

International Atomic Energy Agency

INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Technical Committee Meeting:

7th MEETING OF THE IFRC SUBCOMMITTEE ON

ATOMIC AND MOLECULAR DATA FOR FUSION

16-17 October 1992, Cadarache, France

SUMMARY REPORT

Prepared by R.K. Janev

May 1993

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

INDC(NDS)-278 Distr.:

IAEA Technical Committee Meeting:

7th MEETING OF THE IFRC SUBCOMMITTEE ON

ATOMIC AND MOLECULAR DATA FOR FUSION

16-17 October 1992, Cadarache, France

SUMMARY REPORT

Prepared by R.K. Janev

May 1993

Abstract

A brief proceedings and a summary of the conclusions and recommendations of the 7th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion, held on October 16-17, 1992, in Cadarache, France, are provided.

The report on the activities of the IAEA Atomic and Molecular Data Unit for the period October 1990 - October 1992, is also appended to the present report.

Reproduced by the IAEA in Austria May 1993

93-01805

Contents

1.	Introduction	1
2.	Brief Meeting Proceedings	1
3.	Summary of Conclusions and Recommendations	2
4.	Attachments to the Meeting Conclusions and Recommendations	5

Appendices:

Appendix 1:	List of Meeting Participants	11
Appendix 2:	Meeting Agenda	13
Appendix 3:	Report on Activities of the IAEA	14
	A+M Data Unit	

1. INTRODUCTION

The 7th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion (IFRC A+M Subcommittee) was held on October 16-17, 1992 in Cadarache, France, immediately after the large IAEA Technical Committee Meeting (TCM) on "Atomic and Molecular Data for Fusion Reactor Technology" (October 12-16, Cadarache). The IFRC A+M Subcommittee Meeting was attended by all Subcommittee members, except by Dr. M.F.A. Harrison, as well as by the chairmen of the Working Groups of the preceeding TCM (see <u>Appendix 1</u>).

The purpose of the meeting was to review the Agency's activities in the period October 1990 - October 1992 in the area of atomic and molecular (A+M) and plasma-material interaction (PMI) data for fusion, to analyze the results of the preceeding TCM on A+M data for fusion reactor technology, and to provide the Agency with a set of recommendations regarding its policies, programmes and implementation methodology in the A+M and PMI data area.

2. BRIEF MEETING PROCEEDINGS

The meeting discussed the following main items (see Appendix 2: Meeting Agenda):

- (1) Review of the IAEA activity in the last two year period and assessment of the results of this activity;
- (2) Analysis of the conclusions and recommendations of the Working Group (WG) Reports of the TCM on "A+M Data for Fusion Reactor Technology" and development of scientific recommendations consistent with the WG reports;
- (3) Consideration of the impact of scientific recommendations on the near- and longterm programmes of the IAEA A+M and PMI data activity;
- (4) Formulation of realistic recommendations to the IAEA and IFRC regarding the Agency's data programmes, including priorities;
- (5) Organizational aspects of the A+M and PMI data activity, including establishment of a formal working relationship between the IAEA A+M Data Unit and ITER EDA;
- (6) Discussion of the Subcommittee membership, and extension and modification of the basic Subcommittee documents.

The review of the Agency's A+M and PMI data activity during the past two year period was made on the basis of the report presented by the Head of the A+M Data Unit (see Appendix 3).

The chairmen of the Working Groups presented summaries of the conclusions and recommendations of the TCM on "A+M Data for Fusion Reactor Technology" which were taken as the basis for formulation of Subcommittee's recommendations. The Chairman of the local Organizing Committee of this TCM also provided a brief report on the TCM financial aspects.

The results of the Subcommittee analyses and discussions are summarized in a set of conclusions and recommendations given below.

3. SUMMARY OF MEETING CONCLUSIONS AND RECOMMENDATIONS

- (1) The Subcommittee recognizes the essential and highly beneficial role of the IAEA in the co-ordination of the world efforts on compilation, evaluation and generation of atomic and plasma-material interaction data for fusion. This role is becoming of critical importance with the fusion programme entering into a phase of reactorrelevant plasma experiments and engineering reactor design (ITER).
- (2) The Subcommittee concurs with the conclusion of the international experts forum TCM on "A+M Data for Fusion Reactor Technology" (see IAEA Report INDC(NDS)-277), that the Agency's co-ordinating and integrating role in the area of A+M and PMI data for fusion has to be further strengthened in the immediate future in order to meet in a timely fashion the increased needs for such data and avoid duplication of efforts. The Subcommittee, therefore, strongly recommends that the Agency undertakes necessary actions in this direction.
- (3) The Subcommittee commends the IAEA A+M Data Unit for its numerous accomplishments in the past two years, particularly for its initiatives and leadership in the establishment of recommended databases for the low Z (Be and B) and intermediate-Z (Ti, Cr, Fe, Ni) plasma impurities, He-beam fusion alpha particle diagnostics, radiative cooling rates for major plasma impurities (C and O), particle-surface interaction processes (particle reflection and physical sputtering databases), material properties data (Be, pyrolitic graphites databases) and of the Nuclear Fusion Supplement Series "Atomic and Plasma-Material Interaction Data for Fusion" (Vols. 1-3).
- (4) The significat contribution of the A+M Data Unit to the international effort in fusion energy research should be appropriately recognized within the IAEA and adequate resources should be made available to the Unit for its critical assessment and research co-ordination activities.
- (5) The Subcommittee endorses the Agency programmes in the area of A+M and PMI data for fusion for the period 1993-1994, and finds them highly relevant for the most critical issues of the current and near-future fusion energy research. These programmes (see <u>Attachment 1</u>) are consistent with the recommendations of the Subcommittee to the IAEA given at its 6th Meeting in 1990.

- (6) In view of the increased demands for A+M and PMI data from the fusion research and reactor design community (including the needs for ITER EDA), the Subcommittee concurs with the recommendations of the TCM on "A+M Data for Fusion Reactor Technology" regarding the priorities of the near- and long-term Agency programmes in this area. In particular, the Subcommittee strongly recommends the initiation by the Agency during 1993 of the following Co-ordinated Research Programmes:
 - (a) CRP on A+M and PMI databases for H and He recycling and exhaust in fusion reactor divertors;
 - (b) CRP on radiative cooling rates of fusion plasma impurities; and
 - (c) CRP on H-isotope retention in fusion reactor plasma facing components.

