italy, M. Capitelli;
- CR Models, Kurchatov Institute, Russian Federation, A. Kukushkin;
- ATOM, ATOM-AKM, GKU, Lebedev Institute, Russian Federation, L. Vainshtein;
- HYDKIN, Forschungszentrum Jülich, Germany, D. Reiter;
- MCHF, GRASP2K, FLYCHK, NOMAD, National Institute for Standards and Technology, USA, Yu. Ralchenko;
- DEGAS databases, Princeton Plasma Physics Laboratory, USA, D. Stotler;
- LANL Codes, Los Alamos National Laboratory, USA, J. Abdallah, Jr.;
- HULLAC code, ETHZ, Switzerland, M. Klapisch (new in 2010);
- SDTRIM-SP, IPP Greifswald, Germany, R. Schneider (new in 2010);
- AMD Services, International Atomic Energy Agency, H.-K. Chung.

Online calculation capabilities provided by the CCN include fast codes for electron impact excitation using the Average Approximation by J. Peek and codes for cross section calculations for collisions of bare nucleus with hydrogenic target by A. Dubois, J. P. Hansen and P. D. Fainstein. There are also codes to calculate effective ionization and recombination rates and associated population balance and power loss based on tabulated data obtained using the Los Alamos collisional radiative modelling codes. An interface is provided to the Los Alamos Atomic Physics Codes (Cowan codes) and to some data sets obtained using these codes. Most recently an interface to the FLYCHK code at NIST and tabulated output from FLYCHK for steady state conditions was added. The tabulated data provide charge state distributions and radiative power loss rates as a function of electron temperature and density for atoms from hydrogen up to gold ( $Z=79$ ), and coronal model rate coefficients for direct ionization, excitation-autoionization, radiative recombination, dielectronic recombination and radiative loss per charge state at coronal conditions.

The 2nd meeting of the network was held 27-28 September 2010 and at this meeting it was broadly agreed that the validation of code results is more important than on-line access to the code. Some codes are suitable for on-line use, but in many cases it is better to provide the data that has been generated by expert users. CCN will continue to make codes available through a web interface, but we do not view the online computing capabilities as the key to participation in CCN activities. Instead, the CCN will continue as a flexible network with a flexible and broader group of participants. The CCN web page should provide a database of recommended data and code capabilities, possibly following a decision tree structure. (The Numerical Algorithms Group library documents provide a model of such a decision tree.) Several ideas were proposed as future activities to help CCN members. One proposal is to organize focused meetings along the model of the series of NLTE (non-local thermodynamic equilibrium) kinetics code comparison workshops. The other proposal is to develop the CCN into a structured network that brings together code developers, code users and experimentalists for specific topics for fusion. The CCN meeting in 2010 already brought together code users and code developers and this was considered to be very useful.

### **Code comparison workshops**

The Unit cooperated in the organization of the 7th Non-local Thermodynamic Equilibrium (NLTE) code comparison workshop that was held 05-09 December 2011 at the K+K Maria Theresia Hotel in Vienna. The Agency provided partial support for 3 participants from eligible countries. Hyun Chung was a participant in each previous NLTE workshop back to 1996 and in 2011 she was the local organizer with co-organizers C. Bowen (CEA, France), R.W. Lee (LCLS, USA) and Yu. Ralchenko (NIST, USA). The purpose of the NLTE code comparison workshops is to bring together developers of codes for atomic kinetics in finite density plasmas and to perform detailed comparison of calculations on well-defined test cases. There were 20 participants from 18 institutes from 8 Member States and IAEA. Results were submitted from 19 codes for 5 broad test cases with more than 50 specific cases and these results were discussed in detail. There were also two topical speakers: S. Vinko (Oxford) on the creation and diagnosis of hot solid-density plasmas with an X-ray FEL and S. Bastiani (LULI) on X-ray and time resolved XUV-emission of laser-produced plasmas. The 5 broad test cases included Ne, Ar and W for a range of plasma densities and temperatures. Generally the interest is on high density plasma, but conditions relevant to magnetic fusion were included as well. These workshops lead to a summary publication.

