

# INDC International Nuclear Data Committee

Summary Report of  
IAEA Technical Meeting

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

Prepared by  
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IAEA Headquarters, Vienna, Austria  
20-21 April 2006

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**Abstract**

The 15<sup>th</sup> Meeting of the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council was held on 20-21 April 2006, at the IAEA Headquarters in Vienna, Austria. Work of the Atomic and Molecular Data Unit for the period 2004-2006 was reviewed, and recommendations were made for the 2008-2009 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 June 2004 – March 2006, are also included.

February 2007



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## EXECUTIVE SUMMARY

Prepared by N.J. Peacock

The IFRC Subcommittee on Atomic and Molecular Data for Fusion held their biennial meeting at the IAEA Headquarters in Vienna on 20<sup>th</sup>-21<sup>st</sup> April 2006. Twelve members of the Subcommittee were in attendance, namely, J. Roth (IPP), T. Kato (NIFS), R. Janev (Macedonian Academy of Sciences), N.J. Peacock (UKAEA), M. Crisp (DoE), W.P. West (GA), H. Kubo (JAERI), R. Guirlet (CEA), Yu.V. Martynenko (Kurchatov Institute) and new members G. Mazzitelli (ENEA), I. Mazul (Efremov Institute) and J. Davis (University of Toronto). The additional membership reflects the current fusion requirements for data on plasma-facing materials and plasma-surface interactions.

The A&M Data Unit was represented by Dr. A. L. Nichols (Section Head, Division of Physical and Chemical Sciences, NAPC) and Dr. R.E.H. Clark (Head of the A&M Data Unit).

The purpose of the Meeting was to review the activities of the A&M Data Unit of the IAEA since the last Subcommittee Meeting in June 2004, and to make recommendations to the Office of the Director General concerning the work of the Unit over the next two-year budget cycle.

Dr. A.L. Nichols opened the meeting by welcoming the Committee members. He endorsed the work of the Subcommittee and emphasised the importance of their recommendations to the work programme of the A&M Data Unit with respect to their advisory role to the IFRC. He noted the unfolding needs for A&M data to support the development and operation of the large, internationally managed, fusion device, ITER, at Cadarache, and noted that requirements for IFMIF (International Fusion Materials Irradiation Facility) have already triggered requests for nuclear data involving light elements.

The agenda as distributed before the meeting was accepted.

The Subcommittee received from Dr Clark an overall presentation of the activities of the A&M Data Unit over the period 2004-2006 covering the recommendations of the previous Subcommittee meeting. An itemized summary was given of the progress on the A&M database, the Data Centre Network activities and related computing issues. Summaries of current and planned Co-ordinated Research Projects (CRPs) were highlighted while other Unit activities including a new ICTP Workshop were discussed. The status of interface codes on the network and Unit publications was brought up-to-date.

Data Centre Network (DCN) developments involving co-ordination between eleven international centres, the A&M Data Base, related computer issues and interactions with other data base users were reviewed in detail by D Humbert. A practical demonstration of the ALADDIN system was also given to the Subcommittee.

The Subcommittee recognises the excellent efforts of the Unit over the past two years. Of particular note are the advances in the latest ALADDIN interface access to the Database. Substantial amounts of new A&M data have been entered into the ALADDIN numerical data base. The further possibility of access to the data base associated with ADAS system developed by H P Summers is to be encouraged. A substantial database also exists for plasma-surface interactions. An electronic link to several members of the Data Centre Network (DCN) through a numerical search engine GENIE (GENeral Internet research

Engine) has been established through <http://www-amdis.iaea.org/GENIE>. The Subcommittee noted with gratification the continued progress through consultancies on XML (Extensible Mark-up Language), an appropriate software for comparison of data from disparate data bases. The purpose of the A&M Data Unit in this role is to encourage and coordinate the dozen or so national Data Centres to make their data mutually accessible and comprehensible.

The overall size of the A&M database has grown by approximately a factor of 60% over the past two-year period and has a high level of access by users. The previous recommendation by the Subcommittee that the concept of a code network maintained by the code authors with approved A&M data input and available through the internet has been followed up. The Unit is to be commended for these advances, and this direction should continue to be a priority for the Unit's activities.

In general the Subcommittee finds that the Unit has made extremely effective use of consultancies to further the work of the Unit, particularly on the development of XML standards, the new ALADDIN interface, the availability of computer codes through the Interface and advice on a number of data issues.

Hopefully, the present *ad hoc* increase in funding enjoyed by the Unit for Consultants' Meetings will be made available throughout the next two-year period. However, Dr Nichols remarked that, in general, the priority of the IAEA is to redirect increased funding towards "safeguards" rather than "power and energy applications".

