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**INTERNATIONAL NUCLEAR DATA COMMITTEE**

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IAEA Technical Committee Meeting:

**8<sup>TH</sup> MEETING OF THE IFRC SUBCOMMITTEE ON ATOMIC  
AND MOLECULAR DATA FOR FUSION**

**5 - 6 September 1994, Vienna, Austria**

**SUMMARY REPORT**

**Prepared by R.K. Janev**

**January 1995**

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**IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA**



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8<sup>TH</sup> MEETING OF THE IFRC SUBCOMMITTEE ON ATOMIC  
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## Abstract

A brief account of the proceedings and a summary of the conclusions and recommendations of the 8<sup>th</sup> Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion, held on September 5-6, 1994, in Vienna, Austria, are provided. The Report on the activities of the IAEA Atomic and Molecular Data Unit for the period October 1992 - September 1994, is also appended to the present report.

### Some frequently used abbreviations

IFRC	- International Fusion Research Council
A+M ...	- Atomic and Molecular ..
AMDIS	- Atomic and Molecular Data Information System
AMDU	- Atomic and Molecular Data Unit
CRP	- Co-ordinated Research Programme
RCM	- Research Co-ordination Meeting
AGM	- Advisory Group Meeting
TCM	- Technical Committee Meeting
SM	- Specialist Meeting
CM	- Consultants' Meeting
PMI ...	- Plasma-Material Interaction ...
DCN	- Data Centre Network
NDS	- Nuclear Data Section
INDC	- International Nuclear Data Committee



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## 1. INTRODUCTION

The 8<sup>th</sup> Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion (IFRC A+M Subcommittee) was held on September 5-6, 1994, at the IAEA Headquarters in Vienna, Austria. All Subcommittee members attended the Meeting except Dr. J. Roth. Dr. H. Tawara (Nagoya, Japan) attended the Meeting as an observer. The staff of the IAEA A+M Data Unit attended most of the Meeting sessions and took part in some of the discussions. (see Appendix 1: List of Meeting participants).

The purpose of this regular meeting of the IFRC A+M Subcommittee was to review the Agency activities in the area of A+M and PMI (plasma-material interaction) data for fusion for the period October 1992 - September 1994, and to provide the Agency with recommendations regarding its programmes in the 1995-1996, and beyond

This was the first meeting of the Subcommittee in its expanded form (Dr. P.T. Greenland, Harwell, UKAEA, replacing Dr. M.F.A. Harrison, and the new Subcommittee members being Dr. D.E. Post, PPPL-USA, Dr. J. Roth, IPP Garching, Germany, and Dr. E. Menapace, ENEA, Italy), and the last meeting for two retiring members, Prof. A. Miyahara and Prof. H.W. Drawin.

## 2. BRIEF MEETING PROCEEDINGS

The Meeting was opened by the welcome address of Dr. C.L. Dunford, Head of Nuclear Data Section, and then proceeded according to the adopted Agenda (see Appendix 2) under the chairmanship of Dr. R. McKnight, the Subcommittee chairman.

The first session of the Meeting was devoted to the presentation of IAEA A+M Data Unit activities in the period October 1992 - September 1994 by the Data Unit staff (R.K. Janev, R.A. Langley and J. Botero). The overall A+M data activity was presented by the Unit's head (R.K. Janev), including: co-ordinated research programmes and projects, database establishment programmes, co-ordination of A+M Data Centre Network activities, AMDIS and ALADDIN developments, numerical and bibliographic data related publications, results of the experts meetings in 1993-1994, contacts and collaboration with the atomic, material science and fusion communities, and an overview of the Unit programme plans for 1995-1996. Dr. Botero elaborated on the technical aspects of the establishment and development of the Agency's A+M Data Information System (AMDIS), now on-line accessible via Internet, and on the development of ALADDIN structural and functional features. Dr. R. Langley provided details

on the status and development of the Agency data programmes in the areas of plasma-wall interactions and material properties.

The second session of the Meeting was devoted to the analysis of the work performed by the IAEA and the national A+M and PMI data centres, co-ordinated by the IAEA, in view of the current and near-future needs of the world fusion programme, including ITER EDA. The specific aspects which were addressed in the broad and in-depth discussion included: the present level of availability of A+M/PMI data with regard to the current and near-future (ITER EDA and beyond) fusion needs, the degree of implementation of existing data into fusion application (e.g. modeling, or diagnostic) codes, the adequacy of the present level and forms of data collection, evaluation and generation on national and international level for responding to the dynamic changes and growth of A+M/PMI data needs for fusion, and the role of the IAEA in integrating the efforts and meeting the data needs.

The IAEA data activities of relevance and in support to ITER EDA were analyzed in detail in the third session of the Meeting. For this analysis, Dr. D Post provided an up-to-date insight in the ITER EDA A+M/PMI data needs, particularly those related to the new ITER divertor concept (dynamic gas target divertor). The existing working-level relations and contacts between some parts of the ITER Central and Home Teams and the IAEA A+M Data Unit (and national A+M data centres, as well) provide a useful focussing and relevance of the IAEA A+M Data Unit activities. These relations have formally been endorsed by a decision of the ITER Council at its second meeting (December 1992).

The near- and long-term priorities in the IAEA and Data Centre Network A+M/PmI data activities have been discussed in the fourth session of the Meeting, within the Agency's 1995-1996 budget plan framework. The discussions covered both general priority guidelines and specific priority programmes, including new CRPs (Co-ordinated Research Programmes), experts' meetings, etc. Some technical and financial aspects of the IAEA A+M Data Unit activities have been discussed in session 5. The discussions on technical aspects have focussed on AMDIS, interconversion of various existing databases (specifically ADAS and ALADDIN) and on the interface of numerical databases with the fusion application codes. Among the other operational aspects of the A+M Data Unit activity (such as programmes based on extra-budgetary contributions, cost-free experts, etc), the potential loss of one of the two P-4 positions in the Unit as of June 1996, as planned in the Agency programme and budget for 1995-1996, has occupied most of the discussion.

