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Summary Report of an IAEA Technical Meeting

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

IAEA Headquarters, Vienna, Austria  
17–18 April 2008

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R.E.H. Clark  
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**Abstract**

The 16<sup>th</sup> meeting of the Subcommittee on Atomic and Molecular (A&M) Data for Fusion of the International Fusion Research Council was held on 17-18 April 2008, at the IAEA Headquarters in Vienna, Austria. Activities of the Atomic and Molecular Data Unit for the period 2006-2008 were reviewed, and recommendations were made for the 2010-2011 programme and budget cycle. The discussions, 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 2006 – March 2008, are also included. Of specific concern is the loss of three key personnel early in the upcoming budget cycle, including the A&M Data Unit Head (Dr. R.E.H. Clark), the Section Head for the Nuclear Data Section (Dr. A.L. Nichols), and the Data Unit coordinator for the computational facilities and databases (Dr. D. Humbert). Timely replacements of these key individuals are critical for the continued effective operation of the Atomic and Molecular Data Unit.

November 2008





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## EXECUTIVE SUMMARY

Prepared by W.P. West

The IFRC Subcommittee is very pleased with the progress made by the Atomic, Molecular, and Plasma-Material Interaction Data Unit over the previous two years. The Unit has done an excellent job of following the recommendations of the Subcommittee following the 2006 meeting. Coordinated Research Projects (CRPs) are the basic mechanism the Unit uses for the gathering, generation and documentation of new data needed by the fusion community. The execution of the recommended CRPs has exceeded expectations, given the budgetary and manpower constraints. The completed CRPs are as follows:

- Molecular processes in edge plasmas,
- Atomic and molecular data from plasma diagnostics.

The continuing CRPs are as follows:

- Atomic and molecular data for plasma modelling,
- Tritium inventory in fusion reactors,
- Atomic data for high Z element impurities in fusion reactors,
- Data for surface composition dynamics relevant to erosion processes.

Consultancy and Technical Meetings also contributed valuable information on the timely topics of materials for plasma-facing components and the measurement of isotopic fuel ratios in the core of a burning plasma.

Unit personnel also continued to take leadership roles in international organizations and meetings in the area of atomic and molecular databases. The activities provide excellent leverage for the small unit, resulting in improved access by fusion scientists to worldwide databases. Collaboration with other atomic and molecular data institutes around the world leverages efforts to modernize the database architecture using state-of-the-art eXtensible Markup Language. The Unit has also shown considerable originality in the creation of new pathways\ for fusion scientists to access the required data (e.g. the potential code centre network).

The Subcommittee has recommended three new CRPs to begin over the time period 2008-2011. A fourth topic is recommended if funding allows. The topics of these recommended CRPs are as follows:

- Data requirements for the characterization of size, composition and origins of dust in Tokamaks,
- Data on processes involving light atomic and molecular ions in recombining plasmas,
- Atomic data for tungsten in burning plasma devices,
- Data requirements for the diagnosis of the isotopes of hydrogen and light fusion products such as  $^4\text{He}$  and  $^3\text{He}$  in the core of a burning plasma.

The primary concern of the Subcommittee at this time is the continuity of the management of the existing and new CRPs during 2009 and early 2010 when the Unit's leadership and technical team will have to be completely replaced. The Subcommittee is encouraged by the awareness of the Division Director to the seriousness of this problem, and his apparent aggressiveness in finding highly qualified replacements in a timely fashion.





## 1. Introduction

The 16<sup>th</sup> Technical Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion was held on 17-18 April 2008 at the IAEA headquarters in Vienna, Austria. Twelve members of the Subcommittee were in attendance: J.W. Davis (University of Toronto), R. Guilet (Centre Etudes Nucleaires de Cadarache), J. Roth (Max Planck IPP, Garching), G. Mazzitelli (ENEA, Frascati), K. Ida (NIFS), T. Nakano (JAEA), R.K. Janev (Macedonian Academy of Sciences), Yu. Martynenko (Kurchatov Institute), I. Mazul (Efremov Institute), M. Crisp (Department of Energy, USA), W. West (General Atomics) and R.E.H. Clark (IAEA), as well as A.L. Nichols and D. Humbert from the IAEA Atomic and Nuclear Data Centre (see Appendix 1).

The purpose of the Subcommittee meetings is to review the activities of the A&M Data Unit over the two years prior to each meeting, and to make recommendations to the IFRC committee and the Office of the Director General on the direction the A&M data programme should take over the next two-year budget cycle to meet the pressing needs of the international fusion community.

The meeting was opened with an address from Dr. N. Ramamoorthy, Director of the Division of Physical and Chemical Sciences. He emphasized the importance of the biennial meeting of the Subcommittee to the budget planning process. He mentioned that there had been a recent external review of the entire Nuclear Data Section and that the Section had been found to be effectively and successfully carrying out the goal of providing A&M and nuclear data for a large variety of applications. He also expressed some concern for the near term efficacy of the A&M data work due to the imminent departure of the three key technical leaders, Drs Nichols, Clark and Humbert, in 2009. Dr. Ramamoorthy took the opportunity to note that 2008 marked the 50<sup>th</sup> year of international cooperation on fusion research, to be officially celebrated at the IAEA-sponsored Fusion Energy Conference to be held in Geneva, October 2008.