All these programmes are in line with the recommendations of the Subcommittee at its 6th Meeting as long-term Agency programmes in the A+M and PMI data area; however, their immediate implementation is now becoming an urgent task in view of the rapid evolution of fusion research and reactor design needs. The Subcommittee recommends a selective approach to the collection and evaluation of PMI data, which should be restricted to the most relevant properties and materials, required in the selection process of candidate plasma facing materials.

- (7) The Subcommittee endorses the Agency's experts meeting programme in the A+M and PMI data fields for the 1993-1994 period, and recommends, if feasible, inclusion of a few additional, small meetings, in conjunction with already approved ones, for specification of the scope and participants of the new CRPs (see <u>Attachment 2</u>).
- (8) The IAEA annual publication series "Atomic and Plasma-Material Interaction Data for Fusice" has proved to be a highly effective medium for rapid communication of data information between A+M, PMI and fusion communities. The Subcommittee recommends to explore the possibilities for increasing the publication frequency to two issues per year.
- (9) While continuing to respond to the urgent A+M and PMI needs of the national fusion programmes of its Member States, the Agency's activity in this area should also be strongly related to the needs of the ITER EDA. It is strongly recommended that a formal working relationship be established between the IAEA A+M Data Unit and the ITER EDA Central and Home Teams in areas in which the existing Agency databases, or programmes aimed to establish such databases, can be beneficial to the ITER design process. The Subcommittee Chairman was asked to take action in this regard*.

^{*} In the meantime the Subcommittee Chairman took the necessary actions, resulting in a decision of the ITER Council (December 15-16, 1992, 2nd ITER Council Meeting in Moscow) to establish such formal working relationship.

- (10) The Subcommittee discussed the structure and the size of its membership and concluded that an expansion of the Subcommittee membership with two experts is necessary to cover competently all the areas from the scope of its responsibilities and expertise. Dr. D.E. Post (PPL, Princeton) and Dr. J. Roth (IPP, Garching) have been suggested as best qualified candidates for this purpose.
- (11) The Subcommittee also concluded that in order to reflect more adequately the programmatic scope of its activities, certain modifications in its basic documents, Terms of Reference and Methods of Work, should be appropriate. The modified Terms of Reference and Methods of Work (see <u>Attachments 3 and 4</u>) will be submitted to the IAEA and the IFRC for approval.
- (12) The Subcommittee Chairman was asked to inform the Agency's Director General with the main conclusions and recommendations of this Subcommittee Meeting.

4. ATTACHMENTS TO THE MEETING CONCLUSIONS AND RECOMMENDATIONS

Attachment 1

IAEA Programmes on A+M and PMI Data for Fusion

for 1993 - 1994

- 1. CRP on A+M data for fusion edge plasmas (1988-1994);
- 2. CRP on plasma-interaction induced erosion of fusion reactor materials (1989-1994);
- 3. CRP on atomic data for medium- and high-Z fusion plasma impurities (1991-1994);
- 4. CRP on reference data for thermo-mechanical properties of fusion reactor plasma facing materials (1993-1996);
- 5. IAEA series on "Atomic and Plasma-Material Interaction Data for Fusion" ("Nuclear Fusion" Supplement) (Vol. 4 1993, Vol. 5 1994);
- 6. Technical document on A+M data for fusion reactor technology (1993);
- 7. Publication of CIAMDA-94;
- 8. Publication of two issues of the International Bulletin on A+M Data for Fusion;
- 9. Organization of experts' meetings related to co-ordination of data generation, compilation and evaluation activities (see <u>Attachment 2</u>);
- 10. Continuation of data compilation and evaluation work related to the establishment of A+M and PMI databases, including recommended data parametrization;
- 11. Maintenance and updating of existing recommended A+M and PMI databases;
- 12. Maintenance and upgrading of the ALADDIN data processing and exchange system;
- 13. ALADDIN formatting of new evaluated/recommended databases;
- 14. Data publication and dissemination.

Attachment 2

IAEA A+M and PMI Data Related Meetings for 1993 - 1994

<u>1993</u>

- 1. SM on Hydrogen retention in fusion reactor plasma facing components (17-18 June, Vienna)
- 2. 2nd RCM on Plasma-interaction induced erosion of fusion reactor materials (14-16 June, Vienna)
- 3. AGM on Technical aspects of A+M and PMI data processing and exchange (12th Meeting of A+M Data Centres and ALADDIN Network) (20-21 September, Vienna)
- 4. 1st RCM on Atomic data for medium- and high-Z impurities in fusion plasmas (22-24 September, Vienna)

Additional meetings suggested by the Subcommittees:

- 5. SM to define the scope of the new IAEA CRP on Reference data for thermochemical properties of fusion reactor plasma facing materials, 1990 1994, (September; one day; in conjunction with the ICFRM-6 in Italy)
- 6. SM to define the scope of the new IAEA CRP on Radiative cooling rates of fusion plasma impurities, 1993 1996 (one day, in conjunction with the September meetings, Vienna).

<u>1994</u>

- 1. TCM: 8th Meeting of the IFRC A+M Subcommittee (Vienna);
- 2. AGM: Technical aspects of A+M and PMI data processing and exchange (13th A+M Data Centre and ALADDIN network meeting) (Vienna);
- 3. 1st RCM on Radiative cooling rates of fusion plasma impurities (Vienna);
- 4. 1st RCM on Reference data for thermomechanical properties of fusion reactor plasma facing materials (Vienna);

Additional meeting requested by the Subcommittee:

5. A CM or SM (two days) on an urgent, ITER- related, data issue.

Attachment 3

Suggested Modifications of Subcommittee's Basic Document:

TERMS OF REFERENCE

IFRC Subcommittee on Atomic and Plasma-Material Interaction (Atomic and Molecular) Data for Fusion

The International Fusion Research Council (IFRC) Subcommittee on Atomic and Plasma Material Interaction Data for Fusion will serve as a continuing Subcommittee within the framework of the International Atomic Energy Agency. Its function will be to review periodically the planning and execution of the Agency's Atomic and Plasma-Material Interaction Data for Fusion Programme and to advise the Director General on its direction in accordance with the needs of fusion research and reactor design.