The Subcommittee noted with satisfaction that the Unit has three current CRPs already in progress ("Atomic & molecular data for diagnostics": "Data for molecular processes in edge plasmas"; "Tritium inventory in fusion reactors"), with a fourth ("Data base for edge modelling emphasising hydrocarbon processes") to start this year. A minimum of three CRPs has been a strong recommendation as the core projects of the Unit at previous meetings of the Subcommittee. Further topics recommended for inclusion in the A&M Data Unit future programme include: "Data for surface composition dynamics relevant to erosion processes" (2005); "Data on sticking coefficients for tritium and the role of dust in tritium retention" (2006), essentially an extension of the earlier CRP on tritium inventory; "Atomic data for high Z element impurities in fusion reactors"; "Data for surface composition dynamics relevant to erosion processes"; diagnostics methods for measuring isotope ratios in burning plasmas (H, He, D, T, Be, Li); and "Materials for fusion plasma facing components including liquid walls". The Subcommittee is cognisant of the growing importance of the physics of burning plasmas and the need to involve experts from the ITER design team whenever appropriate.

The decennial IAEA Technical Meeting on Atomic and Plasma-Material Interaction Data for Fusion Science and Technology took place at Jülich in October 2002. The reviews and recommendations from the specialists attending this meeting have an important bearing on the views of the Subcommittee. Summarised in INDC(NDS)-445, October 2003, the meeting considered three main areas of fusion interest where A&M data are required. The first such area is the traditional topic of core physics with the usual features of interest such as transport, enhanced-confinement modes, atomic beam emission and heating, radiation loss and diagnostics, but with an added interest in burning plasmas. The second topic is edge physics - the importance of molecular processes involving hydrocarbons was emphasised in different divertor scenarios usually with low edge temperatures of  $T_e \leq 5$  eV. The third topic is plasma-material interactions (PMI) where the choices of neutron irradiated wall and divertor materials, optimised for sputtering and for erosion/re-deposition mechanisms, were



highlighted as problems requiring further data. The tritium inventory is an important consequence of the choice of wall materials. Most of the new CRPs suggested to the A&M Data Unit address one or other of these new areas. Furthermore, the need to strengthen the collective expertise of the Subcommittee in PMI has now been acted upon.

The Subcommittee endorses the continued publication of the (APID) journal series *Atomic and Plasma-Material Interaction Data for Fusion* with Vol. 13 and 14 in preparation. Furthermore, the Subcommittee agrees that following publication of the forthcoming Volume 65 of the *International Bulletin on Atomic and Molecular Data for Fusion*, although future volumes should be produced on an annual basis rather than biannually. The addition of a newsletter style section to publicise new features of the electronic databases should be included. At least three “Summary Reports” have been produced as INDC(NDS) yellow documents.

The above activities are seen to be the core priorities of the A+M Data Unit.

Apart from these core activities, the Subcommittee recognises the invaluable catalytic effect of the A+M database on international collaboration for fusion. A good example is the training workshop on “Atomic and Molecular Data for Fusion Research” to be held at the International Centre for Theoretical Physics (ICTP) in Trieste, Italy, over the two-week period from 28 August to 8 September 2006.

After careful review and discussion of all aspects of the Unit activities, the Subcommittee made a number of specific recommendations to the A&M Data Unit for the 2006-2008 budget cycle. These recommendations and summaries are:

On the subject of Co-ordinated Research Projects:

(i) In view of the responsiveness of CRPs to the increasing data needs for new plasma scenarios and new materials issues, the simultaneous organisation of four CRPs is endorsed, and this may need to be increased in the future.

(ii) Two CRPs on “Molecular processes in edge plasmas” and “Atomic and molecular data for fusion plasma diagnostics” will be completed on time in 2006 - two volumes of APID will be produced from these CRPs.

(iii) A new CRP on “Atomic and Molecular Data for Plasma Modelling” was initiated in 2005, and data priorities was reviewed at the first RCM in September 2005. The possibility of generating comprehensive databases to satisfy such needs was discussed. Several areas of significant CRP expertise were identified, and a work plan was formulated to generate data for support of fusion plasma modelling.

(iv) The CRP on “Tritium inventory in fusion reactors” was initiated in 2002, and will be extended with a final RCM in 2006. It is recommended that dusty plasmas and sticking coefficients for tritium will be included in the extension and that if needed additional expertise be added to the CRP for this purpose.

(v) The first RCM on “Atomic data for high Z element impurities in fusion reactors” was held in 2005 (there are also on-going studies in ITER). Some investigation of data reduction methods should be included in this CRP to make the data usable in a 2D modelling code.

(vi) Establish a new CRP in 2006 on “Data for surface composition dynamics relevant to erosion processes”. This CRP should include data collection of solid state diffusion of components of refractory metals and metal multi-layers of elements such as Be, B, C, Cu, and W.

(vii) Establish a new CRP in 2007 with the goal of characterising the size, composition and origin of dust in Tokomaks. This CRP should initially consider dust from a variety of elements such as C, W and Be, to be followed by determining the role of dust in the tritium inventory.