Before the first item of business, Dr. Mazzitelli presented a brief memorial for Mario Mattioli, a dedicated plasma spectroscopist who passed away unexpectedly. He had made many contributions to the diagnosis of fusion relevant plasmas using soft x-ray spectroscopy.

The first item of business was to elect an interim chair for the Subcommittee due to the absence of N. Peacock. W. West was elected to serve as chair for this meeting. The election was immediately followed by approval of the agenda as presented by R. Clark (see Appendix 2). A meeting with members of the Department of Nuclear Safety to discuss the safety related issues of dust accumulation in ITER was left open until a schedule could be finalized with M. El-Shanawany.

The agenda included the following presentations by unit staff:

1. General Report on Unit activities since April, 2006 by R. Clark
2. Review of the Data Centre Network (DCN) activities and computer issues by D. Humbert
3. Review of current and planned CRPs by R. Clark
4. Review of other unit activities by R. Clark
5. Discussion of web-based A&M code interfaces and publications by R. Clark and D. Humbert

The full report of the Data Unit activities is included as Appendix 3.

## 2. Review of 2006-2008 Activities

### 2.1 CRPs and Related Meetings

The Data Unit continues to respond to all recommendations of the Subcommittee, although progress is limited by manpower and other budgetary constraints. Over the past several years, budget increases have only occurred in line with the rate of inflation. Active Coordinated Research Projects

(CRPs), the basic tool used by the Unit for data compilations in response to Subcommittee requests are limited to no more than four per year. At the time of the meeting the Unit has three active CRPs, with an additional CRP proposed for 2008. Supporting these very productive CRPs requires a major fraction of the Unit's manpower. Over the past two years, two new volumes of the APID series (Vols 13 and 14) have been edited and printed. The APID series will soon be downloadable from the IAEA website, making access to these timely reports much easier. Comments from the Subcommittee concerning each CRP (and throughout Section 2) are included in square brackets [ ] at the end of each paragraph below.

The CRPs on "Molecular processes in edge plasmas" and "Atomic and molecular data for plasma diagnostics" were completed, and two APID volumes were produced. [*The Subcommittee commends the Data Unit on the completion of these APID volumes, and is pleased to learn that these data are being incorporated into the Aladdin database.*]

A new CRP on "Atomic and Molecular Data for Plasma Modelling" was initiated in 2005, and continued with a second RCM in June 2007. Data from this CRP are already being used in the B2 Eirene edge model, revealing that some scaling laws are inadequate. Good progress has continued with the generation of new data, and the final RCM is planned for 2008. [*The Subcommittee is very pleased that the work of this CRP is being actively used in the fusion modelling community even prior to release as an APID volume. The Unit is encouraged to complete and issue this volume of APID, incorporate these data into the appropriate databases in a timely fashion.*]

The CRP on "Tritium inventory in fusion reactors" (initiated in 2002) held the third and final RCM in 2006. A comprehensive review article has been submitted to *Fusion Science and Technology*. An additional task of including data on the retention by dust was not included in this work, but will be part of a new CRP on dust (see below). An APID on this CRP (Vol. 15) is anticipated in 2008. [*The submission of the first phase of this work as a review article in Fusion Science and Technology is indicative of the high importance of this topic. The Subcommittee recommends the speedy completion of the APID volume because of the importance of this topic to ITER.*]

The second RCM for the CRP on "Atomic data for high Z element impurities in fusion reactors" was held in 2007. Interesting comparisons between various theoretical methods are underway, and a final RCM is planned for 2009. [*Partly because of the issue of Tritium inventory, the choice of first wall material for fusion reactors is non-trivial. Data from this CRP are urgently needed to assess ongoing experiments and for incorporation into plasma models. The Subcommittee recommends the timely completion of the APID volume associated with this CRP.*]

A new CRP on "Data for surface composition dynamics relevant to erosion processes" was initiated in 2007, and the first RCM was held that same year. The CRP will include issues relevant to both theory and experiment. Recommendations from a Technical Meeting (TM) held in 2007 on "Materials for fusion plasma-facing components" were incorporated into the CRP. The second RCM is scheduled for 2009. [*Surface composition dynamics is a relatively new area of study, prompted partly by the high fluxes of incident particles present in fusion devices. This CRP will provide timely support to this developing field, both for experimental and theoretical studies.*]

The initiation of a new CRP on data requirements for the characterization of size, composition and origins of dust in tokamaks was delayed one year due to budgetary constraints. There has also been some internal discussion on the relevance of this CRP to the IAEA from the Department of Nuclear Safety (NS). The Subcommittee invited key NS staff members to discuss the needs for data relevant to dust. [*Following this meeting, the Subcommittee reinforced the recommendation to the Data Unit to pursue a CRP on this topic. More on this topic will appear in Section 4, below.*]