<u>Composition</u>: the Subcommittee shall be composed of fusion and atomic scientists nominated by IFRC.

<u>Methods of Work</u>: the Subcommittee shall determine its own methods of work. The IAEA Nuclear Data Section shall provide the secretariat services to the Subcommittee.

<u>Meetings</u>: the Subcommittee shall be convened at a frequency not exceeding two years, and shall normally meet at IAEA Headquarters. The cost of participation of Subcommittee Members will be borne by the Government or sponsoring institute of the member. No interpretation will be required.

Suggested Modifications of Subcommittee's Basic Document:

METHODS OF WORK

IFRC Subcommittee on Atomic and Plasma-Material Interaction (Atomic and Molecular) Data for Fusion

Under the Terms of Reference of the IFRC Subcommittee on Atomic and Plasma-Material Interaction (Atomic and Molecular) Data for Fusion (herein after referred to as the Subcommittee), as approved by the IAEA Administration 1993, the Subcommittee is authorized to determine its own Methods of Work.

I. Scope and Responsibilities

In addition to the general functions of the Subcommittee, stated in the Terms of Reference, the Subcommittee shall

- periodically review the IAEA programme on A + PMI data for fusion;
- review A + PMI data needs and recommend their priorities;
- assist in specifying and planning topical data meetings and coordinated research programmes;
- assist in maintaining contacts between the IAEA A + PMI Data Unit and the fusion community;
- assist in the coordination of data centres networks.

II. Organization

(1) <u>Chairman</u>: the Chairman shall be a member of the Subcommittee and shall serve for 2 meetings. The Chairman may be renominated by the Subcommittee. The responsibility of the Chairman shall remain in effect between meetings, until the following meeting, and he shall be kept informed by the Subcommittee members and the Scientific Secretary of relevant activities and developments.

- (2) <u>Scientific Secretary</u>: the Scientific Secretary shall be the Head of the A + PMI Data Unit of the IAEA Nuclear Data Section, and shall serve as a member of the Subcommittee.
- (3) <u>Membership</u>: should it become necessary for a Subcommittee member to relinquish his membership, it shall be his responsibility to arrange for his replacement in collaboration with the pertinent IFRC member, and to inform the Chairman and the Scientific Secretary of the Subcommittee of the membership change in writing.

III. Meetings

- (1) <u>Preparation</u>: the preparation of the meetings shall be done timely by the Scientific Secretary of the Subcommittee in collaboration with the incoming and outgoing Chairmen.
- (2) <u>Frequency</u>: the time between meetings of the Subcommittee shall be determined by progress in the field of fusion research and technology pertinent to A + PMI data and development within the IAEA, but shall not exceed two years.
- (3) <u>Proceedings</u>: the proceedings of the meetings shall be written by the Scientific Secretary, and shall be issued as an IAEA report after having been approved by all Subcommittee members. The proceedings of every meeting shall be distributed to the IFRC committees, the A + PMI data centres and to the directors of all major fusion laboratories in Member States.
- (4) Observers: all meetings of the Subcommittee shall be open to observers.

7th MEETING OF THE IFRC A+M SUBCOMMITTEE:

APPENDICES

Appendix 1

List of Participants for the TCM: 7th IFRC Subcommittee Meeting

Cadarache, 16-17 October 1992

<u>IAEA</u>

Dr. R.K. Janev [*]	Atomic and Molecular Data Unit, Nuclear Data Section, Division of Physical and Chemical Sciences, IAEA, Wagramer Str. 5, P.O. Box 100, A-1400 Vienna
FRANCE	
Dr. HW. 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
<u>GERMANY</u>	
Dr. J. Roth	Max-Planck-Institut für Plasmaphysik, Boltzmanngasse 2, D-W 8046 Garching bei München
<u>JAPAN</u>	
Dr. Y. Kikuchi [*]	Nuclear Data Centre, Physics Department, Japan Atomic Energy Research Institute (JAERI), Tokai-mura, Naka-gun, Ibaraki-ken 319-11
Dr. A. Miyahara [•]	Teikyo University, Otsuka, Hachioji, Tokyo

* Member of the IFRC A+M Subcommittee

THE RUSSIAN FED.

Dr. V.A. Abramov [*]	Institut Atomnoi Energii I.V. Kurchatova, Ploshchad I.V. Kurchatova, Moscow D-182, 123182
Dr. V.R. Barabash	D.V. Efremov Scientific Research Institute of Electrophysics Apparatus, P.O. Box 42, St. Petersburg 189631, Metallostroi
<u>U.S.A.</u>	
Dr. R.H. McKnight [*]	Division of Applied Plasma Physics, ER-542, GTN, US Dept. of Energy, Washington, D.C. 20545
Dr. R.A. Phaneuf	Department of Physics, University of Nevada-Reno, M.S. 220, Reno, Nevada 89557-0058
Dr. D.E. Post	Princeton University, Plasma Physics Laboratory, P.O. Box 451, Princeton, NJ 08540
Dr. K.L. Wilson	Physical Res. Division 8347, Sandia National Laboratories, Livermore, CA 94551-0969

Appendix 2

7th IFRC A+M SUBCOMMITTEE MEETING

16 - 17 October 1992, Cadarache, France

Meeting Agenda

FRIDAY, 16 October

14:00 - 14:30	Opening Summary of activity: IAEA A+M Data Unit Report
14:30 - 16:15	WG chairmen reports Development of scientific recommendations, consistent with WG reports
16:15 - 16:30	Break
16:30 - 17:45	Consideration of impact of scientific recommendations on near term and long range IAEA A+M and PMI data activities. Formulate realistic recommendations to IAEA and IFRC.
17:45 - 18:00	TCM summary (Drawin)
SATURDAY, 17 October	
09:00 - 10:30	Membership discussion, other subcommittee matters
10:30 - 10:45	Break
10:45 - 12:15	Organizational aspects of A+M data activities Acceptance of draft recommendations
12:15	Adjournement