On the subject of various forms of Technical Meeting (TM/CM):

The Subcommittee recommends that,

(i) The A+M Data Unit holds a Consultants’ Meeting (CM) in 2006 on diagnostics methods for measuring isotope ratios in burning plasmas (H, He, D, T, Be and Li), possibly leading to a TM in 2007 on this topic.

(ii) A Technical Meeting (TM) on “Materials for fusion plasma facing components”, to be held in 2006, possibly leading to a CRP in 2007 on material properties, and may be including liquid walls.

(iii) The Subcommittee was impressed by the high technical standards and recommendations from the decennial IAEA Technical Meeting at Jülich (INDC(NDS)-445, author R. Clark, 2003). The list of excellent recommendations is an example of how well the IAEA is keeping abreast of current trends and data needs in fusion, and the appendices should be given close attention.

The Subcommittee endorses the efforts of the A+M Data Unit in co-hosting a follow-up Workshop/Summer School (2006 ICTP-IAEA) at Trieste on “Plasma-Wall Interactions”.

(vi) The ICAMDATA meetings are wide ranging and of interest to astrophysicists and fusion scientists alike. They are held on alternate years to the Data Centre Network (DCN) meetings (see below). The Subcommittee recommends active participation by the A&M Data Unit in these meetings accompanied by informal discussions between DCN representatives to discuss progress.

On the subject of Databases and the Data Centre Network (DCN):

(i) The Subcommittee was impressed by the considerable development of the ALADDIN numerical database system, and of the increasing effort by the Unit to adopt a variety of electronic interconnections among databases and codes. GENIE and DANSE are two web search engines which allow simultaneous retrieval of data from different web sites, and continue under development. GENIE is dedicated to numerical atomic data and DANSE to bibliographic atomic and molecular data. The Subcommittee strongly recommends continued development of these two important tools, especially for additional collision processes (e.g. atomic-ion collisions) in the databases and enlargement of the data Network (data from four out of fifteen DCN members are now available on line).

(ii) The Subcommittee members were heartened by the recent progress involving the successful access of the Los Alamos codes on atomic structure and cross section calculations

and the ion collision codes of Dubois and Hansen through Internet interfaces. The Subcommittee recommends continued efforts on similar projects.

(iii) The Subcommittee endorses a Technical Meeting (TM) on the investigation of the establishment of a code centre network that would follow the general form of the existing DCN. This new network should also compile a list of codes and their capabilities, as well as contact persons for these codes.

(iv) The issue of performing modelling calculations in the Unit was raised. It was affirmed that this is not an overall objective of the Unit - the Subcommittee endorsed the primary goal of the Unit in the establishment of databases, and not modelling calculations.

(v) The issue of formulating XML standards was raised - use of XML will increase over time and the Unit should remain involved in the development, but not attempt to play a major role.

On the subject of publications and publicity:

(i) Each A&M Subcommittee member should ensure that his/her Member State representative to the IFRC is familiar and up to date with the work of the Data Unit, and thus make A+M data needs made more visible and an increasingly important topic for the IAEA..

(ii) Member State representatives are reminded of the importance of and the funding for the national data base centres, without which much of the work of the IAEA Data Centre on evaluation and coordination of A+M data would be diminished.

On the subject of Staff:

Increasing data needs and the increasing networking of computers has led to requirements for large amounts of high quality data, which has placed increasing demands on the A+M Unit. It is strongly recommended that additional support from international experts in the areas of ITER performance and plasma-surface interaction physics be made available to the Unit through DCN and Consultants' Meetings (CM). All possibilities should be explored.

On the subject of Subcommittee business:

(i) The chairman welcomed the three new members to the Subcommittee viz. G. Mazzitelli (ENEA, replacing E Menapace), I. Mazul (Efremov Institute) and J. Davis (University of Toronto).

(ii) At the previous meeting of the Subcommittee in 2004, a recommendation was made that there should be at least one additional member added to the Subcommittee with expertise in the area of plasma-facing materials and possibly one other in the field of plasma-surface interaction physics. Accordingly, Professor Igor Mazul (Efremov Institute, St Petersburg) and Professor Jim Davis (University of Toronto) have been invited and accepted to serve on the Subcommittee. This brings increased experience on edge-related fusion problems and ITER design to the business of the Subcommittee.

(iii) The present strength (12 members) and composition of the Subcommittee was discussed, taking into account the established Terms of Reference as a Subcommittee of the IFRC. The present composition of the Subcommittee arising from changes in personnel through

resignations, retirements, co-options etc. was deemed satisfactory for the tasks to be faced in the immediate future.

(iv) The timing of the 2-day biennial meetings was discussed. From a budgetary point of view the earlier in the year the better, while most members favoured somewhat later. Accordingly the timing of late-April seemed a reasonable compromise, providing that sufficient notice of the schedule is sent to the membership.

(v) The Subcommittee recommends that the present composition of the Subcommittee be endorsed by the IFRC.