A Consultancy Meeting (CM) on diagnostic methods for measuring isotope ratios (H, D) and other light elements (He, Be, Li) in burning plasmas was convened in 2006. Gaps in existing data for atomic-based diagnostics were noted, and a larger, more comprehensive meeting on this topic was

recommended. [*The Subcommittee recommended the initiation of a CRP on this topic in the 2010-2011 budget cycle, with an additional advisory meeting to recommend specific goals for the CRP.*]

## 2.2 External Meetings, Data Centre Network Collaboration and Related Work

A workshop on “Atomic and Molecular Data for Fusion Research” was held at the International Centre for Theoretical Physics (ICTP) in Trieste, Italy on August 28 – September 29, 2006. This was the second such workshop, and over 20 students attended, along with 5 lecturers. The ICTP staff handled most of the administrative facets of this workshop which was designed to give students and professionals new to fusion research an in-depth introduction to the available atomic and plasma-material interaction data, modelling resources, and applications to fusion science. The lectures have been documented for future reference. Following the recommendation of the Subcommittee in 2006, the unit has proposed a third ICTP workshop on plasma-wall interactions with a target date within 2009. [*The Subcommittee recognizes the long-term positive effects these summer-school style workshops have on the fusion community, and strongly support their continuation.*]

Formal cooperation was proposed by a former ICTP workshop participant between the Birla Institute of Technology in Jaipur, India, and the IAEA A&M Data Unit. Once approved, the collaboration led to a successful workshop on the challenges of plasma spectroscopy for future fusion research machines. Approximately 130 participants (about 30% from outside India) discussed in some detail the future of plasma spectroscopy for fusion, with a focus on ITER. [*The strong support of the IAEA in promoting the extension of fusion energy research into developing countries is an extremely worthwhile activity, and the Unit was able to take advantage of a very good opportunity that will likely pay dividends in future years.*]

The Unit remains very active in the organization and execution of the ICAMDATA meetings, and the Subcommittee has encouraged the Unit to remain active in this endeavor. ICAMDATA meetings are held on alternate years with Data Centre Network (DCN) meetings. The unit plays a key leadership role in the DCN, and the institutes of all DCN member are strongly involved in the ICAMDATA meetings. The DCN also plays an important role in the development and promulgation of international standards for atomic and molecular databases. Under the DCN umbrella, the unit is active in the modernization of searchable atomic, molecular and plasma-material interaction databases by means of the eXtensible Markup Language (XML). A major part of the work is being carried out at the National Institute of Standards and Technology (USA), Oak Ridge National Laboratory (USA), and the Paris Observatory (France). [*The Subcommittee notes that the Unit is following previous advice to maintain a strong role in these activities, but not to take a dominant role due to limited Unit resources.*]

At the 2006 meeting, the Subcommittee was enthusiastic about the establishment of a code centre network. The goal of this work is to allow fusion researchers to access atomic structure and collision modelling codes to calculate specific data of interest. A preliminary meeting of key individuals was held, and a TM is scheduled for 2008. In addition, the ability to access atomic structure and collision cross-section codes at Los Alamos National Laboratory (USA) and other codes elsewhere has continued, with new features being added to the web interfaces. Some of these codes will remain accessible only to registered users because of their complexity and large CPU time consumption. [*Presently this effort represents only a small percentage of the Unit’s activities, and the Subcommittee feels continuation at this level is highly justified. The Subcommittee was impressed by the range of capabilities that are becoming available through internet access to computational tools.*]

The development of OpenADAS, in collaboration with H. Summers and A. Whitford at the University of Strathclyde represents an important addition to the accessible A&M databases. A test version of an interface to many ADAS data files has been written and presented to the DCN – this interface should become available in late 2008. [*The Subcommittee strongly recommends the continued pursuit of openADAS because this database is commonly used by the major fusion laboratories, but the cost for membership is prohibitive to smaller institutions. Open access to the basic data will help these smaller institutes with their development of and studies with benchmarking codes and analysis tools.*]

## 2.3 Database Maintenance

The Unit has remained active in the maintenance and expansion of the Aladdin and GENIE databases. Both databases of numerical atomic, molecular, and plasma-material interaction data are now accessible from the IAEA website. GENIE allows searches of several DCN databases via the web, while data from the CRPs and associated APIDs has been added to Aladdin. Retrievals of data continue to increase at a rate of 30% per year. Further work on DANSE, a bibliographic database, has not been undertaken due to manpower limitations. Ultimately these databases will be reorganized using the XML Atomic and Molecular Schema. [*The Subcommittee recognizes this work as the most essential activity of the Unit.*]

The Unit continues to coordinate the work of an extrabudgetary project on the properties of irradiated graphite. After a series of annual meetings, the initial database is scheduled to be available by June 2009. A second phase has been proposed to the sponsors of this work by the participants.