The Subcommittee conclusions and recommendations on the considered topics were formulated during the last (sixth) session of the Meeting. During this session the Subcommittee discussed also some membership matters. Two Subcommittee members, Prof. A. Miyahara and Prof. H.W. Drawin, have informed the Subcommittee about their retirement and requested relief from their Subcommittee membership. The Subcommittee chairman thanked warmly Profs Miyahara and Drawin for their remarkable contributions to the work of the Subcommittee for so many years, while the scientific secretary of the Subcommittee conveyed the Agency appreciation for their dedicated work in the Subcommittee. Profs. Miyahara and Drawin informed the Subcommittee that they have arranged with their country's authorities that their replacements in the Subcommittee will be, respectively, Dr. Hiro Tawara (National Institute for Fusion Science, Nagoya) and Dr. Mario Matioli (Research Department for Controlled Fusion, CEN Cadarache).

### 3. SUMMARY OF MEETING CONCLUSIONS AND RECOMMENDATIONS

The in-depth discussions of the Subcommittee on the topics of the Agenda have led to the following conclusions and recommendations.

#### Conclusions

- 1) The Subcommittee recognizes the outstanding response of the Agency to the recommendations made by the Subcommittee at its 7<sup>th</sup> Meeting in 1992 (Cadarache, France). Four CRPs have been initiated specifically to address critical data needs for fusion energy development.
- 2) The Subcommittee highly commends the IAEA A+M Data Unit (AMDU) for its efficiency and competence in carrying out the Agency A+M data programmes during 1993-1994, and for the substantial progress made during this period in establishing the A+M Data Information System (AMDIS) and making on-line accessible (via Internet) the IAEA A+M/PMI databases to the fusion community and other users. The Subcommittee also notes with satisfaction the continuing and planned efforts to further improve the accessibility of all IAEA fusion related A+M/PMI databases, including the bibliographic database.
- 3) The Subcommittee notes that the IAEA AMDU has started the implementation of Subcommittee's recommendation to establish a working relationship with ITER Joint

Central and Home Teams, which had been recognized and endorsed by the ITER Council. The participation of the AMDU staff in ITER Divertor Modelling and Database Expert Groups, which began in 1994, should provide an important co-ordination and focus for the A+M and PMI activities of both the IAEA and the A+M Data Centre Network

- 4) The co-ordination of the A+M Data Centre Network activities by the IAEA continues to be instrumental for the effective and rational use of presently available resources for these activities, for focussing the efforts on well identified priorities and for integration and further processing of the data compilation and evaluation results. The IAEA AMDU plays a similar and equally important role in the area of data generation (through CRPs, research projects and other actions) The Subcommittee notes that in the period 1993-1994, the Agency has successfully fulfilled these two functions.
- 5) The Subcommittee endorses the Programme Plans for the period 1995-1996 in the area of A+M/PMI data for fusion (see Attachment 1) as well as the list of experts' meetings for the same period (Attachment 2). These programmes are in line with the recommendations made by the Subcommittee at its previous meeting. The Subcommittee, however, suggests to include several additional items in the programme and meeting plans, subject to availability of funds, or for inclusion in the next (1997-1998) programme and budget planning cycle.
- 6) The Subcommittee views with extreme concern the impacts of the budget reductions for the Agency A+M/PMI data activities for the period 1995-1996. These budget reductions are in direct contradiction with the recommendations made by the Subcommittee at its 7<sup>th</sup> Meeting in September 1992, and will jeopardize the ability of IAEA to maintain the database breadth and activity required for present-day and future fusion activities.

### Recommendations

- 1) The Subcommittee strongly recommends that the reduction for the AMDU not be carried out in 1995-1996 as planned. This action would disrupt critical plasma surface interaction and materials properties activities which could not be completed in any alternate way. The coordination activities of the AMDU which bring together data center activities throughout the world result in a consolidation and distribution of data for fusion which has a programmatic impact disproportionately larger than the resources expended to support the activity. Staff reductions would be correspondingly damaging to the program.

- 2) The Subcommittee recognizes the important role that cost free visitors play in Agency activities, a role that takes on added importance in times of budget limitations. Accordingly, the Subcommittee urges the Agency to evaluate the priorities of tasks to be carried out in the future and to provide tasks descriptions that would be of use to data center participants in assessing support for visitors to the Agency.
- 3) The Subcommittee recommends that the Agency continue its involvement in the ITER process while at the same time recognizing a continuing obligation to continue its support of the ongoing and active fusion programs throughout the worldwide fusion energy community.
- 4) The Subcommittee recognizes that where issues of synergistic effects are of concern in the area of plasma material interaction, radiation effects should be considered in collaboration with the nuclear data group of Nuclear Data Section.
- 5) The Subcommittee recommends that the Agency adds additional CRPs and experts meetings in its 1995-1997 programme, as delineated in Attachments 1 and 2.