The NLTE code comparison workshops are highly appreciated by the participating researchers and the plan developed to organize a similar code comparison workshop for computation of spectral line-shapes in plasmas (SLSP). Accordingly the First SLSP code comparison workshop was held 02-05 April 2012, also at the K+K Maria Theresia Hotel in Vienna with Hyun Chung as local organizer and E. Stambulchik (Weizmann Institute of Science, Israel) as the lead organizer. There were 22 participants from 9 countries; the Agency provided partial support to 7 participants from eligible countries. Participants submitted and discussed results from 19 codes on 15 test cases involving ion dynamics, broadening of Rydberg lines and Stark broadening due to electric and magnetic fields, and ranging in complexity from Lyman and Balmer lines in H-like systems to various lines in Ne-like Al. The meeting was very successful and it is planned to make it the first of series similar to NLTE.

### **Planned future CCN activities**

As discussed at the CCN meeting we intend to focus more on code results than on on-line availability of codes. We would like to make available results from the Flexible Atomic Code (FAC) by M. Gu (USA), from the ATOM code by L. Vainstein (Lebedev Institute, Russia) and perhaps also from the HULLAC code (M. Klapisch, USA). We also would like to initiate a database relevant to molecular dynamics modelling, working with S. Irle (Nagoya University) and others. The biennial schedule places the next CCN meeting in 2012 and we plan to devote that meeting to data evaluation activities, development of guidelines for assessment of uncertainties in theoretical data, and development of a prioritized list of data needs. We are interested in a possible code comparison workshop in the area of plasma-material interaction studies.

### **A3.3. Review of Coordinated Research Projects**

Over the years the Unit has started one new coordinated research project (CRP) in most years. A CRP normally runs for three research coordination meetings (RCM) spaced 18 months to 2 years apart. An overview of our CRP work is found on the web page <http://www-amdis.iaea.org/CRP/> from where there are links to each individual project. The CRPs that are active or about to start are these.

- 2007-2011: Data for Surface Composition Dynamics Relevant to Erosion Processes
- 2008-2012: Characterization of Size, Composition and Origins of Dust in Fusion Devices
- 2009-2013: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions
- 2010-2014: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV
- 2011-2015: Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma
- 2012-2016: Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials
- 2013-2017 (tentative): Plasma-material Interaction for Irradiated Tungsten and Tungsten Alloys

We discuss the CRPs individually.

### **2007-2011: Data for Surface Composition Dynamics Relevant to Erosion Processes**

This CRP is concerned with erosion, redeposition and material migration for mixed materials: Be, C, W. Research coordination meetings were held in Oct 2007, Mar 2009 and Sep 2010. The participants are:

- Alain Allouche, CNRS / Université de Provence, France
- Russell Doerner, University of California at San Diego, USA
- James Davis, University of Toronto, Canada
- Guangnan Luo, Chinese Academy of Sciences, China
- Rinad Zalavutdinov, Russian Academy of Sciences, Russia
- Yury Martynenko, RRC Kurchatov Institute, Russia
- Predrag Krstic, Oak Ridge National Laboratory, USA
- Karl Krieger, IPP Garching, Germany
- Kai Nordlund, University of Helsinki, Finland
- Daiji Kato, National Institute for Fusion Science, Japan

The group has done a great deal of work concerning mixed wall materials in fusion devices, as is reflected in publications by CRP participants. However, the subject does not lend itself well to contributions to a database such as ALADDIN. (In fact, one reason to start the wiki-style Knowledge base on our web pages is to accommodate the kind of information that is associated with this mixed materials CRP.) An attempt was made to assemble contributions for a joint journal article, but this was not successful. The output of the CRP will be the sequence of three INDC (yellow) meeting reports and the related conference contributions and journal publications by CRP participants. The INDC report for the 3rd RCM has not yet appeared.

### **2008-2012: Characterization of Size, Composition and Origins of Dust in Fusion Devices**

The formation of dust and the trapping of tritium in dust is a significant concern for ITER and it is a major issue for the licensing of ITER as a nuclear device. The ITER team must be able to verify in real time that the amount of dust in the device and the amount of tritium in the dust is within the licensing limits. The CRP on Dust in fusion devices was initiated in order to collect data for dust properties such as the distribution of particle size and composition and the origins in fusion machines. Research coordination meetings were held in Dec 2008, Jun 2010 and Dec 2011. The participants are:

- Christian Grisolia, CEA, France
- Volker Rohde, IPP Garching, Germany
- Joerg Winter, Bochum, Germany
- Carmine Castaldo, ENEA Frascati, Italy
- Naoko Ashikawa, NIFS, Japan
- Anna Widdowson, CCFE, UK
- Phil Sharpe and Paul Humrickhouse, INL, USA
- Charles Skinner, PPPL, USA
- Suk-Ho Hong, NFRI, Korea

In connection with this CRP the Garching group (led by V. Rohde) developed a dust database. Images have been made of 10s of thousands of dust particles from the AUG tokamak; they are classified by origin and, using automated image analysis software, classified by size and shape and many other parameters. At present (April 2012) the infrastructure for this database exists only at Garching, but a desired output of the CRP is to have this database and the associated analysis tools accessible for contributions from plasma experiments from around the world. The A+M Data Unit would desire to host the database then. A survey article based on contributions from all CRP participants is planned.