The IAEA computational facilities play an important role in the maintenance and modernization of the databases. Dr. Humbert gave the Subcommittee a detailed presentation on the status and future plans for the servers, high-level computational hardware and storage facilities. Extreme satisfaction was expressed in the present capabilities and future plans.

## 2.4 Overall Assessment of 2006-2008 Activities

The IAEA Data Unit on Atomic, Molecular and Plasma-Materials Interaction for Fusion is extremely productive and remains a key player in the international effort to coordinate similar databases and make their use transparent to users worldwide. Unit personnel have taken a leadership role in ICAMDATA and the DCN to provide data not only to fusion science, but also to the related plasma processing and astrophysics communities.

The Unit remains very responsive to the recommendations of the IFRC Subcommittee, and pursues data accumulation and generation highly relevant to the urgent needs of the fusion community. The continued line of CRPs and the associated APID series of database work documents is clear evidence of their efficient responsiveness.

The Unit has also launched important initiatives in data generation and dissemination. The code centre network is a very good example of this type of initiative. Outreach workshops, such as the ICTP and the Birla Institute workshop, are good examples of the Unit reaching out to the needs of developing countries.

The Subcommittee is very pleased with the continued progress made by the Data Unit over 2006-2008.

# 3. Personnel and Management Issues

## 3.1 Personnel Issues

The imminent departure of the two technical staff members of the Data Unit (Drs. Clark and Humbert) coupled with the near simultaneous departure of the Section Head (Dr. Nichols) has the potential to seriously impact on the performance of the A+M Data Unit and the continuity of ongoing CRPs. This issue was brought up at the initial address to the Subcommittee by Dr. Ramamoorthy (Division Director), with discussion continuing within the Subcommittee through the final session of the meeting. The level of concern among the Subcommittee members for the near term health of the Data Unit is significant. This concern is assuaged to some extent by the obvious shared concern of Drs. Nichols and Ramamoorthy. The plan to aggressively pursue replacements for these three positions starting very soon after the Subcommittee meeting is judged to be essential and very wise in the eyes of the Subcommittee, and the highest priority issue for the Unit during the next biennial budget cycle.

### 3.2 Management Issues

During the discussion about the serious personnel issues the Unit will face during 2009, the topic of the management structure of the A&M Data Unit was addressed. This is the first time in several meetings that the Subcommittee discussed management issues. The issue was felt to be important both to address the personnel and budgetary health of the Unit, and to understand how the review of the Subcommittee was communicated within the upper level management of the IAEA.

The Subcommittee was surprised to learn that management of the budget planning process for the Unit flows through the Department of Nuclear Energy, while personnel issues flow through the Department of Nuclear Sciences and Applications which contains the Nuclear Data Section headed by Dr. Nichols. Thus, two of the essential elements of the management of the Data Unit flow through separate paths to the Director General. A third important element of the management of the A+M Data Unit is represented by the reports from biennial reviews of the Data Unit by the IFRC Subcommittee, which flows through a third distinct path to the Director General via the IFRC. The Subcommittee worries that this multi-path management scheme encumbers the Unit Head with management-related overhead tasks, and has the potential to provide inconsistent guidance and budget for future activities of the Unit. The Subcommittee gives very high marks to Dr. Clark for his ability to maintain the health and high performance of the Unit over his years of employment. A unification of the management paths of the Data Unit should be considered prior to the appointment of a new Unit Head in 2009.

## 4. Recommendations and Conclusions

### 4.1 Coordinated Research Programs (CRPs)

The CRP entitled “Tritium inventory in fusion reactors” should be brought to a close in 2008 with the preparation and issue of APID Volume 15.

The CRP on “Atomic and molecular data for plasma modelling” should hold the final RCM in 2008, and be brought to a close in 2009. A new volume of the APID series should be produced from the work of this CRP.

The CRP on “Atomic data for high Z element impurities in fusion reactors” should hold the final RCM in 2009. A new volume of the APID series should result from this work in 2010.

The CRP on “Data for surface composition dynamics relevant to erosion processes” should continue through 2010. Progress of this CRP will be reviewed at the next meeting of the Subcommittee.

The initiation of a CRP on dust was proposed for 2007, but was delayed for budgetary reasons and by the concerns of safety experts in the IAEA Department of Nuclear Safety and Security. The concerns of the safety experts seem to focus on the development of safety criteria for ITER, which is well underway. The Subcommittee understands that the capability to predict ITER compliance to these regulations is presently unsatisfactory, as is the capability to deploy diagnostic systems to demonstrate compliance. This CRP will be oriented toward providing engineers and scientists with the data needed to measure and predict dust production and accumulation in tokamaks, and to develop new dust diagnostic systems. Following this meeting, the Subcommittee reinforced the recommendation to the Data Unit to pursue a new CRP on “Data requirements for the characterization of size, composition and origins of dust in Tokamaks” (post meeting note: CRP on “Characterization of size, composition and origins of dust in fusion devices” was approved on 30 April 2008 - first Research Coordination Meeting is scheduled for December 2008).