#### 4. ATTACHMENTS TO THE MEETING CONCLUSIONS AND RECOMMENDATIONS

##### **Attachment 1: Programme Plans for 1995-1996**

##### **A. CRPs for 1995-96 Period**

- 1) "Plasma-interaction induced erosion of fusion reactor materials" (Completion: 1996)
- 2) "Radiative cooling rates of fusion plasma impurities" (Completion: 1997)
- 3) "Atomic and plasma-material interaction data for divertor performance optimization of fusion reactors" (Completion: 1997)
- 4) "Collection and evaluation of reference data for thermo-mechanical properties of fusion reactor plasma facing materials" (Completion. 1997)
- 5) "Reference data for tritium retention and release in fusion reactor plasma facing components" (Completion: 1997)

##### **Recommended additional CRPs to be initiated in 1995-1997 time period:**

- 1) Atomic and molecular data to support modeling of molecular processes in edge and divertor plasmas with an emphasis on hydrogen.
- 2) State selective charge exchange processes data for modeling and diagnostics applications

## **B. Establishment of Numerical Databases**

- 1) Collision processes of He atoms with electrons, protons and multiply charged ions  
(Completion: 1995)
- 2) Database on chemical erosion (Completion: 1995)
- 3) Collisional database for Be and B (Completion: 1996)

## **Attachment 2: Experts' Meetings for 1995-1996**

### **A: 1995**

- 1) 3rd RCM on Plasma-interaction induced erosion of fusion reactor materials
- 2) 1st RCM on A+M and PMI data for divertor performance optimization of fusion reactors
- 3) 1st RCM on Tritium retention and release in plasma facing components
- 4) AGM on Technical aspects of A+M data processing and exchange  
(13<sup>th</sup> A+M data centre network meeting)

### **B: 1996**

- 1) 2nd RCM on Radiative cooling rates of fusion plasma impurities
- 2) 2nd RCM on Collection and evaluation of reference data for thermo-mechanical properties of fusion reactor plasma facing materials
- 3) TCM: 9<sup>th</sup> A+M Subcommittee Meeting

## **Meetings to be added to the existing agenda for the years 1996-1998:**

### **1996**

- 1) TCM on Molecular Processes in Edge and Divertor Plasmas
- 2) Expert Group Meeting on the Atomic and Molecular Data Needs for Disruption Modeling
- 3) Expert Group Meeting on Effects of Radiation on Particle Erosion Processes

### **1997**

- 1) TCM to Assess Status of Database for Plasma-Interaction Induced Erosion of Fusion Reactor Materials-Post CRP Meeting
- 2) 1st RCM on A+M Data Needs for Molecular Processes in Edge and Divertor Plasmas
- 3) 1st RCM on State Selective Charge Exchange Processes

## **Appendices**





**Appendix 1**

**IAEA Technical Committee Meeting  
8<sup>th</sup> Meeting of the IFRC Subcommittee  
on Atomic and Molecular Data for Fusion  
5-6 September 1994, IAEA Headquarters, Vienna, Austria**

**MEETING AGENDA**

**Monday, 5 September**

Mtg. Room C-07-VI

9:30-10:00    **Opening**  
Adoption of Agenda

**Session 1:    Review of the IAEA A+M/PMI Data Activities**

10:00-10:30    **Report on the IAEA A+M Data Unit activities since the last Subcommittee Meeting**

10:30-11:00    **Status of AMDIS, ALADDIN and Numerical and Bibliographic A+M Databases**

11:00-11:30    *Coffee Break*

11:30-12:30    **Status of PMI Databases and data collection and evaluation activities**

12:00-12:30    **Comments on the Reports**

12:30-14:00    *Lunch Break*

**Session 2:    Assessment of Agency's and National A+M/PMI Data Programmes in View of the Current and Near-Future Fusion Needs**

14:00-15:30    **Presentations by Subcommittee Members and policy considerations**

- \* **Specific aspects to be addressed:**
  - **present level of overall A+M/PMI data availability vs. current and near-future fusion needs;**
  - **degree of implementation of available data into fusion application codes (including ITER EDA);**
  - **level of interaction of A+M/PMI data producers and users;**
  - **status of A+M/PMI data activities in the national and international fusion programmes and policies;**
  - **capacity and effectiveness of present forms of responding to fusion A+M/PMI data needs (IAEA and national efforts).**

15:30-16:00    *Coffee Break*

**Session 3:    Activities in Support to ITER EDA R+D Programme**

16:00-18:00    **Presentations by Subcommittee Members and discussion**

- \* **Aspects to be addressed:**
  - **status of established programmatic, working-level and formal relationships between ITER EDA and IAEA and national A+M/PMI data activities;**
  - **needs, possibilities and means for stronger interaction with ITER Central and Home Teams and involvement in the ITER EDA R+D programmes (on the national and IAEA level);**
  - **specific actions: ITER oriented programmes and their support, formal aspects, others.**

**Tuesday, 6 September**

**Session 4: Near- and Long-Term Priorities in the IAEA and Data Centre Network A+M/PMI Data Programmes**

- 9:00-10:30 Programme analysis and determination of priorities
- Near- and long-term A+M/PMI data needs for fusion;
  - Agency 1995-96 programme and budget plan framework;
  - General priority guidelines;
  - Specific priority data programmes, (CRPs, experts' meetings, etc) beyond 1996.

10:30-11:00 *Coffee Break*

**Session 5: Operational Aspects of A+M/PMI Data Activities**

- 11:00-12:30 - **Technical aspects:** common data format, ADAS-ALADDIN database interconversion, interfaces to fusion application codes
- **Financial aspects:** operation of IAEA A+M Data Unit and some national A+M Data Centres under reduced 1995-96 (and beyond) budgets programmes based on extrabudgetary contributions, cost-free experts, etc)
  - A+M data publications (Bulletin, CIAMDA, Nucl. Fusion A+M Suppl.).