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

Period Covered: October 1990 - October 1992

Prepared by R.K. Janev

October 1992, Vienna

 To: 7th Meeting of the IFRC Subcommittee on A+M Data for Fusion
 October 16-17, 1992
 Cadarache, France

Report on Activities of the IAEA A+M Data Unit

for the period October 1990 - October 1992

Contents

1.	Introduction	1
2.	A+M and PMI Programme Definition and Implementation	2
3.	A+M and PMI Data Status and Needs Assessments, and Data Evaluation	4
4.	Co-Ordinated Research Programmes (CRPs) and Projects	6
5 .	Database Establishment Programme	10
6.	Co-Ordination of A+M and PMI Data Centre Network Activities: Data Processing and Exchange	13
7.	A+M/PMI Database and ALADDIN System Maintenance and Development	15
8.	A+M and PMI Data Publication and Dissemination	16
9 .	International Bulletin on Atomic and Molecular Data for Fusion	19

Attachments:

Attachment 1: IAEA Programmes on A+M and PMI Data for Fusion
Attachment 2: Proposal for Co-ordinated R+D Programme Tasks for ITER
Attachment 3: Members of A+M and PMI Data Centre Network
Attachment 4: ALADDIN Formatted Recommended and/or Evaluated Data

1. INTRODUCTION

The IAEA A+M Data Unit operates within the IAEA Nuclear Data Section and is responsible for the execution of Agency's programmes in the area of atomic and molecular (A+M) and plasma-material interaction (PMI) data for fusion. The objectives of these Agency's programmes are to establish an international bank of recommended atomic, plasma-wall interaction and material properties data for fusion energy research and reactor design, to promote, co-ordinate and integrate the world's efforts in providing the fusion community with evaluated A+M and PMI data, and to disseminate the data information to national fusion laboratories, international fusion projects and other users in the Agency's Member States. In implementing these objectives, the IAEA A+M Data Unit conducts, organizes and initiates the following activities:

- (a) Organization of international forums and assistance to standing advisory bodies for definition and review of Agency's programmes in this area;
- (b) Co-ordination of data compilation and evaluation programmes of national A+M and/or PMI data centres;
- (c) Initiation and co-ordination of international programmes for enhancement of fusion related data generation and evaluation efforts;
- (d) Initiation, assistance and participation in the establishment of recommended A+M and PMI databases for fusion;
- (e) Maintenance, up-dating and development of evaluated and recommended A+M/PMI databases at the IAEA;
- (f) Maintenance and development of ALADDIN data system for storage, processing and exchange of A+M/PMI data;
- (g) A+M/PMI data publication and dissemination;
- (h) Publication of the bibliographic International Bulletin on Atomic and Molecular Data for Fusion (semi-annually), and of the Computerized Index for Atomic and Molecular Data (CIAMDA) (periodically); and
- (i) Maintenance of a continuing working interaction with the fusion, A+M and PMI communities.

In conducting these activities in the reporting period, the IAEA A+M Data Unit has enjoyed a strong support and assistance of the fusion, atomic physics and material science communities, which has been provided through a continuous, working-level interaction and collaboration. This support and interaction has been essential for all the A+M Data Unit accomplishments and for maintaining a close correlation and compatibility of Agency's programmes in this area with the changes and developments in the fusion research programmes. Of particular importance for the achievements in the areas of data compilation, evaluation, processing and exchange was the strong and coherent collaboration of the Unit with the A+M Data Centre Network (A+MDCN).

The IAEA A+M Data Unit's activities in the reporting period are briefly described below. It should be noted that in this period the A+M Data Unit operated with reduced staff, because the substitution of one professional staff member (Mr. J.J. Smith by Dr. J. Botero) was delayed by one year. Thus, in the reporting period the Unit operated with 1.5 effective professional staff and one secretary.

2. <u>A+M AND PMI DATA PROGRAMME DEFINITION AND IMPLEMENTATION</u>

2.1. **Programme Definition**

Under its Terms of Reference, the Subcommittee on Atomic and Molecular Data for Fusion of the Agency's International Fusion Research Council (IFRC) is authorized "to review periodically the planning and execution of the Agency's atomic and molecular data programme and to advise the Director General on its direction in accordance with the needs of fusion reactor design". The Subcommittee is composed of about ten prominent fusion and atomic physics scientists, nominated by the IFRC. The IAEA A+M Data Unit, which is executing the Agency's A+M Data programmes, annually reports to the IFRC on its activity. The major role in the definition and the supervision of the Agency's A+M data programmes is played by the IFRC A+M Subcommittee. The Subcommittee exercises this role through a continuous interaction with the Head of A+M Data Unit and at its biennial meetings. The last, 6th IFRC A+M Subcommittee meeting was convened on 27-28 September 1990 in Vienna. Besides a comprehensive review of work performed by the IAEA A+M Data Unit for the preceding two years (based on a detailed report from the Data Unit), the most important items on the agenda of this Subcommittee meeting were the establishment of short- and long-term priorities in the fusion related A+M data compilation, evaluation and generation activities of the A+M Data Unit and the international programmes under its co-ordination or supervision, the enhancement of the data evaluation effort in the international A+M Data Centre Network, and the extension of the Agency's data activity in the area of plasma-material interaction data The proceedings and the conclusions and recommendations of this Subcommittee meeting are given in the IAEA report INDC(NDS)-244/M9.

Another major element in the process of the IAEA A+M and PMI programme definition is the Technical Committee on Atomic and Molecular Data for Fusion, which meets periodically to assess the overall impact of A+M and PMI data activities on the development of fusion energy research programmes, and to determine the general directions and policies in the data activities for a longer period. At its last meeting, the IFRC A+M Subcommittee decided that the Agency organize in 1992 such a meeting in relation with the short- and long-term A+M and PMI data priorities in the engineering design of next-step reactor-level fusion devices (such as ITER). The IAEA A+M Data Unit devoted much of its efforts in the 1991-92 period to the organization of this major meeting (TCM on "A+M Data for Fusion Reactor Technology", October 12-16, 1992, Cadarache, France), both in determining its programme and ensuring a highly competent participation from the fusion, A+M and PMI communities. In the TCM programme definition and selection of TCM participants, the advices and suggestions of the IFRC Subcommittee members were closely followed, as well as those of a number of colleagues from the fusion, A+Mand PMI communities (Drs. F. Engelmann, D. Post, G. McCracken, R. Hulse, R. Phaneuf, W.L. Wiese, Yu. Prokofiev, V. Pistunovich).