A new CRP on data for light ions in cold, recombining divertor plasmas should be initiated in 2009. New data on two- and three-body recombination and multi-step recombination processes involving

$H_2^+$ ,  $H_3^+$ ,  $He^+$  and Be ions are needed for a full definition of the ITER divertor. These ions will also be important in the new JET divertor with the ITER-like wall.

A new CRP on tungsten should be initiated in 2010 as a follow-on from the existing CRP on high Z elements, but will focus strictly on tungsten data for plasma modelling and diagnostic interpretation. The detailed goals of this CRP will be assessed after the final RCM for the existing CRP, but they should be designed to provide continued support to the tungsten wall programmes at Asdex-Upgrade and JET.

Should budgetary constraints allow, another CRP should be initiated during the 2010-2011 timeframe to focus on data requirements for the diagnosis of the isotopes of hydrogen and light fusion products such as  $^4He$  and  $^3He$  in the core of a burning plasma. Diagnostic data on these species is an important issue for ITER and beyond. New atomic data with improved accuracy are necessary to design diagnostic systems and interpret measurements. Cross sections for the accurate determination of the penetration of auxiliary heating beams with an injection energy in the range of 1 MeV should be included in this CRP, as these data are needed for both heating profile determinations and diagnostics based on beam spectroscopy. A Technical Meeting may be useful to recommend specific well-focused goals for this CRP.

#### 4.2 Other Recommendations

The Unit should continue close collaborations with other atomic and molecular data centres around the world under the umbrella of the Data Centre Network. Development of unified web access, greatly strengthened by the new XML schema, will benefit all plasma modelling and spectroscopic interpretation efforts, including those in fusion science. Inclusion of the ADAS database through the development of "openADAS" should also be encouraged.

The Unit should continue active participation in the ICAMDATA and ICPEAC meetings. ICAMDATA is the primary communications vehicle for scientists who participate in atomic and molecular database generation and maintenance, and the Unit should maintain sufficient budget for both technical members to attend and present papers. ICPEAC is the primary international conference for atomic collision physicists, and the Unit Head must attend this meeting to keep abreast of developing knowledge identified with atomic collision theory and experiments.

Through the ICAMDATA meetings and the DCN, the Unit should continue to encourage the development and application of evaluation criteria to define the accuracy of data contained in each database. Scientists involved in plasma modelling and diagnostic interpretation are very eager to incorporate evaluation of the effects of reasonable uncertainties on empirical scaling and model predictions. Evaluations of data contained in databases are not commonplace, frequently leaving plasma researchers without the necessary information to evaluate their own results.

### 5. Concluding Remarks

The IFRC Subcommittee is very pleased and impressed with the progress made by the Atomic, Molecular and Plasma-Material Interaction Data Unit over the previous two years. The Unit has made an excellent job of adopting and carrying out the 2006 recommendations of the Subcommittee. The execution of the recommended CRPs has exceeded expectations, given the budgetary and manpower constraints. Staff within the Unit have successfully leveraged their own activities by taking leadership roles in international atomic and molecular data organizations. The Unit has also shown considerable originality in the creation of new pathways for fusion scientists to access the data that they need, e.g. potential code centre network.

The Subcommittee has recommended three new CRPs to begin over the time period from 2008 to 2011. A fourth topic is recommended if budgets allow. The primary concern of the Subcommittee is the continuity of the management of the existing and new CRPs during 2009 and early 2010 when the

Unit Head and his technical co-worker will both be replaced. The Subcommittee is encouraged by the awareness of the Division Director to the seriousness of this problem, and his apparent aggressiveness in finding highly qualified replacements in a timely fashion.





### IAEA Technical Meeting: 16<sup>th</sup> Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

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## Appendix 2

### IAEA Technical Meeting: 16<sup>th</sup> Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

17-18 April 2008, IAEA Headquarters, Vienna, Austria

#### Meeting Agenda

Thursday, April 17

**Meeting Room: F08-14**

09:30 – 10:00    Opening. Welcome to Subcommittee members.  
Adoption of Agenda, selection of interim Chairman

Session 1: General Report on Activities since April 2006

10:00 – 11:00    General report on 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  
2008-2009 period, *R. Clark*

15:30 – 16:00    *Coffee break*

16:00 – 17:30    Session 3 (continued)

Friday, April 18

**Meeting Room: F08-14**

Session 4: Review of Additional Unit Activities

09:00 – 10:30    Review of activities, *R. Clark*

10:30 – 11:00    *Coffee break*

Session 5: Code Interfaces and Publications

11:00 – 12:30    Status of interfaces to codes on the Internet and Unit publications, *R. Clark and D. Humbert*