### **2009-2013: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions**

The purpose of this CRP is to generate data for processes including excitation, ionization, recombination and heavy particle collisions for atoms and molecules (hydrides) and their ions of Li, Be, B, C, N

and O. Research coordination meetings were held in Nov 2009 and May 2011; the final RCM is expected in Q1 2013. The participants are:

- Pierre Defrance, Université Catholique de Louvain, Louvain-la-Neuve, Belgium
- Igor Bray and Dmitry Fursa, Curtin University of Technology, Perth, Australia
- Ratko Janev, Macedonian Academy of Sciences and Arts, Skopje, Macedonia
- Luis Méndez, Universidad Autónoma de Madrid; Madrid, Spain
- James Brian Mitchell, University of Rennes I, Rennes, France
- Mitch Pindzola and Teck Lee, Auburn University, Alabama, USA
- Dave Schultz, Oak Ridge National Laboratory, Tennessee, USA
- Hidekazu Takagi, Kitasato University, Sagamihara, Japan
- Jianguo Wang and Ling Liu, IAPCM, Beijing, China
- Baoren Wei, Fudan University, Shanghai, China
- Mats Larsson and Asa Larson, Stockholm University, Sweden
- Ioan Schneider, Department of Physics, University of Le Havre, France
- Viorica Stancalie, INFLPR, Bucharest, Romania
- John Curry and Joseph Reader, NIST, USA

Discussions at the 2nd RCM identified some high priority items for the remainder of this CRP. In the area of heavy particle collisions they are cross sections for  $H^+ + N$ ,  $H + N^+$ ,  $H^+ + O$  and  $H + O^+$ . In the area of electron-molecule collisions the light element hydrides are the most important: LiH, BeH, BH, BeH<sub>2</sub>, BH<sub>2</sub> and possibly their ions. Data need to be assessed.

#### **2010-2014: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV**

Tungsten is the divertor material of choice for ITER and it is being used on several present experiments including JET and AUG. This CRP was established to generate experimental and calculated data for radiative and collisional atomic processes involving tungsten ions interacting with plasma from the source region in the edge into the plasma core. The first RCM was held in Dec 2010 and the second RCM is scheduled Aug 2012. The participants are:

- Rajesh Srivastava, Indian Institute of Technology at Roorkee, India
- Alfred Müller, Justus-Liebig-Universität Giessen, Germany
- Nobuyuki Nakamura, University of Electrocommunications, Tokyo, Japan
- Alexander Ryabtsev and Rimma Kildyarova, RAS Institute of Spectroscopy, Troitsk, Russia
- Wan-Ü Lydia Tchong-Brillet, LERMA, and Jean-François WYART, UPS, France
- Peter Beiersdorfer and Joel Clementson, Lawrence Livermore National Laboratory, USA
- Chenzhong Dong, Northwest Normal University, Lanzhou, China
- Fumihiro Koike, Kitasato University, Japan
- Malvina Trzhaskovskaya and Vladimir K. Nikulin, St Petersburg, Russia
- James Colgan, Los Alamos National Laboratory, USA
- Valeriy Lisitsa and Alexander Kukushkin, Kurchatov Institute, Moscow, Russia
- Nigel Badnell, University of Strathclyde, UK
- Yuri Ralchenko, National Institute of Standards and Technology, USA

There are still gaps and uncertainties in the basic data for tungsten. Key data needs identified at the first RCM: rate coefficients for electron impact ionization in a strongly ionizing regime, charge exchange cross sections for  $H + W^{q+}$  for any charge state and for H energy up to 1 MeV (for the ITER neutral beam), spectroscopic data for  $W^{1+}$  and  $W^{2+}$  associated with erosion of a tungsten wall, and VUV and EUV data quite broadly (many lines are still unidentified).