12:30-14:00 *Lunch Break*

**Session 6: Formulation of Meeting Conclusions and Recommendations**

14:00-15:30 Meeting conclusions

15:00-16:00 *Coffee Break*

16:00-17:30 Meeting recommendations

17:30 Adjourn of the Meeting

**IAEA Technical Committee Meeting: 8<sup>th</sup> Meeting of the  
IFRC Subcommittee on Atomic and Molecular Data for Fusion**

5-6 September 1994, IAEA Headquarters, Vienna, Austria

**LIST OF PARTICIPANTS**

Dr. H.-W. Drawin	Dept. de Recherches sur la Fusion Contrôlée, Association EURATOM-CEA, Centre Etudes Nucléaires de Cadarache, B.P. No. 1, F-13108 Saint-Paul-lez-Durance, France
Dr. E. Menapace	ENEA A+M Data Center, C.R.E. "E. Clementel", Viale Ercolan 8, I-40138 Bologna, Italy
Dr. Y. Kikuchi	Nuclear Data Centre, Physics Department, Japan Atomic Energy Research Institute (JAERI), Tokai-mura, Naka-gun, Ibaraki-ken 319-11, Japan
Dr. A. Miyahara	Teikyo University, Otsuka, Hachioji, Tokyo, Japan
Dr. H. Tawara (Observer)	National Institute for Fusion Science, Furo-cho, Chikusa-ku, Nagoya 464-01, Japan
Dr. V.A. Abramov	Scientific Research Centre "Kurchatov Institute", Ploshchad I.V. Kurchatova, Moscow D-182, 123182, Russian Federation
Dr. P.T. Greenland	Building 424, AEA Technology, Harwell Laboratory, Didcot, Oxon OX11 0RA, United Kingdom
Dr. R.H. McKnight	Division of Applied Plasma Physics, ER-542, GTN, US Dept of Energy, Washington, D.C. 20545, U.S.A.
Dr. D.E. Post	ITER EDA, San Diego Joint Work Site, 11025 N. Torrey Pines Rd., La Jolla, CA 92037, U.S.A.

IAEA

Dr. R.K. Janev IAEA Atomic and Molecular Data Unit, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, AUSTRIA

Dr. Ch.L. Dunford IAEA Nuclear Data Section, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, AUSTRIA

Dr. R.A. Langley IAEA Atomic and Molecular Data Unit, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, AUSTRIA

Dr J. Botero IAEA Atomic and Molecular Data Unit, Wagramerstrasse 5, P O Box 100, A-1400 Vienna, AUSTRIA

**REPORT ON ACTIVITIES OF THE IAEA A+M DATA UNIT  
TO THE IFRC SUBCOMMITTEE FOR A+M DATA FOR FUSION**

**Period covered: October 1992 - September 1994**

**Prepared by R.K. Janev**

**September 1994, Vienna**

To: 8th Meeting of the IFRC Subcommittee  
for Atomic and Molecular Data for Fusion  
September 5-6, 1994, Vienna, Austria

Report on Activities of the IAEA A+M Data Unit  
for the period October 1992 - September 1994

R.K. Janev

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2. Co-ordinated Research Programmes and Projects
3. Co-ordination of the A+M Data Centre Network Activities
4. Database Establishment Programmes
5. AMDIS and ALADDIN Developments
6. Data Related Publications
7. International Bulletin on A+M Data for Fusion
8. Experts Meetings 1993-1994
9. Interaction with Atomic, PMI and Fusion Communities
10. Programme Plans for 1995-1996
11. Organizational Matters

## **1. Introductory Remarks**

The activities of the IAEA A+M Data Unit in the period since the last IFRC A+M Subcommittee Meeting (October 16-17, 1992, Cadarache) were focussed on implementing the Subcommittee conclusions and recommendations formulated at that meeting. The recommendations of the Technical Committee Meeting on "Atomic and Molecular Data for Fusion Reactor Technology" (October 12-16, 1992, Cadarache) have also served as guidelines for the A+M Data Unit activity in the reporting period. A strong effort was made to find a way for establishing a working-level relationship with the ITER EDA Central and Home Teams, as well as to formalize this relationship.

Starting June 1993, the A+M Data Unit was joined by Dr. R.A. Langley from the Oak Ridge National Laboratory who took the responsibility for the PMI data programmes of the Unit. Dr. Langley has already been previously (1980-1981) associated with the Unit and his transition time to the new duties was, therefore, very short.

The execution of the programmes in the reporting period was, in general, fairly smooth, despite of the deferral of some operating funds (on the level of about 10%) to the consecutive year.

Among the major accomplishments of the Unit's activity in the 1993-1994 period is the establishment of AMDIS, an on-line accessible Atomic and Molecular Data Information System comprising both the numerical (ALADDIN) and bibliographic databases. Most of the credit for this accomplishment goes to Dr. J. Botero.

The current A+M Data Unit staff consists of three professionals and one documentation clerk/secretary.

A more detailed account of the Unit's activities in the reporting period follows.

## **2. Co-ordinated Research Programmes and Projects**

The co-ordinated research programmes (CRPs) and the supporting individual research projects continue to represent the most important form through which the A+M Data Unit stimulates the generation of new A+M and PMI data for fusion. All of the CRPs are, however, also used as instruments for data collection and evaluation. The individual research projects are normally selected to support and strengthen some parts of an ongoing CRP, or to generate a piece of specific data information necessary to fill certain gaps in an existing data base (or improve the accuracy of some existing data).

### **2.1. CRPs Running During 1993-1994 Period**

#### **2.1.1. CRP on "Atomic and molecular data for fusion plasma edge studies"**

This CRP, initiated in 1988, has been extended in 1992 for additional two years and will be completed in 1994. Eleven laboratories participated in this CRP, including two national A+M data centres. The interim results of this CRP have been published in vol. 2 of the IAEA Series on "Atomic and Plasma-Material Interaction Data for Fusion" (end of 1992) and the final results will be published as a data compendium ("Atomic and

Molecular Processes in Fusion Edge Plasmas") by Plenum Publ. Corp. in 1995. The table of contents of this compendium is given in Attachment 1. Other colleagues from the atomic physics community have been invited (and have accepted) to contribute to this compendium. A significant part of the produced data has been included into the ALADDIN database.