### Summary

The Subcommittee has recognised the efforts of the A+M Data Unit to address all of the recommendations from the previous meeting. The Unit has been remarkably effective in meeting the goals while operating with very limited staffing numbers.

Respectfully submitted on behalf of the Subcommittee,

Nicol J. Peacock  
Chairman

## 1. Introduction

The 15<sup>th</sup> Technical Meeting of the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council was held on 20-21 April 2006 at the Agency Headquarters in Vienna. The main objectives of the meeting were to review and assess the Agency activities in the area of atomic and molecular data and plasma-surface interaction data for fusion for the period June 2004 – March 2006, and to provide recommendations to the Agency regarding the A+M programme for the years 2008-2009.

The meeting was attended by twelve Subcommittee members (see [Appendix 1](#)). Dr. N. Peacock served as the chairman of the meeting. Dr. R. Clark, Head of the Atomic and Molecular (A+M) Data Unit of the IAEA served as the Scientific Secretary of the Meeting. Twelve members of the Subcommittee were in attendance, including J. Davis (University of Toronto), R. Guirlet (Euratom-CEA), J. Roth (IPP), G. Mazzitelli (ENEA), T. Kato (NIFS), H. Kubo (JAEA), R. Janev (Macedonian Academy of Sciences), Yu.V. Martynenko (Kurchatov Institute), I. Mazul (NIIIEFA), N.J. Peacock (UKAEA), M. Crisp (DoE) and W.P. West (GA). The A+M Data Unit was represented by Dr. A.L. Nichols (Head, Nuclear Data Section, NAPC), Dr. R.E.H. Clark (Head of the A&M Data Unit) and D. Humbert (A&M Data Unit).

## 2. Meeting Proceedings

Dr. A. Nichols opened the meeting by welcoming the Committee members. He strongly endorsed the work of the Subcommittee and emphasized the importance of their recommendations to the future work programme of the A+M Data Unit and of their advisory role to the IFRC. He noted the announcement of the site selection for ITER as an important event in fusion energy research, and anticipated the Subcommittee addressing issues related to ITER in their recommendations to the A+M Data Unit.

The agenda as distributed before the meeting was accepted (see [Appendix 2](#)).

The first item of business was the membership of the Subcommittee. Prof. Menapace, ENEA Italy, had retired since the previous meeting, and the Italian government had nominated Prof. G. Mazzitelli to serve on the Subcommittee in the future. Following the recommendation from the previous Subcommittee meeting, Prof. I. Mazul of Russia was nominated to join the Subcommittee to enhance the plasma-surface interaction expertise (full IFRC has endorsed his nomination). Prof. J. Davis had also been invited to join the Subcommittee to add expertise on co-deposition processes - this action came too late for full IFRC review and approval, although Prof. Davis was invited to attend the meeting as an observer with full membership expected before the next Subcommittee meeting. Profs. Mazzitelli, Mazul and Davis were welcomed by the Subcommittee. For the current membership of the DCN, see [Appendix 3](#).

During the morning session of the first day, the A+M Unit staff presented a report on their activities over the previous two-year period, including a review of the Data Centre Network (DCN) and the electronic databases. Each recommendation from the previous Subcommittee had been addressed through specific actions by the A+M Unit. Various issues involving the DCN were reviewed, including the increased possibilities of linking the databases through a common search engine.

The focus of the afternoon session was a review of Co-ordinated Research Projects (CRP), Technical Meetings (TM) and workshops. A review of current CRPs was presented, along

with the proposed dates for final results to be published in the journal *Atomic and Plasma-Material Interaction Data for Fusion*. Topics of highest priority for new CRPs were discussed in detail, with the Subcommittee making a number of specific recommendations. These recommendations appear in the executive summary of the Subcommittee.

During the morning session of the second day, data dissemination methods used by the A+M Unit were reviewed. The status of the main publications of the Unit was reviewed: *International Bulletin on Atomic and Molecular Data for Fusion* (the Bulletin) and the *Atomic and Plasma-material Interaction Data for Fusion* (the APID) journal. Both publications are up to date.

Substantial updates to the interfaces to the electronic databases had taken place over the past two years, and the current interfaces were demonstrated.

A report on the development of an XML (Extensible Mark-up Language) schema for A+M data was presented. There is substantial interest among the Data Centres on the development of a universal format for data transmission that is compatible with modern Internet capabilities.

The text of the A+M Unit report is attached as Appendix 4.

After receiving various presentations from the staff, the Subcommittee reviewed the status of the A+M Unit. The Subcommittee recognized the efforts of the Unit to address all of the recommendations from the previous meeting, and concluded that the Unit has been remarkably effective in meeting the goals while operating with restricted staffing numbers.

The final session of the meeting was devoted to formulating recommendations for the Unit and setting priorities for Unit activities. The results of this session are included in the next section.