#### **2011-2015: Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma**

This CRP is concerned with collisional and radiative processes of H, H<sup>+</sup>, H, He, He<sup>+</sup>, He<sup>2+</sup>, He<sup>-</sup>, H<sub>2</sub>, H<sub>2</sub><sup>+</sup>, H<sub>3</sub><sup>+</sup>, HeH<sup>+</sup>, He<sub>2</sub><sup>+</sup> and their isotopic variants (H, D, T). The emphasis is on obtaining complete data sets that are resolved with respect to vibrational excited state of the molecules. The participants are:

- Roberto Celiberto and Mario Capitelli, Polytechnic of Bari, Italy

- Ursel Fantz and Dirk Wunderlich, MPI for Plasma Physics, Garching
- Christian Jungen, CNRS and Paris-Sud, and Ioan Schneider, Le Havre
- Viatcheslav Kokoouline and Talat Rahman, University of Central Florida
- Predrag Krstic, Oak Ridge National Laboratory
- Xinwen Ma, Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou
- Ousmanou Motapon, University of Douala, Cameroon
- Ann E. Orel, University of California at Davis
- Detlev Reiter, Forschungszentrum Jülich
- Keiji Sawada, Shinshu University, Japan
- Xavier Urbain and Pierre Defrance, Catholic University of Louvain (UCL, Belgium)
- Jung-Sik Yoon and Mi-Young Song, National Fusion Research Institute (NFRI), Korea

At the first RCM participants reviewed their work and work plans. There are many gaps still, both with respect to isotopic species and with respect to excitation state. For ITER modelling it is very much desired to have one trusted and recommended data collection for H and He and their molecules and ions.

### **2012-2016: Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials**

At their meeting in 2010 the IFRC subcommittee on A+M data recommended to the Unit to seek to start two new CRPs in the 2012-2013 biennium: one on plasma interaction with beryllium walls and one on plasma interaction with irradiated tungsten. In order to prepare the proposal for the Beryllium CRP a Consultancy Meeting was held in May 2011 with S. Brezinsek, D. Kato, R. Doerner and W. Jacob. The proposal was approved by CCRA in Aug 2011 and the first RCM is scheduled for Sep 2012. The confirmed participants and their projects are:

- R. Doerner and D. Nishijima, PISCES Laboratory, UCSD: "Research on Beryllium PMI using the PISCES facilities".
- D. Borodin with A. Kreter, A. Huber, S. Brezinsek and A. Kirschner, FZ Jülich: "Development of models for plasma interaction with Be surfaces on the basis of dedicated experiments".
- M. Probst and A. Mauracher, Innsbruck: "Quantum Chemical and Molecular Dynamics Simulations on the Interaction of Fusion-Relevant Atoms with Pure and Hydrogenated Beryllium Surfaces".
- S. Irlé and H. Nakamura, Nagoya: "Parameterization and Application of the Density-Functional Tight-Binding Method for Plasma-Wall Interactions on Be Surfaces".
- K. Nordlund and C. Björkas, University of Helsinki: "Molecular Dynamics Simulations of D and Plasma Impurity Interactions with Be-containing Fusion Reactor Materials".
- Ch. Linsmeier and W. Jacob, IPP Garching: "Beryllium-containing Plasma-facing Materials: Formation, Erosion, Hydrogen Retention and Release".

It is desired to have CCFE and ITER represented in the CRP as well, either as a participant or through another arrangement if formal participation runs up against legal obstacles.

The CRP is concerned with physical and chemical sputtering and trapping and transport of hydrogen (H,D,T) for beryllium-based surfaces. The CRP will emphasize data for the relevant mixed materials, especially Be-(H,D,T,He), Be-C, Be-N, Be-O. The most important projectiles are H, D, T, He, Be, C, N, O, Ne and Ar.

### **Option for 2013-2017: Plasma-material Interaction for Irradiated Tungsten and Tungsten Alloys**

This CRP is in the Programme and Budget to start in 2013 with the overall objective to enhance the knowledge base on interaction of H and He in plasma with tungsten-based plasma-facing materials in the nuclear environment of a fusion reactor. The most important issue is how tritium retention and tritium removal will be influenced by radiation damage and alloy formation. The CRP must include study of the effects of irradiation on surface microstructure. It is intended to use the PSI meeting and the Hydrogen satellite meeting, in May 2012, to inventorize active work and then to prepare a proposal for CCRA near the end of 2012.