2.1.2. CRP on "Atomic data for medium- and high-Z fusion plasma impurities"

This CRP has been initiated in 1991 and will be completed in December 1994. Nine laboratories participated in its work. The first results of this CRP have been published in Physica Scripta T37 (1991). The final document of this CRP will be published as a topical issue of Physica Scripta in 1995.

2.1.3. CRP on "Plasma-interaction induced erosion of fusion reactor materials"

The first three year period of this CRP expires in 1994. On recommendation by the CRP participants (ten laboratories) and of the Subcommittee, the CRP has been extended for additional two years. The emphasis of the work within this CRP in the reporting period was on physical, chemical and RES erosion processes. In the coming period the emphasis will be placed on erosion properties of the ITER plasma facing candidate materials (Be and high-Z materials)

2.2. CRPs Initiated in 1994

Following the Subcommittee recommendations given at the previous meeting (Cadarache, October 1992), the A+M Data Unit initiated in 1994 two new CRPs. Both CRPs have already been approved by the Agency.

2.2.1. CRP on "Radiative cooling rates of fusion plasma impurities"

(June 1994 - June 1997, nine participating laboratories).

The principal scientific investigators of this CRP include: H.P. Summers (JET), R.E.H. Clark (Los Alamos), M.S. Pindzola (Auburn Univ.), V. Abramov (Kurchatov Institute), T. Kato (NIFS, Nagoya), R. Marchand (INRS, Québec), K. Berrington (QUB, Belfast), K. Katsonis (GAPHYOR, Orsay) and S. Mukherjee (IACS, Calcutta).

The main objective of this CRP will be to generate as accurate as possible (within the collisional-radiative model) radiative power loss functions for the individual charge states of most important fusion reactor impurities (of both low- and high-Z). One of the projects of this CRP (H. Summers) will deal with the problem of interconversion of ADAS- and ALADDIN-formatted data (i.e. linkage of the JET-ADAS and IAEA-ALADDIN databases).

The first meeting of the participants of this CRP planned for November 10-11, 1994.

2.2.2. CRP on "Collection and evaluation of reference data for thermomechanical properties of fusion reactor plasma facing materials"

This CRP is now in the stage of constituting its composition. About 10-12 participants are expected to join this CRP including two from the ITER Central Teams (San Diego and Garching). The CRP activity will be focussed on ITER relevant materials but, at the same time, will cover a broader range of reactor relevant candidate materials. Among the objectives of this CRP is also to work out the most convenient format for data storage and exchange (still within the general ALADDIN philosophy).



The first meeting for this CRP is planned for the end of November 1994.

### 2.3. Individual Research Projects

The number of individual research projects in the reporting period has dropped from eight (in 1990-1992) to only one (Dr. I. Mihailescu, Romania). This fact was a consequence of the funding difficulties experienced already in the period 1991-1992

### 3. **Co-ordination of A+M/PMI Data Centre Network Activities**

The A+M/PMI Data Centre Network (currently consisting of 16 national data centres) is still the main instrument for an organized and co-ordinated approach to the A+M and PMI data collection and evaluation effort for the fusion research needs. However, only a relatively small part of the data centre funds is provided exclusively for these activities, and there is a general tendency of reduction of these funds. The data centres are, therefore, gradually reorienting their activities towards pure scientific research, or towards data needs in other application fields (lasers, radiobiology, environment, etc). This phenomenon deserves appropriate attention by the Subcommittee before its size will start to seriously affect the capacity of the Network to respond to the fusion research needs.

The 12th Data Centre Network meeting (AGM on "Technical aspects of A+M and PMI data processing and exchange") was held on September 20-21, 1993 with participation of representatives from all data centres, except from the QUB-Belfast data centre. The emphasis of the meeting was on co-ordination of the data collection and evaluation programmes and their focussing on ITER EDA needs, and on the development of ALADDIN functional and structural features. The spirit of cooperativeness in the Network, both on the whole and bilaterally, is very high. The 12th Data Centre Network meeting discussed the frequency of the Network meetings and concluded that, under the present funding situation in the Agency and because of the existence of advanced electronic communication tools, the Network meetings should be held every second year. The next Network meeting was, therefore, scheduled for 1995.

### 4. **Database Establishment Programmes**

The A+M Data Unit has completed and/or continued the work on establishment of the following numerical databases:

- 1) "Recommended cross sections for collision processes of hydrogen atoms with electrons, protons and multiply charged ions".  
(Completed and introduced into ALADDIN system. Hard copy of this database was published in vol. 4 of "Atomic and Plasma-Material Interaction Data for Fusion", 1993).
- 2) "Atomic collision database for Li-beam interaction with fusion plasmas".  
(Completed and ALADDIN formatted. Published in 1993 as IAEA INDC(NDS)-267).
- 3) "Particle interchange reactions involving plasma impurity ions and H<sub>2</sub>, D<sub>2</sub> and HD".  
(Completed and ALADDIN formatted. INDC(NDS) report in preparation).