### **3. Recommendations and Conclusions**

After reviewing the work of the A+M Unit over the past two years and discussing data needs for fusion research, the Subcommittee formulated the following statement with respect to the performance of the Unit and recommendations for the next two-year budget cycle (2008-2009):

The Subcommittee recognizes the excellent efforts of the Unit over the past two years. Of particular note are the advances in the latest version of the ALADDIN interface access to the database and the substantial possible addition of data access through the Open ADAS project. The numerical database currently contains 7657 entries for atomic and molecular processes, of which approximately 3000 entries were made in the past two-year period. A substantial database also exists for plasma-surface interaction. The APID series also represents significant data efforts.

The Subcommittee noted with gratification the continued progress through consultancies on XML (Extensible Mark-up Language) to produce appropriate software for data comparison from disparate databases. The role of the A+M Unit in this work is to encourage and coordinate the Data Centres to make their data mutually accessible and comprehensible. The Unit is to be commended for these advances, and it is recommended that these efforts continue in the future.

The Subcommittee finds that the Unit has made extremely effective use of consultancies to further the work of the Unit, particularly with respect to the development of XML standards, the new ALADDIN interface, the availability of computer codes through the Internet, and advice on a number of data issues. The Subcommittee hopes that significant funding for consultants will continue to be made available to the Unit in the next two-year period.

The Subcommittee's recommendations on CRPs from the previous meeting are brought up to date through the following observations:

The two recently completed CRPs (**Data for Molecular Processes in Edge Plasmas** and **Atomic and Molecular Data for Fusion Plasma Diagnostics**) have generated two new volumes of the APID journal.

The CRP on **Tritium inventory in fusion reactors** will conclude in 2006, with another APID volume to be issued.

A new CRP on **Atomic and Molecular Data for Plasma Modelling** held the first RCM in September 2005.

A new CRP on **Atomic data for high Z element impurities in fusion reactors** held the first RCM in November 2005.

A new CRP on **Data for surface composition dynamics relevant to erosion processes** will be initiated in 2006.

A new CRP should be initiated in 2007 with the goal of characterizing the size, composition and origin of dust in tokamaks. This CRP should consider dust from a variety of plasma-facing components – initially C, W and Be. Other materials used in some fusion devices should be considered, such as Mo, B and Ti. Dust may also come from other elements in the machine, such as RF antennas. Diagnostics of the dust is important, as well as the production and behaviour of dust in fusion devices. A follow-on could be the role of dust in the tritium inventory.

The Subcommittee recommended participants for a CM in 2006 on the changing core concentrations of hydrogen isotopes and light elements in burning plasmas (He, possibly Be from walls and other elements added for diagnostic purposes). Possible methods to be considered are charge exchange, diagnostic beam injection and ionic e-fluxes. An evaluation should be made of the relative merits of nuclear and atomic diagnostic techniques. Depending on the outcome of the CM, a TM may be proposed for 2007, possibly leading to a new CRP in 2008 or 2009.

The Subcommittee proposed that the Unit hold a TM in 2006 on materials for fusion plasma-facing components, with an emphasis on Be and Be-composites relevant to the JET ITER-like wall project, and the trapping of tritium. These discussions could lead to a CRP starting in 2008. Liquid materials, such as lithium, and other non-ITER materials could be included in that CRP, depending on the outcomes of the TM.

The Subcommittee recognizes the value of the A+M Data Unit's involvement in the ICAMDATA meeting to foster the development of XML and other data issues. This meeting allows collaboration among many users of A+M data, especially with the astrophysics community. These interactions have led to consultancies on XML development.

The Subcommittee noted with approval the continued use of workshops as a semi-permanent feature of the activities of the Unit.

The Unit is now fully stretched to undertake existing work. Any additional projects relating to ITER would require increased resources; IFMIF-related studies of materials would also require more resources. Virtually all plasma-material interactions will be affected by neutron exposure, and highly relevant projects needed for ITER and beyond would require significant additional resources.

A proposal was made for a TM (possibly in 2008) to examine techniques to calculate the molecular dynamics, including quantum surface effects, for sputtering or erosion by low temperature plasmas, such as in the ITER divertor regions. Experimental validation of results, particularly hydrocarbon chemistry, should also be included in such an initiative.

A further proposal was made for a TM to address hydrocarbon deposition and tritium retention on cold surfaces, for example in the shadow region of ITER - this behaviour is a significant concern for diagnostic mirrors.

A TM was recommended to discuss A+M data needs in the study of hydrocarbon influxes due to chemical erosion, sputtering etc. - the hydrocarbon concentration in the divertor region need to be known. This meeting would be a follow on to the CRP on A+M data for plasma modelling.