### A3.4. Publications

A discussion on the future of Atomic and Plasma-Material Interaction Data for Fusion (APID) was introduced by Ms Sophy LeMasurier of the Publishing Section. APID volumes 1-6 were published as informal supplementary issues to the journal Nuclear Fusion. With Volume 7A (1998) they became detached and were issued as books in their own right. Recent issues have received some cosmetic treatment to make them look more journal-like, but it has been impossible to apply real and useful journal features to the publications. (The articles are not indexed in the usual services.)

The present status of APID is not acceptable. Options for discussion:

1. Launch a new journal. This looks too resource-heavy, not warranted by the publication frequency of APID.
2. Seek to re-establish APIDs as special issues of Nuclear Fusion. A Nuclear Fusion Board of Editors decision would be made on a case-by-case basis. Nuclear Fusion guards its citation performance and that will be a criterion for acceptance as a special issue. In general NF Special Issues are limited and are invited on the basis of journal development and reader interest. There would be a tough peer review. All-in-all this option does not appear to offer a stable platform to replace APID.
3. Publish in the open access IOP "Journal of Physics: Conference Series". This is the proposed solution to be discussed further.

The Institute of Physics Journal of Physics: Conference Series (JPCS) is searchable and archival journal platform. The presentation follows IOPs house style. Articles receive DOIs, they have an HTML abstract, hyperlinked references, citation info, and papers are properly indexed. It would be possible to create links from and to Nuclear Fusion for cross-promotion to the NF community. Publication is fast, inexpensive (~40 € per paper plus any printing) and Open Access. We can create a print run in our style and the solution appears to meet provisions of IAEA publishing and dissemination policy (IAEA identity; copies to Member States; pdfs on [iaea.org](http://iaea.org)).

Some requirements and challenges must be recognized. JPCS imposes a peer review burden on the conference organizers, so on the CRP Scientific Secretary in our case. Authors must follow the JPCS templates (LaTeX or MSWord) to the letter. The publication will not appear in the IAEA online catalog. For copyright reasons it is suggested that each paper incorporate an appropriate acknowledgement to IAEA.

### A3.5. Other Activities of the Unit

#### Development of XML Schema for Atoms, Molecules and Solids (XSAMS)

XSAMS version 0.1, the first public version, was released in Sep 2009 immediately after the Data Centre Network meeting that year, following a development path that started at the DCN meeting in 2003. In Summer 2010 the Virtual Atomic and Molecular Data Centre (VAMDC) decided to adopt XSAMS for their databases. This meant implementations on about 25 different databases mainly oriented towards astrophysics. It also meant that problems were identified and developments and modifications to XSAMS were made for the needs of VAMDC. A CM on XSAMS was held at IAEA in Nov 2010 where the main topics were treatment of line shapes and molecular spectroscopy. Another CM on XSAMS took place at NIST in Oct 2011 primarily to review the developments in the VAMDC XSAMS and for outreach to database developers in the USA. In Feb 2012 the VAMDC held its annual meeting in Vienna and a CM was held on XSAMS during that meeting. It was agreed to adopt VAMDC XSAMS as International XSAMS version 1.0, subject to some fine-tuning by VAMDC before their next release in Summer 2012.

The current status of XSAMS is that it is in active use with about 25 implementations in connection with VAMDC, which also offers an extensive infrastructure for data discovery and data access via XSAMS. There is still a lack of user tools and user (plasma or astrophysicist) experience; the experience belongs to the database developers.

## **Joint ICTP-IAEA Workshop on Fusion Plasma Modelling Using Atomic and Molecular Data**

The Unit has organized workshops at ICTP under a title similar to the one above in 2003 (one week), 2006 and 2009 (2 weeks), and also a workshop in Birla, India, in 2008. We obtained support again for a one-week workshop at ICTP that was held 23-27 Jan 2012. Lecturers and their topics were:

- Detlev Reiter: Edge Plasma Modelling
- Kai Nordlund: Molecular Dynamics Modelling for Plasma-wall Interaction
- Yuri Ralchenko: Atomic Collisions and Spectroscopy
- Hyun-Kyung Chung: Collisional-radiative Modelling
- Kaoru Ohya: Impurity Transport Modelling and Plasma-wall Interaction
- Alain Allouche: DFT Modelling of Fusion Materials Exposed to Plasma
- Paolo Giannozzi: Quantum Simulations of Materials Using Quantum ESPRESSO
- Beta Ziaja-Motyka: Modelling of Warm Dense Matter
- Mourad Telmini: Electron-molecule Collisions
- Yaming Zou, Roger Hutton, Joel Clementson: EBIT Experiments

The first four speakers carried the main load with 2 or 3 lectures each. The workshop was addressed to young researchers in fusion energy. Lecturers described experimental and (mainly) computational methods by which one obtains atomic, molecular and plasma-material interaction data for use in plasma modelling. There were 20 further participants that each presented a poster and a 5-minute introduction to their poster and they much appreciated the workshop.