- 4) "Radiative losses and electron cooling rates for H, He, C and O".  
(Completed and ALADDIN formatted INDC(NDS) report in preparation).
- 5) "Recommended cross section database for collisions of He atoms with electrons, protons and multiply charged ions". (In progress).
- 6) Databases for chemical sputtering. (In progress).
- 7) Database for tritium retention. (In progress).
- 8) Database for thermo-mechanical properties of selected materials (Be, C-C, W, Be-, Ti-, Si-carbides). (In progress)

A two week consultancy visit of Prof. L.P. Presnyakov (P.N. Lebedev Physical Institute of Russian Academy of Sciences, Moscow) has resulted in generation of large set of total and state selective electron capture cross section data for the intermediate-to-high energy collisions of H(1s) with medium- and high-Z incompletely stripped ( $q=3-10$ ) ions (Al, Si, Ti, V, Fe, Ni, Cr, Mo, W). (IAEA Report INDC(NDS)-291)

In the work on establishing the above databases, the A+M Data Unit collaborated (on a voluntary basis) with several institutions: Technische Universität-Wien (Li-beam database), University of Utah (particle interchange reactions), University of Québec (radiative losses and cooling rates of low-Z impurities) and IPP-Garching (chemical erosion).

## 5. AMDIS and ALADDIN Developments

An important step towards the accessibility (or dissemination) of the numerical databases contained in the ALADDIN system is the establishment (in July 1993) of the Atomic and Molecular Data Information System (AMDIS). AMDIS currently allows on-line (via Internet) search and retrieval of numerical data from the ALADDIN database, and work now is in progress to extend this possibility also to the bibliographic database. AMDIS resides on an IBM RS6000 AIX computer system with state-of-the-art hardware and software. The system will be portable to any UNIX system and terminal independent. AMDIS is one of the five Agency's on-line accessible data systems (see [Attachment 2](#)).

The ALADDIN developments include two aspects: data content and functional features. The data content of ALADDIN has been significantly augmented by adding to the system the newly established databases mentioned in Section 4 of this report. Input to the ALADDIN data bank has been received also from other data centres. The developments in ALADDIN functional features include: an interface for the on-line users to facilitate the data search (menu-driven, user-friendly), extension of ALADDIN dictionaries to explicitly include the evaluation functions (in both text and Fortran formats), graphical interface for local users, addition of various routines (e.g. for non-linear regression, Post Script output, etc.) to the software, etc. A C-version of ALADDIN for PC's is under development.

## 6. Data Related Publications

### A. Published

- 1) "Cross Sections for Collision Processes of Hydrogen Atoms with Electrons, Protons and Multiply Charged Ions" (R.K. Janev and J.J. Smith)  
Vol. 4 of "Atomic and Plasma-Material Interaction Data for Fusion" (IAEA, Vienna, 1993).
- 2) "Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion" (R.K. Janev, H.W. Drawin, eds) (Elsevier, Amsterdam, 1993).

### B. In preparation

- 1) Material Properties Data Compendium for Fusion Reactor Plasma Facing Components  
Vol. 5 of "Atomic and Plasma-Material Interaction Data for Fusion" (1994) (see Attachment 3, for content).
- 2) "Atomic and Molecular Processes in Fusion Edge Plasmas" (ed. R.K. Janev) (Plenum Publ. Corp., New York, 1995) (see Attachment 1, for content).

Several IAEA INDC(NDS) reports have been published or are being prepared for publication containing the completed databases mentioned in Section 4.

## 7. International Bulletin on A+M Data for Fusion and CIAMDA-3

The semi-annual publication of the bibliographic Bulletin continued during the reporting period. Volumes 46 and 47 of the Bulletin were published on time (June 1993 and December 1993, respectively), but the publication of Vol. 48 has been delayed for about three months due to the delay of the input from the Oak Ridge data centre. The preparation of Vol. 48 for publication is now in progress.

In an attempt to test the usefulness of the Bulletin to the readership and to update its distribution list, a questionnaire was sent to all Bulletin recipients (about 1000 addresses) inquiring about their further interest in this publication. Responses were obtained from about 850 addresses, all positive.

The results of this enquete have shown that the Bulletin remains a highly valuable publication for the broader scientific community and its publication must be continued. The Bulletin is also used as a medium to convey to the readership news regarding the ALADDIN data bases and the A+M/PMI data needs of the current fusion research. Because of the planned shut down of the Agency's IBM main frame by the end of 1994, the A+M Data Unit took measures to transport all the stored bibliographic information to its IBM RS6000 AIX computer system, i.e. to incorporate it into the AMDIS. The bibliographic and the ALADDIN data bases will be relationally connected in AMDIS, which will also be reflected (by a flag) in the Bulletin.

The publication of CIAMDA-3 (the Computerized Index of bibliographic Atomic and Molecular Data for fusion), scheduled previously for 1994, had to be postponed for 1995 due to the necessity for deferral of a part of 1994 funds to 1995. This gave the Unit time to work on a new format of CIAMDA-3 and on the technology of its production.

#### **8. Expert Meetings in 1993-1994**

The following experts meetings have been organized during the 1993-1994 period:

##### A: 1993

- 1) 2nd RCM on "Plasma-interaction induced erosion of fusion reactor materials (14-16 June, 1993)  
Meeting results presented in IAEA Report INDC(NDS)-283 (1993)
- 2) SM on "Tritium retention in fusion reactor plasma facing components" (17-18 June, 1993)  
Number of participants: 14  
Meeting results contained in IAEA Report INDC(NDS)-284 (1993)
- 3) AGM on "Technical aspects of atomic and molecular data processing and exchange (12<sup>th</sup> Meeting of the A+M Data Centre Network) (Sept 20-21, 1993)  
Meeting results contained in IAEA Report INDC(NDS)-294 (1994)
- 4) 1st RCM on "Atomic data for medium- and high-Z impurities in fusion plasmas" (September 22-24, 1993)  
Meeting results in IAEA Report INDC(NDS)-292 (1994)
- 5) CM on "Requirements for CRP on collection and evaluation of reference data for thermo-mechanical properties of fusion reactor plasma facing materials (22-23 September, 1993)  
Number of participants: 3  
Meeting results in IAEA Rept INDC(NDS)-289 (1994)
- 6) CM on "Atomic and plasma-surface interaction data needs for plasma disruption modeling" (8-9 November, 1993)  
Number of participants: 4  
Meeting results in IAEA Rept. INDC(NDS)-293 (1994)