Input for the IAEA A+M/PMI activity programmes, particularly those involving short-term tasks, is also provided by various experts' meeting discussing the data needs for specific fusion research problems. Examples of these types of meetings are given in <u>Section 3</u>. The overall process of the IAEA A+M and PMI data programme definition and various steps and elements involved in its implementation, are shown in Attachment 1.

The role played by the A+M Data Unit and the A+M Data Centre Network in this process, as well as other activities of the Unit, are also shown schematically in this Attachment.

2.2. Interaction with the Fusion, A+M, and PMI Physics Communities

Both the IAEA A+M Data Unit and several of the national A+M data centres are in a continuous interaction and working relationship with the world's leading fusion research laboratories. This interaction allows to follow the dynamics of A+M data needs evolution in the fusion research programmes and to provide a prompt response to the data need changes. In the reporting period, this interaction has been particularly stimulated by the conceptional design activities on ITER. The interaction with the fusion community included not only delivery of required A+M data and exchange of information on data needs and sources, but also joint work on database establishment, data implementation into fusion modelling and diagnostic codes and the formulation of certain short-term data activity projects.

The most useful forms of this interaction in the reporting period were the expert meetings (see Section 3 below), organized on specific subjects, and attended by active atomic physicists, fusion researchers and representatives of national A+M data centres. Under Special Service Agreements (see Section 4.5.), the Agency invited a number of experts from the fusion, A+M and PMI communities to provide advice and assistance to the IAEA A+M Data Unit in carrying out certain projects from the Unit's database establishment (or completion) programme and ALADDIN system development (see Section 5).

In order to strengthen the working-level interaction with the fusion community, and provide a direct implementation of the available evaluated/recommended A+M and PMI data into fusion application codes, the A+M Data Unit in the reporting period undertook a series of broad consultations to formulate a programme through which part of its future activity could be directly related to certain ITER EDA R+D tasks. The areas in which the IAEA co-ordinated A+M and PMI data activities could make a direct contribution to the ITER EDA R+D programme are: (i) radiative cooling of the plasma edge, (ii) particle recycling and helium exhaust, and (iii) optimization of neutral beam heating and/or diagnostic systems. The rationele and more details on the possible involvement of the IAEA co-ordinated A+M and PMI activities in the ITER EDA related R+D programme are given in Attachment 2. Significant input to the formulation of this draft proposal was given by several Subcommittee members (in particular by Dr. M.F.A. Harrison) and by a number of colleagues from the fusion community (Drs. F. Engelmann, D.E. Post, D. Reiter). The content of this document will certainly undergo further modifications (in response to the detailed definition of ITER EDA R+D programme), but it represents the frame within which a useful working relationship with the ITER teams can be established.

3. <u>A+M AND PMI DATA STATUS AND NEEDS ASSESSMENTS, AND DATA</u> <u>EVALUATION</u>

3.1. Evaluation of thermo-mechanical properties data of carbon-based plasma facing materials (CM, Vienna, December 17-21, 1990)

A small group of experts performed a critical analysis of the available thermophysical and thermo-mechanical data for carbon-based materials (various types of graphites, doped graphites, carbon fiber composites) presently considered as candidate materials for fusion reactor plasma facing components. The consultants' group also formulated the scope and the structure of the Agency's material properties database for fusion, the *ALADDIN* dictionaries for formatting material properties data, and prepared an ALADDIN file of evaluated data for anisotropic pyrolytic graphites. Specific recommendations were also formulated regarding the Agency's future activity in this data area. Results of this evaluation effort are described in more detail in the report INDC(NDS)-246/MO.

3.2. He-beam database for alpha particle diagnostics of fusion plasmas (CM, Vienna, June 3-5, 1991)

The objectives of this consultants' meeting were to assess the needs and the available data for the He-beam based diagnostics of fusion plasmas, including the alpha particle diagnostics of fusion reactors, to perform a critical evaluation of the existing data and recommend selected data sets for use in He-beam attenuation and diagnostic codes. These objectives of the meeting were fully achieved. Many of the participants provided newly generated cross section data for the collision processes of the atoms

with other plasma constituents. Many of the meeting participants committed themselves to continue the data generation and evaluation effort at their home laboratories in order to improve the completeness and quality of the required He-beam data base. The results of the meeting are described in the report INDC(NDS)-253/N2 and most of the evaluated data are presented in Vol. 3 (1992), of the IAEA series on "Atomic and Plasma-Material Interaction Data for Fusion".

3.3. Atomic database for Be and B (CM, Vienna, June 10-12, 1991)

Berrylium and boron have become increasingly important impurities in many recent large tokamak experiments, and are likely to be present in the ITER machine. The consultants' meeting on the collisional database of these impurities was organized with the idea to assess the available data information and, through additional cross section calculations performed by the participants before the meeting, to improve the completeness of the database. These meeting goals have been achieved, resulting in the establishment of complete sets of recommended data for the most important collision processes of these plasma impurities. The proceedings and the main results of the meeting can be found in the report INDC(NDS)-254, and the recommended data have been published in Vol. 3 (1992) of the IAEA series on "Atomic and Plasma-Material Interaction Data for Fusion".

3.4. Atomic and Molecular Data for Fusion Plasma Impurities (AGM, Vienna, September 25-27, 1991)

The objectives of the meeting were to provide a review of the available spectroscopic and collisional data information for all the impurities (both low- and high-Z, molecular) present in operating large tokamak devices, and anticipated in the future fusion reactors. A specific objective of the meeting was to determine the scope and priorities of an initiated Agency's Co-ordinated Research Programme (CRP) in this data area. The Advisory Group has produced a set of assessments and recommendations regarding the data status and needs for spectroscopic and collisional properties of plasma impurities, which should serve as guidelines for the Agency's activity in this data area, and for the programmatic scope of the above mentioned CRP. These assessments and recommendations are reproduced in the report INDC(NDS)-257/N8.