12:30 – 14:00    *Lunch*

Session 6: Review of Unit Status

14:00 – 14:45    Review of status of A+M Unit, *Subcommittee members*

Session 7: Recommendations for New Projects, Setting of Priorities

14:45 – 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*

### Activities of the Atomic and Molecular Data Unit (April 2006 - March 2008)

R.E.H. Clark and D. Humbert  
A+M Data Unit, Nuclear Data Section, IAEA, Vienna, Austria

#### 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 [1]. Recommendations from that meeting have been closely followed by A+M staff. A detailed summary of the progress made with respect to these recommendations is given in Section II. Database activities, Data Centre Network activities and computing issues are described in Section III. Current and planned CRPs are described in Section IV, while other Unit activities are summarized in Section V. Methods of data distribution, including interfaces to computer codes and publications, are outlined in Section VI. Finally, a synopsis of the work of the Unit from April 2006 to March 2008 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 the April 2006 meeting. A detailed summary of each recommendation and the resulting progress on the part of the A+M Unit are given below.

- In view of the appropriateness and responsiveness of IAEA CRPs to the increasing data needs for new plasma scenarios and new materials issues, the simultaneous organisation of four CRPs is endorsed, and may need to be increased in the future.  
*The budget for the Nuclear Data Section determines the number of active CRPs. Currently the A+M Unit has three active CRPs with a proposal for a fourth CRP to begin in 2008.*
- Two CRPs on “Molecular processes in edge plasmas” and “Atomic and molecular data for fusion plasma diagnostics” will be finished on time in 2006 and two volumes of the APID will be produced from these CRPs.  
*Volumes 13 and 14 of the APID [2, 3] cover the above CRPs, and have been edited and printed.*
- 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 expertise were identified, and a work plan was formulated to generate data for support of fusion plasma modelling.  
*The second RCM for this RCM was held in June, 2007 [4]. Significant progress has taken place in developing comprehensive databases. Data are already being used in applications such as B2 EIRENE.*
- The CRP on “Tritium inventory in fusion reactors” (initiated in 2002) will be extended with a final RCM in 2006. It is recommended that dusty plasmas and sticking coefficients for tritium be included in the extension and that, if needed, additional expertise be added to the CRP for this purpose.  
*The third RCM was held in 2006 [5], but a decision was taken that additional work on dusty plasmas was not feasible within the existing work load of the CRP. A new CRP on characterization of size, composition and origin of dust in fusion reactors will be proposed for commencement in 2008. The CRP on tritium inventory had formulated specific*

*recommendations related to tritium and material considerations for fusion devices. A comprehensive review article authored by members of the CRP has been submitted to Fusion Science and Technology. More complete papers from the CRP will be published in Vol. 15 of APID [6].*

- The first RCM on “Atomic data for high Z element impurities in fusion reactors” was held in 2005. There are on-going studies in ITER. Included in this CRP should be some investigation of data reduction methods to make the data usable in 2D modelling codes.  
*The second RCM was held in September, 2007 [7]. Significant progress on data generation was reported. There are some investigations of data reduction methods taking place, especially at Los Alamos National Laboratory. A number of interesting comparisons among different theoretical methods and between theory and experiment have taken place. A final RCM is planned for 2009.*
- 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.  
*This CRP was initiated in 2007 with a first RCM in October 2007 [8]. The CRP includes both experiments and theory, such as quantum molecular dynamics. A number of specific areas for collaboration between theory and experiment were identified. The second RCM is scheduled for 2009.*
- Establish a new CRP in 2007 with the goal of characterising the size, composition and origin(s) of dust in Tokomaks. This CRP should consider dust from a variety of elements such as C, W, Be for a start. A follow-on activity could be identifying the role of the dust in defining the nature of the tritium inventory.  
*A proposal for the establishment of this CRP is in process. The initiation of the CRP was delayed to 2008 for budgetary reasons.*
- The A+M Data Unit should hold a Consultancy Meeting (CM) in 2005 on diagnostics methods for measuring isotope ratios in burning plasmas (H, He, D, T, Be, Li), possibly leading to a TM in 2007 on this topic.  
*A CM was held in December 2006 [9]. Data needs for atomic-based diagnostics were summarized, and gaps in existing data were noted. The consensus was that there is sufficient need for a larger and more comprehensive meeting on this topic.*
- 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 (might including liquid walls?).  
*TM was held December 2006 [10]. Suggestions from this TM have been incorporated into the CRP on erosion processes.*
- In addition the Subcommittee was impressed by the high technical standards and the recommendations from the decennial IAEA Technical Meeting at Jülich [11]. The appendices should be given close attention - list of excellent recommendations is an example of how well the IAEA keeps abreast of current trends and data needs in fusion.  
*The Unit continues to follow the recommendations from the TM to the extent possible within budgetary constraints. Excellent progress continues to be made.*
- The Subcommittee endorses the efforts of the A+M Data Unit in co-hosting a follow-up Workshop/Summer School (ICTP-IAEA, 28 August – 9 September 2006) at Trieste on “Plasma-Wall Interactions”.  
*A proposal for another ICTP workshop has been put forward with a target date within the first half of 2009.*
- The ICAMDATA meetings are wide ranging and of interest to astrophysicists and fusion scientists alike. They are held on alternate years to the meetings of the Data Centres Network (DCN), 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.