##### B: 1994

- 1) TCM: 8<sup>th</sup> Meeting of the IFRC A+M Subcommittee (September 5-6, 1994)
- 2) AGM on "Atomic and particle-surface interaction data for divertor physics design studies" (November 7-9, 1994)  
Expected number of participants: 10

- 3) 1st RCM on "Radiative cooling rates of fusion plasma impurities" (November 10-11, 1994)  
Expected number of participants: 8
- 4) 1st RCM on "Collection and evaluation of reference data for thermo-mechanical properties of fusion reactor plasma facing materials" (November 29 - December 1, 1994)  
Expected number of participants: about 10

**Note:** As mentioned earlier, the planned AGM on "Technical aspects of A+M and PMI data processing and exchange" (13<sup>th</sup> A+M Data Centre Network meeting) has been postponed to 1995.

## **9. Interaction with Atomic, PMI and Fusion Communities**

The A+M Data Unit makes efforts to maintain an active relationship with the atomic, PMI and fusion communities through various ways of interaction. The senior A+M Data Unit staff members serve on the advisory boards of several international conferences in the fields of atomic, plasma and PMI physics and participate in the work of these conferences (usually at no cost to the Agency)

The Head of the Data Unit attended the ITER EDA workshop on ITER divertor physics design (February 23-25, 1994, Garching), while Dr. Langley attended a similar workshop on material properties database for ITER in-vessel components (July 14-15, 1994, Garching). Dr. Langley also made two short working visits to ORNL (at no cost to the Agency).

## **10. Programme Plans for 1995-1996**

### **10.1. CRPs for 1995-96 Period**

- 1) "Plasma-interaction induced erosion of fusion reactor materials" (Completion: 1996)
- 2) "Radiative cooling rates of fusion plasma impurities" (Completion: 1997)
- 3) "Atomic and plasma-material interaction data for divertor performance optimization of fusion reactors" (Completion: 1997)
- 4) "Collection and evaluation of reference data for thermo-mechanical properties of fusion reactor plasma facing materials" (Completion: 1997)
- 5) "Reference data for tritium retention and release in fusion reactor plasma facing components" (Completion: 1997)

### **10.2. Establishment of Numerical Databases**

- 1) Collision processes of He atoms with electrons, protons and multiply charged ions (Completion: 1995)

- 2) Database on chemical erosion  
(Completion: 1995)
- 3) Collisional database for Be and B (Completion: 1995)

### 10.3. Experts' Meetings for 1995-1996

#### A: 1995

- 1) 3rd RCM on Plasma-interaction induced erosion of fusion reactor materials
- 2) 1st RCM on A+M and PMI data for divertor performance optimization of fusion reactors
- 3) 1st RCM on Tritium retention and release in plasma facing components
- 4) AGM on Technical aspects of A+M data processing and exchange  
(13<sup>th</sup> A+M data centre network meeting)

#### B: 1996

- 1) 2nd RCM on Radiative cooling rates of fusion plasma impurities
- 2) 2nd RCM on Collection and evaluation of reference data for thermo-mechanical properties of fusion reactor plasma facing materials

### 10.4. AMDIS and ALADDIN, Bulletin and CIAMDA-3

- 1) Maintenance and further development of AMDIS and ALADDIN systems  
(continuous task);
- 2) Publication of a new ALADDIN Manual, including a C-version  
(Completion: 1995);
- 3) Publication of CIAMDA-3 (Completion: 1995);
- 4) Publication of the bibliographic bulletin (semi-annually)

## 11. **Organizational Matters**

The operation of the A+M Data Unit in 1995-1996 will be affected by the budget cuts introduced in the Agency's Programme and Budget plans for this period. The A+M Data Unit budget for 1996 includes termination of one P-4 position in the Unit in the second half of 1996. If this is implemented some of the programmes will have to be reduced. The contract of Dr. J. Botero with the Agency expires in June 1995, and Dr. Botero is currently not planning to ask for extension of his contract for additional two years. The process of replacement of Dr. Botero with another staff member will introduce a period of reduced activity of the Unit in the data operation area.

ATOMIC AND MOLECULAR PROCESSES IN FUSION EDGE PLASMAS

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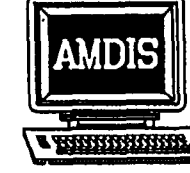

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- Ch. 3. S. Trajmar and I. Kanik  
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Electron-molecular ion collision processes
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## ON LINE DATABASES