#### **4. Concluding Remarks**

Following a detailed presentation of the work of the A+M Unit over the past two-year period, the A+M Subcommittee of the IFRC recognized the high level of success of the Unit staff in achieving their goal of establishing databases for A+M and plasma-surface interaction data for fusion research. Following detailed discussions on data needs and priorities, the Subcommittee formulated an extensive list of recommendations for the Unit for the next two-year period. The Subcommittee also recognized that there are more recommendations than can be achieved by the Unit without additional resources. However, due to the progress with ITER, the Subcommittee notes the need for considerable new data in a number of areas. Hopefully, at some point, these needs for additional data will result in an increase of resources for the A+M Unit to achieve their re-defined objectives.



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**IAEA Technical Meeting:  
15<sup>th</sup> Meeting of the IFRC Subcommittee on Atomic and Molecular  
Data for Fusion**

20-21 April 2006, IAEA Headquarters, Vienna, Austria

**Agenda**

Thursday, April 20

**Meeting Room: C-07-VI**

09:30 - 10:00    Opening. Welcome to Subcommittee members  
Adoption of Agenda

Session 1: General Report on Activities since June 2004

10:00 - 11:00    General report on the activities, *R. Clark*

11:00 - 11:30    *Coffee break*

Session 2: Data Centre Network, Database Activities and Computer Issues

11:30 - 12:30    Review of DCN, databases and computing issues, *D. Humbert*

12:30 - 14:00    *Lunch*

Session 3: Review of Current and Planned CRPs

14:00 - 15:30    Results from recent CRPs, review of current CRPs and new CRPs to start in  
2006-2009 period, *R. Clark*

15:30 - 16:00    *Coffee break*

Session 4: Review of Additional Unit Activities

16:00 - 17:30    Review of activities, *R. Clark*

Friday, April 21

**Meeting Room: C-07-VI**

Session 5: Code Interfaces and Publications

09:00 - 10:30      Status of interfaces to codes on the Internet and Unit publications, *R. Clark and D. Humbert*

10:30 - 11:00      *Coffee break*

Session 6: Review of Unit Status

11:00 - 12:30      Review of status of A+M Unit, *Subcommittee members*

12:30 - 14:00      *Lunch*

Session 7: Recommendations for New Projects, Setting of Priorities

14:00 - 15:30      Recommendations for any new projects as well as setting priorities for Unit activities, *Subcommittee members*

15:30-16:00      *Coffee Break*

Session 8: Subcommittee Business and Formulation of Meeting Conclusions

16:00 - 17:30      Membership issues, other business, meeting conclusions, *Subcommittee members*

17:30 -              *Adjournment of Meeting*

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- CRAAMD, Jun, Yan
- ENEA, Mazzitelli, G.
- GAPHYOR, LPGP, Katsonis, K.
- IAEA, Atomic and Molecular Data Unit, Clark, R.E.H.
- JAEA, Kubo, H.
- KAERI, Rhee, Y.
- Kurchatov Institute, Martynenko, Yu.V.
- Max-Planck-Institut für Plasmaphysik, Eckstein, W.
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**IAEA Technical Meeting:  
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**Activities of the Atomic and Molecular Data Unit  
July 2004 - March 2006**

**I. Introduction**

The Atomic and Molecular (A+M) Data Unit has continued to make significant progress in supplying data relevant to fusion energy research during the two years since the last meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion. The Unit has followed the recommendations from the previous Subcommittee meeting. A detailed summary of the progress on those recommendations is given in Section II. Database activities, Data Center Network activities and computing issues are described in Section III. A summary of current and planned CRPs is given in Section IV, while other Unit activities (including a new ICTP Workshop) are summarized in Section V. Methods of data distribution, including interfaces to computer codes and publications, are described in Section VI. Finally, a summary of the work of the Unit for this time period is given in Section VII.

**II. Progress on Subcommittee Recommendations**

The A+M Subcommittee of the IFRC made a number of recommendations to the A+M Data Unit during its previous meeting. These recommendations have resulted in specific actions by the Unit. A detailed summary of each recommendation and the resulting progress on the part of the A+M Unit are given below.

1. *Recommendation:* The two CRPs on “Molecular processes in edge plasmas” and “Atomic and molecular data for fusion plasma diagnostics” should be concluded on time in 2004, and two volumes of *APID* to be produced from these CRPs.

*Progress:* All manuscripts for volumes 13 and 14 of *APID* have been prepared and assembled. All of these manuscripts have undergone review, and recommended improvements have been completed by the authors. Both volumes are now undergoing final editing within the IAEA, and should be published in the near future. Data from participants are undergoing evaluation for inclusion in the ALADDIN numerical database.

2. *Recommendation:* The CRP on “Tritium inventory in fusion reactors” (initiated in 2002) will be extended, with a final RCM to be held in 2006. It is recommended that dusty plasmas and sticking coefficients for tritium will be included in the extension and that if needed additional expertise be added to the CRP for this purpose.

*Progress:* The CRP on tritium inventory has been extended and will hold a final RCM in September 2006. However, the introduction of new topics has proven to be problematic,

and the current intention is to include at least some of the outstanding dust issues in the new CRP on erosion processes (starts in 2006).