*The Unit Head continues to serve on the Programme Committee of the ICAMDATA, and DCN members continue to be active at the ICAMDATA meetings. Significant discussions take place at each ICAMDATA meeting on DCN issues. A notable example is the work on XML schema that arose originally in discussions among DCN members and astrophysicists at ICAMDATA.*

- The Subcommittee was impressed by the considerable development of the Aladdin numerical database system and of the increasing effort by staff on the use of a variety of electronic interconnections among databases and codes. GENIE and DANSE are two web-search engines under development to allow simultaneous retrieval of data from different web sites. 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 (four out of fifteen DCN members now available on line).

*Work has continued on GENIE with more databases now searchable as well as additional options on the numerical searches. Due to the existing collaboration on bibliographic data, as well as staffing limitations, further work on DANSE has not been undertaken.*

- The Subcommittee was heartened by the recent progress achieved in successfully accessing 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 effort on similar projects.

*Work on these interfaces has continued. The interface to the Los Alamos codes has undergone substantial improvement with a number of new features. The ion collision work now includes ionization by ion collision as well as excitation and charge transfer.*

- The Subcommittee endorses a Research Co-ordination Meeting (RCM) on the investigation of the establishment of a code centre network. It is recommended that the network follow the general form of the existing DCN. It was recommended that the network would also compile a list of codes and their capabilities as well as contact persons for those codes.

*After a preliminary meeting to assess interest, a second TM is scheduled for 2008.*

- The issue of performing modelling calculations in the Unit was raised. It was affirmed that this is not one of the overall objectives of the Unit. The Subcommittee endorsed the goal of the Unit in establishing databases, but not modelling calculations.

*The A+M Unit continues to focus on the objective of providing data for support of fusion research, and does not have any active modelling activities. Much of the data are of great interest to modellers, and the Unit responds to requests for such data, but does not undertake modelling calculations independently.*

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

*The Unit has continued to arrange meetings on XML [12, 13]. The major work has been carried out at NIST, Oak Ridge National Laboratory and the Paris Observatory. The Unit has incorporated the resulting schema in the ALADDIN database. Preliminary results will be presented at the ICAMDATA meeting in 2008. The DCN has endorsed the idea of using the final XML schema as the future method for data exchange, replacing the ALADDIN system, which has become outdated.*

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

The Unit server has remained stable during the two-year period (2006-2008). As noted at the 2006 meeting, all servers are now administered through the System Development Unit of the Nuclear Data

Section. This arrangement continues to work very well. The IAEA has now consolidated the location of all servers with the result that the AMDU machine is now physically located with MTIT, rather than within the Section. This arrangement gives the added benefit of stability of the power source: several times a year the electrical power supply to A tower is interrupted for testing and maintenance, which disrupts services on the web - the power is fully maintained in the new location, and these disruptions do not occur.

The Section has now added two new 64-bit computers to their facilities, and Unit staff have used them to carry out calculations of atomic structure and cross sections for atomic ions of argon for addition to the A+M databases. Further resources continue to be added and made available for use by all Units in the Section. Plans are also being made to upgrade the AMDU server in the near future.

The Data Centre Network (DCN) held a meeting in 2007 [14]. Updates were made to the list of priorities among Data Centres (available on the homepage of the A+M Unit). As mentioned previously, the topic of formulating XML standard formats for A+M data was also raised. There was general acceptance that this is the proper method to adopt for data exchange, and that the development of standards should proceed. This work has progressed through several consultancies, as discussed in more detail below.

The topic of membership to the DCN was thoroughly discussed. A number of Member States that are not represented on the DCN have significant interest in A+M data related to fusion. Representatives from such Member States should be identified and invited to DCN meetings as observers for mutual benefit - such participants would be exposed to the work of the DCN, and would add new resources to the DCN.

Substantial work has continued on updating the ALADDIN numerical database system. The resulting interface is much more flexible and easy to use. All data have been reviewed and some entries removed as better data are now available. Substantial amounts of new data continue to be added to the database by means of CRPs and CMs. This database is very well known and is referenced often in fusion related conferences around the globe - retrievals of data have increased by approximately 30% per year.

#### **IV. Coordinated Research Projects (CRPs)**

One CRP ended in 2006; two new CRPs were initiated in 2007 and 2008, while a further CRP should begin in 2009. A fourth CRP continues through until 2008.

The final RCM on “Tritium Inventory in Fusion Reactors” was held in 2006 [5]. A set of recommendations and conclusions was formulated, and a summary of the major findings for proposed plasma-facing components was prepared as a journal article to be submitted to *Nuclear Science and Technology*. More complete articles from each participant will be published in Volume 15 of the *APID* [6].