OF THE INTERNATIONAL ATOMIC ENERGY AGENCY

 <p><b>Database name</b> Power Reactor Information System (PRIS)</p> <p><b>Type of database</b> Factual</p> <p><b>Producer</b> International Atomic Energy Agency In co-operation with 29 IAEA Member States</p> <p><b>IAEA contact</b> IAEA, Nuclear Power Engineering Section, P.O. Box 100 A-1400 Vienna, Austria Telephone (43) (1) 2360 Telex (1)-12645 Facsimile +43 1 234564 Electronic mail via BITNET/INTERNET to ID NES@IAEA1.IAEA.OR.AT</p> <p><b>Scope</b> Worldwide information on power reactors in operation, under construction, planned or shutdown, and data on operating experience with nuclear power plants in IAEA Member States.</p> <p><b>Coverage</b> Reactor status, name, location, type, supplier, turbine generator supplier, plant owner and operator, thermal power, gross and net electrical power, date of construction start, date of first criticality, date of first synchronization to grid, date of commercial operation, date of shutdown, and data on reactor core characteristics and plant systems, energy produced, planned and unplanned energy losses, energy availability and unavailability factors, operating factor and load factor</p>	 <p><b>Database name</b> International Information System for the Agricultural Sciences and Technology (AGRIS)</p> <p><b>Type of database</b> Bibliographic</p> <p><b>Producer</b> Food and Agriculture Organization of the United Nations (FAO) in co-operation with 172 national, regional, and International AGRIS centres</p> <p><b>IAEA contact</b> AGRIS Processing Unit c/o IAEA, P.O. Box 100 A-1400 Vienna, Austria Telephone (43) (1) 2360 Telex (1)-12645 Facsimile +43 1 234564 Electronic mail via BITNET/INTERNET to ID: FAS@IAEA1.IAEA.OR.AT</p> <p><b>Number of records on file from January 1993 to date</b> more than 130 000</p> <p><b>Scope</b> Worldwide information on agricultural sciences and technology, including forestry, fisheries, and nutrition.</p> <p><b>Coverage</b> Agriculture in general; geography and history, education, extension, and information, administration and legislation, agricultural economics, development and rural sociology; plant and animal science and production, plant protection, post-harvest technology, fisheries and aquaculture, agricultural machinery and engineering, natural resources, processing of agricultural products, human nutrition, pollution, methodology</p>	 <p><b>Database name</b> Nuclear Data Information System (NDIS)</p> <p><b>Type of database</b> Numerical and bibliographic</p> <p><b>Producer</b> International Atomic Energy Agency In co-operation with the United States National Nuclear Data Centre at the Brookhaven National Laboratory, the Nuclear Data Bank of the Nuclear Energy Agency, Organisation for Economic Co-operation and Development in Paris, France, and a network of 22 other nuclear data centres worldwide</p> <p><b>IAEA contact</b> IAEA Nuclear Data Section, P.O. Box 100 A-1400 Vienna, Austria Telephone (43) (1) 2360 Telex (1)-12645 Facsimile +43 1 234564 Electronic mail via BITNET/INTERNET to ID: RNDS@IAEA1.IAEA.OR.AT</p> <p><b>Scope</b> Numerical nuclear physics data files describing the interaction of radiation with matter, and related bibliographic data.</p> <p><b>Data types</b> Evaluated neutron reaction data in ENDF format, experimental nuclear reaction data in EXFOR format, for reactions induced by neutrons, charged particles, or photons, nuclear half-lives and radioactive decay data in the systems NUDAT and ENSDF, related bibliographic information from the IAEA databases CINDA and NSR; various other types of data</p> <p><b>Note</b> Off-line data retrievals from NDIS also may be obtained from the producer on magnetic tape</p>	 <p><b>Database name</b> Atomic and Molecular Data Information System (AMDIS)</p> <p><b>Type of database</b> Numerical and bibliographic</p> <p><b>Producer</b> International Atomic Energy Agency In co-operation with the International Atomic and Molecular Data Centre network, a group of 16 national data centres from several countries.</p> <p><b>IAEA contact</b> IAEA Atomic and Molecular Data Unit, Nuclear Data Section Electronic mail via BITNET to: RNDS@IAEA1; via INTERNET to ID: PSM@RIPCR301.IAEA.OR.AT</p> <p><b>Scope</b> Data on atomic, molecular, plasma-surface interaction, and material properties of interest to fusion research and technology</p> <p><b>Coverage</b> Includes ALADDIN formatted data on atomic structure and spectra (energy levels, wave lengths, and transition probabilities); electron and heavy particle collisions with atoms, ions, and molecules (cross sections and/or rate coefficients, including, in most cases, analytic fit to the data), sputtering of surfaces by impact of main plasma constituents and self sputtering, particle reflection from surfaces; thermophysical and thermochemical properties of beryllium and pyrolytic graphites</p> <p><b>Note</b> Off-line data and bibliographic retrievals, as well as ALADDIN software and manual, also may be obtained from the producer on diskettes, magnetic tape, or hard copy</p>	 <p><b>Database name</b> International Nuclear Information System (INIS)</p> <p><b>Type of database</b> Bibliographic</p> <p><b>Producer</b> International Atomic Energy Agency In co-operation with 87 IAEA Member States and 16 other international organizations</p> <p><b>IAEA contact</b> IAEA, INIS Section, P.O. Box 100, A-1400 Vienna, Austria Telephone (43) (1) 2360 2842 Telex (1)-12645 Facsimile +43 1 234564 Electronic mail via BITNET/INTERNET to ID ATIEH@NEP01.IAEA.OR.AT</p> <p><b>Number of records on file from January 1976 to date</b> more than 1.3 million</p> <p><b>Scope</b> Worldwide information on the peaceful uses of nuclear science and technology; economic and environmental aspects of other energy sources.</p> <p><b>Coverage</b> The central areas of coverage are nuclear reactors, reactor safety, nuclear fusion applications of radiation or isotopes in medicine, agriculture, industry, and pest control, as well as related fields such as nuclear chemistry, nuclear physics, and materials science. Special emphasis is placed on the environmental, economic, and health effects of nuclear energy, as well as, from 1992, the economic and environmental aspects of non-nuclear energy sources. Legal and social aspects associated with nuclear energy also are covered</p>
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For access to these databases, please contact the producers. Information from these databases also may be purchased from the producer in printed form. INIS and AGRIS additionally are available on CD-ROM

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**Atomic and Plasma-Material Interaction Data for Fusion,  
Vol. 5: (Material properties data compendium for fusion  
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