3.5. Atomic and Molecular Database for H-Recycling and He-removal from Fusion Reactors (CM, Vienna, June 11-12, 1992)

Hydrogen recycling in the divertor of a fusion device and helium removal from the divertor are important parameters defining the performance of the fusion reactor power and particle exhaust system.

The accurate knowledge of the atomic physics aspects of these transport phenomena is indispensible for a successful prediction of the divertor performance, and for its design. The Consultants' Group critically analyzed all the atomic and plasma-surface interaction (PSI) data information required for the corresponding modelling codes, and formulated an optimum ("standard") scheme for the A+M and PSI processes to be included in these codes.

The Group also identified all the A+M and PSI processes for which new data information is required to satisfy the necessary accuracy of the modelling codes. A set of urgent actions has been recommended to the Agency to improve the A+M and PSI physics basis of the modelling codes. The results of this meeting are described in the report INDC(NDS)-274.

4. CO-ORDINATED RESEARCH PROGRAMMES (CRPs) AND PROJECTS

4.1. CRP on "Atomic and Molecular Data for Fusion Plasma Edge Studies" (period: 1988-1992; number of participating laboratories: 11)

The purpose of this CRP was to improve the available database for the A+M collision processes involved in the edge plasma regions of fusion devices through both direct data generation and data collection of evaluation efforts. This CRP also included a spectroscopic data part. The emphasis in this activity was placed on completion of the spectroscopic and collisional databases for the basic plasma edge constituents (including all forms of hydrogen and its isotopes), molecular impurities, and low-charge states of most abundant atomic impurities. Two Research Coordination Meetings (RCMs) were organized during the activity on this programme, one of which during the reporting period (17-19 June 1992, Vienna). An interim report on the results achieved within this CRP has been published in Vol. 2 (1992) of the IAEA series "Atomic and Plasma-Material Interaction Data for Fusion". The numerical data generated or evaluated within this CRP has been introduced in the corresponding ALADDIN files. The final product of the research and evaluation activities of the Programme will be published during 1993.

4.2. CRP on "Plasma-Interaction Induced Erosion of Fusion Reactor Materials" (period: 1989-1994; number of participants: 10)

The objective of this CRP is to establish a co-ordinated effort, involving the most active experimental laboratories and theoretical groups in the field, directed in collection, evaluation and generation of data for all particle-surface and plasmamaterial interaction processes resulting in erosion of candidate plasma facing materials in fusion reactors. The final goal of this effort is to prepare a comprehensive data compendium on the erosion characteristics of fusion reactor candidate materials under various plasma-material interaction conditions (particle fluxes, fluences, material composition, temperature, etc.) which should provide an expert guidance to the fusion reactor designers in the process of reactor material selection. The material erosion rates should preferably be determined under realistic plasma-wall interaction conditions, i.e. they should include the effects of material redeposition, various synergistic effects, the material structural and other changes during the reactor operation, etc. Emphasis in the CRP is currently given on the carbon based materials (including carbon fiber composites), B-, Si- and Ti-doped graphites and berrylium. A RCM was held within this CRP activity (15-17 May 1991, Vienna) and some of the obtained results are published in Vol. 1 (1991) of the IAEA series on "Atomic and Plasma-Material Interaction Data for Fusion". It is likely that the work of this CRP will be extended to the erosion processes characterizing the off-normal plasma operation phenomena (such as plasma disruption, run-away electrons effects, etc.).

4.3. CRP on "Atomic Data for Medium- and High-Z Fusion Plasma Impurities" (period: 1991 - 1994; participating institutions: 9)

With increasing the atomic number of plasma impurities, both the spectroscopic and (especially the collisional data information became increasingly scarce. However, medium -Z impurities, such as Si, Ti, Cr, Fe and Ni, seem to be inavoidable in most of the current fusion devices, and high-Z elements (such as Mo, Ta, W) are candidate base structure divertor plate materials. The purpose of this CRP is, therefore, to promote a strong co-ordinated research effort to improve the spectroscopic and collisional database for these plasma impurities. This information is needed for the prediction of plasma cooling effects of these impurities, their transport in various plasma regions, as well as for the study of other associated phenomena (e.g. impurity recycling). The data generation, compilation and evaluation work within this CRP has considerably progressed, particularly for the metallic impurities. The work of this CRP is supported by the activity of several other experimental and theoretical groups, formally not members of the CRP. A first compendium of compiled, evaluated and generated collisional data on metallic plasma impurities (with emphasis on Ti, Cr, Fe and Ni) was published as a topical issue of Physica Scripta (T37, 1991).

4.4. Individual Research Contract Projects

In order to enhance the data generation and evaluation efficiency of the above coordinated research programmes, but also to assist the IAEA A+M Data Unit in the execution of other data related programmes (e.g. completion of specific databases), the Agency in the reporting period has financially supported eight Research Contracts with selected laboratories and theoretical groups from the developing countries. Three of these contracts were related to atomic and molecular processes in the fusion plasma edge, two of them have supported the completion of the database for H-beam attenuation in fusion plasmas, two of these projects were related to the plasmamaterial interaction data programmes, and one contract was related to the data compilation work. The list of individual Research Contracts supported by the Agency in the reporting period is given in Table 1.

<u>Table 1</u>. Individual Research Contracts for A+M/PMI Data

- (1) Calculations of cross sections for ionization of hydrogen and helium atoms by multiply charged ions (Centro Atomico Bariloche, Argentina; Dr. V.H. Ponce, Dr. R. Rivarola).
- (2) Studies of ion-impact excitation processes pertinent to fusion plasmas (Indian Association for Cultivation of Science, Jadavpur, India; Prof. S. Mukherjee).
- (3) Measurements of electron-impact ionization of molecules (including hydrocarbons) (Institute of Physics, Belgrade, Yugoslavia; Dr. N. Djuric).
- (4) Molecular spectroscopy relevant to fusion plasmas (Dept. of Physics, Univ. of Belgrade, Yugoslavia; Prof. N. Konjevic).
- (5) Spectroscopic and transport studies of plasmas near material walls (Institute of Atomic Physics, Bucharest, Romania; Dr. I. Mihailescu).
- (6) Experimental investigation of micro-structural changes of modified SS-316 under energetic alpha particle irradiation (Institute of Atomic Energy, Beijing, China; Dr. Jinan Yu).
- (7) Evaluation of A+M data for metallic impurities in plasmas (Institute of Applied Physics and Computational Mathematics, Beijing, China; Dr. Baolin Jia).
- (8) Investigation of the microstructure of first-wall structural materials (Nuclear Materials Institute, Chengdu, China; Dr. Zhongqui Sheng).