3. *Recommendation:* Establish a new CRP in 2005 on “Atomic data for high-Z element impurities in fusion reactors” - included some investigation of data reduction methods to make the data usable in a 2D modelling code. There are on-going studies in ITER.

*Progress:* A Technical Meeting to formulate the new CRP was held in 2005, and the first RCM was held in November 2005. During the RCM, the current status of data for heavy elements was reviewed. Capabilities of the CRP participants were reviewed. A detailed work plan for the first period of the CRP was formulated.

4. *Recommendation:* Establish a new CRP in 2006 on “Data for surface composition dynamics relevant to erosion processes”.

*Progress:* The new CRP will be formulated during 2006, with the first RCM planned for November 2006.

5. *Recommendation:* Hold a CM in 2005 on diagnostics methods for measuring isotope ratios in burning plasmas (H, He, D, T, Be, Li), possibly leading to a TM on this topic in 2007.

*Progress:* Plan to hold a CM in 2006 in order to generate current ideas for the formulation of the new CRP. The new CRP is included in the 2007 Budget.

6. *Recommendation:* Materials for fusion plasma-facing components - TM to be held in 2006, possibly leading to a CRP 2007, on material properties (may be include liquid walls).

*Progress:* A TM will be held later in 2006. However, there is no possibility of initiating another CRP for the Unit in 2007 - may be possible in 2008, depending on budget constraints.

7. *Recommendation:* The committee were impressed by the increasing effort by the Unit to use a variety of electronic interconnections among databases and codes. GENIE and DANSE are two web-search engines which allow simultaneous retrieval of data from different web sites, and are under development. GENIE is dedicated to numerical atomic data and DANSE to bibliographic atomic and molecular data. The Subcommittee strongly recommends continued development of these two important tools, especially for the additional processes (atomic-ion collisions) and databases to the searches (four out of fifteen DCN members now available).

*Progress:* A+M Unit staff have continued to develop the search engines, with the addition of more databases to the search list. Work has been underway to prepare a uniform designation of processes among data centres. The Unit has worked with key consultants to prepare a list of processes and is working on methods of implementation in the Data Centre Network. Work on the XML standard is also relevant to this issue (see item 12 below).

8. *Recommendation:* The subcommittee were heartened by the recent progress in achieving successful access to the Los Alamos codes on atomic structure and cross-section calculations, and the ion collision codes of Dubois and Hansen through Internet interfaces. The Subcommittee recommends continued efforts on similar projects.

*Progress:* Collaboration on these projects has continued. More features have been added to both interfaces. The Los Alamos codes now have the possibility to calculate configuration-average quantities as well as data for individual shells. Extensive error checking has been added to the heavy-particle interface. In addition, cross-section calculations for excitation from heavy-particle collisions will be added in the near future through collaboration with Dubois and Fainstein.

9. *Recommendation:* The Subcommittee endorses a TM on the investigation of the establishment of a code centre network. It is recommended that this new network follow the general form of the existing DCN, and also compile a list of codes and their capabilities as well as contact persons for those codes.

*Progress:* A TM to discuss the possibility of a code centre network was held in May 2005. There was a strong feeling among the participants that this is a very worthwhile objective. Individual code centres are proposing methods of making their capabilities available for the fusion community. In some cases, the codes will be accessible through an on-line interface, possibly with user registration required. In other cases, the codes will require expertise to carry out calculations; thus, expert centres have offered to run limited calculations for the required data if the number of such requests is reasonable. Each code centre is contributing information to be included in a web page on the A+M Unit home page, detailing the available capability and link to access each code centre.

10. *Recommendation:* The issue of undertaking modelling calculations in the Unit was raised. The Subcommittee affirmed that this is not in the overall Unit objectives, endorsing the goal of the Unit to establish databases, but not to carry out modelling calculations.

*Progress:* The Unit continues to emphasise the establishment of databases, and not to provide modelling capabilities. In connection with this philosophy, there has been considerable discussion with the ADAS project (mainly with H. Summers) on the possibility of making ADAS data, but not modelling capabilities, accessible through a web interface. A successful agreement has been reached - the ADAS project is working on creating an "open ADAS" interface for this purpose. Such an interface would be jointly developed and would reside in final form on the A+M Unit server. One hoped is for this system to be linked to the GENIE search engine to allow access to cross-section data from the ADAS project and for comparison with other databases.

11. *Recommendation:* The issue of formulating XML standards was raised. The Subcommittee felt that the use of XML will increase over time - the Unit should stay involved in the development, but should not attempt to play a major role.

*Progress:* The A+M Unit hosted several consultants on XML development. This issue was also raised in the last DCN meeting and endorsed as a desirable method for data exchange. There is a proposal for a panel discussion at the ICAMDATA meeting in 2006.