The CRP on “Atomic and Molecular Data for Plasma Modelling” held a second RCM in 2007 [4]. Progress on generating comprehensive databases to fill the data needs was debated and summarized, and the work plan was modified accordingly; the final RCM is planned for 2009. Data from the CRP have already been used in modelling calculations, revealing that there are some areas in which the scaling laws are inadequate and new data have been generated in response.

The second RCM on “Atomic Data for Heavy Element Impurities in Fusion Reactors” was held in 2007 [7]. Participants’ presentations revealed that a great deal of progress had been made in this work. A number of very interesting comparisons between different theories and between theory and experiment had been made, providing important information on the ranges of validity of different theoretical methods. Large amounts of data for fusion-related materials have been generated, and the agreed work plan was updated to take into account the accomplishments. A third and final RCM is planned for 2009.



## V. Other Unit Activities

A workshop on “Atomic and Molecular Data for Fusion Research” was held at the International Centre for Theoretical Physics (ICTP) in Trieste, Italy on 28 August to 9 September 2006 [15]. This was the second such A+M workshop at Trieste, involving over 20 students and 5 lecturers. The workshop was well received by all participants – a two-week workshop was judged to be a considerable improvement over the previous one week workshop. Many administrative facets of the workshop were managed by ICTP staff, and these preparative functions proceeded with much less difficulty for A+M staff.

The two workshops in 2003 [16] and 2006 have impacted positively in the field of A+M physics related to fusion. A number of the student participants have maintained their interest in A+M data, and subsequently attended a number of international conferences and formed research collaborations as a direct result of the workshops. Hopefully, these workshops will continue to be held by the A+M Unit in the future. Therefore, a proposal for a third workshop has been prepared and submitted for consideration by the ICTP. This proposal has been assigned a high priority in a recent IAEA review, and would be expected to be held in the first half of 2009 if approved by the ICTP review panel.

A former ICTP workshop participant (Dr. Ram Prakesh) now has a position at the Birla Institute of Technology (BIT) in Jaipur, India. He has maintained contact with the A+M Unit, and sought cooperation between the IAEA and BIT on an international workshop devoted to challenges in plasma spectroscopy for future fusion research machines. Formal cooperation with the IAEA was approved, and the workshop was held in Jaipur on 20-22 February, with approximately 130 participants (approximately 33% from outside India). This workshop was particularly successful, and provided the opportunity for much significant interaction through informal discussions. The presentations and resulting debates were of particular importance to the Indian attendees due to their involvement in diagnostics studies for ITER.

The A+M Unit continued to sponsor individual consultancies over the previous two years 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.

A+M Unit staff continue to coordinate the work of the extrabudgetary project on the properties of irradiated nuclear graphite. The Steering Committee for this project meets yearly in Vienna to review progress and set priorities [17-19]. They are scheduled to complete the first phase to establish the initial database by June 2009, with the possible initiation of a second phase of development if sufficient funding is available from the sponsors.

## VI. Data Distribution

The main data distribution methods are the on-line databases and access to computational tools, and normal forms of hardcopy publication.

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. Over the previous two years, these publications have continued with the preparation and issue of Volume 66 of the Bulletin [20] and Volumes 13 and 14 of the APID. Written contributions are now being collected for Volume 15 of the APID on tritium inventories.

Work has continued to develop the interface for on-line access to several computational tools. Our interface to the Los Alamos codes now allows the calculation of atomic structure parameters, electron impact excitation and ionization cross sections, photoionization and autoionization. Data can be calculated for any ionization stage of any element of interest to the fusion physics community. Energy levels can be specified as fully-coupled fine structure levels or configuration-averaged quantities. Work has begun to allow registered users to undertake large-scale calculations: jobs will be submitted

in the background to be run under a controller, allowing a user to submit a job through the web interface and log out. At a later time the user will be able to log in again, check if the job has finished, and retrieve the data if completed (this service should be operational in late 2008).

The interface to the heavy-element code has more comprehensive error-checking functions, and now can calculate excitation cross sections as well as charge transfer. Work by Pablo Fainstein on collisional ionization has also been incorporated as an option.

There will be a meeting of the proposed members of a code centre network in 2008. Terms of reference will be developed at the meeting, along with soliciting levels of commitment. Participants' capabilities will be summarized and added to the web site of the A+M Unit. Subsequent meetings should occur every two years.

Collaboration with Hugh Summers on OpenADAS has continued. Alan Whiteford has now written a test version for an interface to many ADAS data files, allowing access to such data without the user having to be a member of ADAS. This project has been approved by the ADAS steering committee and should be generally available in late 2008. A preliminary version of the interface was presented to the DCN in 2007. As soon as a working OpenADAS becomes available, an ADAS representative will be invited to join the DCN.

## **VII. Summary**

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

The recommendations of the A+M Data for Fusion Subcommittee of the IFRC remain an invaluable tool in ensuring that the work of the Unit is highly focused on the important data needs and their priorities. As can be judged from this report, staff within the A+M Data Unit follow these recommendations as closely as the budget and staffing numbers permit.

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