4.5. Special Service Agreement Programme

To accelerate the programme on establishment of specific (some of them purposeoriented) recommended databases, the A+M Data Unit in the reporting period has extensively used the Agency's Special Service Agreement form for inviting individual visiting consultants to advise or assist the Unit in the completion (through additional data generation) and/or evaluation of specific sets of data. The visiting consultants' programme included visits (in the range from one week to two months) of 15 toplevel experts from the research areas relevant to the database projects. The joint work of these experts with the A+M Data Unit staff was essential for the completion or development of the recommended A+M and PMI databases described in the next Section.

The list of visiting consultants under the Special Service Agreement programme is given in <u>Table 2</u>.

<u>Table 2</u>: List of Visiting Experts under Special Service Agreement

Name/Institution		Duration	Data Programme
1.	Prof. E.W. Thomas Georgia Tech., Atlanta USA	two weeks	Ion backscattering
2.	Dr. W. Eckstein IPP Garching, Germany	one week (cost-free)	Ion backscattering
3.	Dr. P.S. Krstic Inst. of Physics, Belgrade Yugoslavia	three weeks	He ²⁺ + H(n) collisions (low-E region)
4.	Prof. E.W. Thomas Georgia Techn., Atlanta USA	one month	Reflection, Phys. Sputtering
5.	Dr. R.A. Phaneuf ORNL, Oak Ridge, USA	three weeks	$H+C^{6+}$, O^{8+} el. capture (state selective)
6.	Dr. H. Tawara NIFS, Nagoya, Japan	three weeks	_ " _
7.	Dr. R. Marchand INRS, Varennes, Canada	three weeks	Radiative cooling rates for C and O impurities
8.	Dr. D.T. Kato NIFS, Nagoya, Japan	one month	e-He excitation data (evaluation, parametrization)
9.	Dr. V.A. Abramov Kurchatov Inst., Moscow Russia	one month	H-recycling database
10.	Dr. P.S. Krstic Inst. of Physics, Belgrade Yugoslavia	two months	Be^{4+} , B^{5+} + H(n) (low-E region)
11.	Dr. E.A. Solov'ev Univ. of St. Petersburg Russia	four weeks	C^{6+} , O^{8+} + H(n) (low-E region)

12. Dr. V. Barabash two weeks Be-materials properties Efremov Inst., St. Petersburg Russia 13. Prof. I.V. Komarov three weeks $A^{q+} + H$ ionization Univ. of St. Petersburg (low-E region) Russia 14. Dr. G.P. Yushko two weeks ALADDIN up-grade Efremov Inst., St. Petersburg Russia

5. DATABASE ESTABLISHMENT PROGRAMME

5.1. Recommended Database for State-Selective Electron Capture (in collaboration with ORNL, Oak Ridge, NIFS, Nagoya, and JAERI)

A recommended cross section database has been established for the state-selective electron capture in collisions of fully stripped carbon and oxygen ions with ground state hydrogen atoms. The database contains more than 80 cross sections in the energy range relevant to fusion applications. This database is of paramount importance in the "charge-exchange recombination spectroscopy "diagnostics of central (hot) plasma regions" of the presently operating large tokamaks. The recommended cross sections are fitted to an analytical expression containing less than ten fitting parameters, and having appropriate physical behaviour in the asymptotic regions. The database has been ALADDIN formatted and stored in the IAEA ALADDIN databank. The data evaluation procedure and the recommended cross section data will be published in ADNDT (1993).

5.2. Recommended Database for Light Ion Reflection from Surfaces

(in collaboration with the IPP Garching and the Georgia Institute of Technology, Atlanta)

A critical assessment of all the available theoretical and experimental data on the particle and energy reflection coefficients for the ions of hydrogen and helium isotopes backscattered from a large number of elemental solid surfaces, was performed. The covered impact energy range extends from about 10 eV up to several hundred keV. Only the normal incidence case was considered. The data for self-ion reflection have also been included in this assessment. The recommended data have been fitted to a six-parameter analytical expression (nine parameters for the self-ion reflection), with an rms deviation below 5% in all cases. The recommended particle "number" and "energy" reflection coefficients, in their parametrized form, have been stored in the A+M Data Unit's ALADDIN system, and distributed to fusion

laboratories and other interested research groups. This database has also been published in hard-copy format (IAEA report INDC(NDS)-249 (1991)), and in a condensed form (with elements of the background physics and assessment procedure) in Nucl. Instr. Meth. Phys. Res. B <u>69</u> (1992) p. 427.

5.3. Recommended Database for Physical Sputtering of Fusion Relevant Materials under Light Ion Impact

(in collaboration with the Georgia Institute of Technology, Atlanta, and the Institute of Applied Physics and Computational Mathematics, Beijing)

The available theoretical and experimental data for physical sputtering of a large number of elemental and composite fusion relevant materials under normal incidence bombardment of hydrogen- and helium-isotope ions have been critically assessed and a set of recommended sputtering yield coefficients (as function of incident ion energy) has been established. The considered energy range extends from the threshold to several hundred keVs. The case of self-ion sputtering for the most important first wall candidate materials has also been included in this assessment. The recommended sputtering yield coefficients have been fitted to a single analytical expression containing only one fitting parameter. The recommended data are being stored in the IAEA ALADDIN system, and a hard-copy version of the database, as well as journal publication, are now in preparation.