### **III. Data and Computing Issues**

The Unit server has remained stable during the two-year period (2004-2006). For purposes of uniformity and security, all Section servers are now administered through the Systems Development Unit of the Nuclear Data Section. This arrangement has worked very well, allowing Unit staff to free themselves from most systems administrative details. In addition, when the Section introduces new computer systems, the Unit is able to make use of these additional resources. With the Section now adding new 64-bit computers to their facilities,

this will result in more extensive resources being made available to run (for example) codes to calculate heavy-particle collisions.

The Data Centre Network met in 2005. During the course of the meeting an update was made to the list of priorities among the Data Centres. The updated list is available on the A+M Unit homepage. As mentioned previously, the topic of formulating XML standard formats for A+M data was raised. There was general acceptance that this is the proper method to use for data exchange, and that the development of standards should proceed. This work has progressed through several consultants, as discussed in more detail below.

Work continues on the ALADDIN numerical database system. A new, more flexible interface is now in its testing stage. Substantial amounts of new data have been entered into the databases.

#### **IV. Co-ordinated Research Projects (CRPs)**

Two CRPs ended in 2004, while two new CRPs were initiated in 2005 and another will be initiated in 2006.

The CRP “Data for Molecular Processes in Edge Plasmas” was extended for an additional year, and held its final RCM in 2004. Results from the CRP have been submitted as a new issue of the APID journal.

The CRP “Atomic and Molecular Data for Fusion Plasma Diagnostics” was also extended for an additional year, and held its final RCM in 2004. Results from this CRP will constitute another issue of the APID.

The CRP on “Tritium Inventory in Fusion Reactors” held a second RCM in 2004. The final RCM of this CRP will be held in September 2006.

A new CRP on “Atomic and Molecular Data for Plasma Modelling” was initiated in 2005. A review of data priorities was undertaken at the first RCM in September 2005. The possibility of generating comprehensive databases to fill such needs was discussed. Several areas of significant CRO expertise were identified, and a work plan was formulated to generate data for support of fusion plasma modelling.

A second new CRP on “Atomic Data for Heavy Element Impurities in Fusion Reactors” was also initiated in 2005, with the first RCM held in November 2005. “Heavy element” was defined to be elements heavier than magnesium. Data for both collisional and radiative processes are needed for fusion research purposes, and a vital element of the resulting databases will be the inclusion of estimates of accuracy for all quantities. A detailed work plan for the first two years of the CRP was formulated at the RCM.

#### **V. Other Unit Activities**

A new workshop on “Atomic and Molecular Data for Fusion Research” will be held at the International Centre for Theoretical Physics (ICTP) in Trieste, Italy, over the two-week period from 28 August to 8 September 2006. This workshop will be an official ICTP workshop, rather than only hosted by ICTP (the difference is in the level and type of support offered by ICTP). The workshop is being advertised through the ICTP workshop webpage, with a deadline for application of 18 May 2006:

The A+M Unit sponsored a number of individual consultants during the past two-year period to provide advice on a number of data issues. Consultants have contributed to the XML development, the new interface to the ALADDIN numerical database, and the addition of new data to the various A+M databases.

## **VI. Data Distribution**

The main data distribution methods of the Unit are the on-line databases, publications and on-line access to computational tools.

The main publications of the Unit are the *International Bulletin on Atomic and Molecular Data for Fusion* (the Bulletin) and the *Atomic and Plasma-material Interaction Data for Fusion (APID)* journal. During the last two-year period these publications have continued with the latest issue, volume 65 of the Bulletin, and volume 13 and 14 of APID in their final stages of editing.

The new method of data distribution is the on-line interface to computational tools. An early version was the interface to the average approximation method for the calculation of electron impact excitation cross sections of atomic ions. This allowed a user to obtain an approximate cross section for transitions between non-relativistic electron configurations for a range of energies using an approximation to distorted wave theory (“average approximation” of Peek and Mann). That interface has averaged five to ten users per week over the past two years, indicating a continuing need for such a capability. Over the past two years, this capability has been extended significantly to two new areas.

Work has continued towards the improvement of on-line access to several computational tools. The interface to the Los Alamos codes continues to be developed with the addition of several new features. The heavy-element code has more comprehensive error-checking functions, and will have the capability to calculate excitation cross sections in the near future. There are also the beginnings of a code centre network, which will allow many more computational resources to be used widely in the fusion community.

## **VII. Summary**

Staff within the A+M Data Unit have continued to work towards the goal of establishing databases of atomic, molecular and plasma-material interaction data for fusion energy. The databases continue to expand in order to meet the needs of the fusion community. Appropriate meetings are held to determine the data priorities, and CRPs have been established to develop the data in the areas recommended. The Unit continues to explore the most efficient means of disseminating data as new tools become available.

The recommendations of the IFRC Subcommittee remain an invaluable tool in ensuring that the work of the Unit remains focused on the important A+M data needs and their priorities. As can be judged from this report, the A+M Data Unit follows these recommendations closely.

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