Some conclusions are offered for future such events. ICTP offers an excellent environment. The contact between plasma modellers, atomic and molecular physicists and materials modellers is valuable. A future workshop can have a more advanced nature than the one that was held in 2012; the ICTP is very willing to host advanced events. We expect to make an effort each year to obtain a slot for an event at ICTP and to emphasize the scientific workshop aspect.

### **Meetings held during Jan 2010 – Apr 2012**

- CM on XML Schema for Atomic and Molecular Data (24-26 Mar 2010, NIFS)
- TM of IFRC Subcommittee on A+M Data for Fusion Research (27-28 Apr 2010)
- 2nd RCM of CRP on Dust in Fusion Devices (21-23 Jun 2010)
- 3rd RCM of CRP on Surface Composition Dynamics (13-15 Sep 2010)
- TM of the International Code Centres Network (27-28 Sep 2010)
- Cooperate in TM on Analysis of ITER M&T (23-25 Nov 2010, Monaco)
- CM on XML Schema for Atomic and Molecular Data (17-19 Nov 2010)
- 1st RCM of CRP on Tungsten from 1 eV to 20 keV (13-15 Dec 2010)
- 2nd RCM of CRP on Light Elements in Edge and Divertor (23-25 May 2011)
- CM on Erosion and Tritium Retention in Beryllium PMI (30-31 May 2011)
- 1st RCM of CRP on State-Resolved Data for H and He (10-12 Aug 2011)
- TM of A+M/PMI Data Centres Network (7-9 Sep 2011)
- CM on XML Schema for Atomic and Molecular Data (3-5 Oct 2011, NIST)
- 3rd RCM of CRP on Dust in Fusion Devices (30 Nov – 02 Dec 2011)
- Cooperate in 7th NLTE Code Comparison Workshop (5-9 Dec 2011)
- TM on Improving the Database for Physical and Chemical Sputtering (12-13 Dec 2011)
- TM on Ab Initio-Based Methods for Plasma-Material Interaction (14-15 Dec 2011)
- ICTP-IAEA Workshop on Fusion Plasma Modelling (23-27 Jan 2012, Trieste)
- CM on Procedures for Evaluation of A+M+PMI Data for Fusion (7-9 Feb 2012, NIFS)
- CM on XML Schema for Atoms, Molecules and Solids (20-22 Feb 2012)
- Cooperate in SLSP Code Comparison Workshop (2-5 Apr 2012, Vienna)
- TM of IFRC Subcommittee on A+M Data for Fusion Research (26-27 Apr 2012)

### **Meetings attended during Jan 2010 – Apr 2012**

- EFDA SEWGs on dust and tritium removal, 8–11 Jun 2010, Garching (BJB)
- 8th IC on Dissociative Recombination, 16-20 Aug 2010, Tahoe City (BJB)

- 7th ICAMDATA, 21-24 Sep 2010, Vilnius, Lithuania (BJB + HKC)
- ADAS Workshop, 3-6 Oct 2010, Armagh, UK (BJB)
- 14th IC on RPHDM, 4-8 Oct 2010, Marbella, Spain (HKC)
- Annual Meeting of EU PWI TF, 3-5 Nov 2010, Vienna (BJB + HKC)
- EFDA SEWGs of PWI TF, 31 Jan – 2 Feb 2011, Tervaniemi, Finland (HKC)
- Annual meeting of the VAMDC, 28-31 Mar 2011, Cambridge, UK (BJB)
- 13th International Workshop on PFMC, 9-13 May 2011, Rosenheim (BJB)
- 6th International Workshop on Warm Dense Matter, 05-09 June, Pacific Grove, CA (HKC)
- 17th APiP, 19-22 Jul 2011, Belfast, UK (BJB)
- 7th IC on Inertial Fusion Sciences and Applications, 12-16 Sep 2011, Bordeaux Lac (HKC)
- ADAS Workshop, 6-8 Oct 2011, Auburn (BJB)
- Annual Meeting of EU PWI TF, 28-29 Nov 2011, Bratislava (HKC)



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