5.4. Recommended A+M Database for H-Beam Penetration into Fusion Plasmas

A comprehensive recommended database for all collision processes of ground state and excited hydrogen atoms colliding with electrons, protons, alpha particles and other fully stripped (Be^{4+} , B^{5+} , C^{6+} , O^{8+}) and arbitrary stripped (A^{q+} , q > 8) ions, has recently been completed by the IAEA A+M Data Unit staff. The database contains recommended cross sections for more than sixty individual reactions in the energy range from a few eVs (or the threshold, for electron impact processes, and typically $\sim 100 \text{ eV/amu}$ for heavy particle collision processes) (up to several MeV (or MeV/amu for heavy particle collisions). The database is also supplemented by a number of generalized (scaled) formulae for the reactions involving highly excited states and/or ions in high charge states (q > 8), which makes the entire database complete and self-consistent. The primary mission of this database is to meet the needs for modelling of neutral hydrogen beam penetration into fusion plasmas, but it can also be used in other (e.g. diagnostic) fusion applications. The recommended cross section data are presented by analytic-fit functions, having appropriate, physically based, asymptotic behaviour and containing usually not more than 10 fitting parameters. The entire database is ALADDIN formatted and stored in the Agency's A+M database. A handbook, containing a hard-copy version of this database and all the associated information (data sources, assessment procedures, data accuracies, etc.), is now in its final stage of preparation.

- 12 -

5.5. Recommended A+M Database for He-Beam - Fusion Plasma Interaction

(in collaboration with the JET Team A+M Group, FOM Institute, Amsterdam, National Institute for Fusion Science, Nagoya).

The establishment of this database has been initiated during the work at the Consultants' Meeting on "He-beam database for alpha particle diagnostics of fusion plasmas" (see 3.2.). A large part of the existing database has already been evaluated, and recommended cross section for all processes involving the ground state of He have been established. The part of the database involving collisions of excited He-atoms, particularly the transitions between excited states, is still of inadequate accuracy (50 - 100%) at low collision energies. These data uncertainties, however, do not have a significant impact on the calculation of He-beam attenuation in a plasma (due to the low population of excited states during the beam penetration). Part of the evaluated and recommended data are published in Vol. 3 (1992) of the IAEA Series on "Atomic and Plasma-Material Interaction Data for Fusion", and some of them are stored in the Agency's ALADDIN database. It is expected that this database will be completed by the end of 1993.

5.6. Recommended A+M Database for Li-Beam Edge Plasma Diagnostics

(in collaboration with the Technical University, Vienna)

Neutral Li-probing beams are becoming a standard technique for diagnostics of edge plasmas in present tokamak fusion devices. The further developments of this technique, and its extension to reactor level edge plasmas, in particular, depend on the establishment of a complete database for all collisional processes of ground-state and excited Li atoms with plasma electrons, protons and impurity ions. The part of the evaluated database involving Li and Li[•] collisions with electrons and protons is now being completed and stored in the ALADDIN system. The cross sections for electron-loss processes by multiply charged impurity ions are described by a scaling relationship, valid only for ion charge states above q = 5. The entire A+M database for the Li-beam attenuation kinetics in fusion plasmas is expected to be finished by May 1993.

5.7. Collisional Database for Be and B Plasma Impurities

(in collaboration with the Los Alamos National Laboratory, the Queen's University of Belfast, St. Petersburg University, Argonne National Laboratory, University College London, Oak Ridge National Laboratory, and Institute of Physics, Belgrade)

The establishment of the recommended collisional database for Be and B plasma impurities has been initiated by the work performed during and in connection with the IAEA Consultants' Meeting on this subject held on 10-12 June 1991 in Vienna (see 3.3.). Recommended cross sections have been established for all the electron-impact

collision processes involving ground-state Be and B atoms and ions, and their first few excited states. The part of the database involving collisions of Be^{q+} and B^{q+} ions with edge plasma neutrals (H, H₂ and He) is less complete, and its completion is envisaged during 1993 through collaboration with the instituions cited above.

5.8. Recommended Radiative Cooling Rates for Carbon and Oxygen Plasma Impurities

(in collaboration with the University of Quebec, Varennes)

Using the available IAEA recommended database for collision processes involving carbon and oxygen plasma impurities, accurate calculations were performed for the radiative cooling rates of these impurities in a fusion plasma within a wide range of plasma parameters (temperature and density). The temperature dependences of recommended cooling rates for each ion have been represented by analytic-fit functions (for a number of fixed plasma densities around 10¹⁴cm⁻³) containing nine fitting parameters. The recommended radiative cooling rates (together with the associated plasma electron energy cooling rates) due to the carbon and oxygen impurities have been published in the report INDC(NDS)-255, and in a more condensed form (but including the background physics) in Vol. 2 (1992) of the IAEA Series on "Atomic and Plasma-Material Interaction Data for Fusion" (p. 117).

5.9. Evaluated Thermo-Mechanical Properties Data for Beryllium

(in collaboration with the Efremov Institute of Radio-Physical Aparatus, St. Petersburg)

The establishment of a comprehensive evaluated database for the thermo-physical and thermo-mechanical properties of beryllium materials has been initiated in May 1992. In collaboration with Dr. V. Barabash (Efremov Institute, St. Petersburg), the available data for a large number of cast and plasma-sprayed Be materials have been collected, critically assessed, and stored in the ALADDIN material properties database. In view of the intense work currently underway in several laboratories on characterization of different types of Be-materials, the compilation and evaluation work related to this database will continue during 1993.

6. <u>CO-ORDINATION OF A+M AND PMI DATA CENTRE NETWORK</u> <u>ACTIVITIES: DATA PROCESSING AND EXCHANGE</u>

6.1. A+M/PMI Data Centre Network Co-ordination

The main part of the fusion related A+M and PMI data compilation effort is currently being performed by the international A+M/PMI Data Centre Network, the members of which are given in <u>Attachment 3</u>.

A number of the data centres (such as those at NIST-Gaithersburg, ORNL, NIFS-Nagoya, JAERI, IPP-Garching, Efremov Inst.-St. Petersburg) are also performing data assessment work by their own staff or through consultants' services. Almost all of the data centres are also involved in data generation projects, which are directly related to the A+M and PMI needs for fusion. Several of the Data Centre Network members also participate in the Co-ordinated Research Programmes conducted by the A+M Data Unit. The membership of the Network has slightly increased in the recent two years owing to the limited and selective expansion of the co-ordinated data activity in the area of plasma-material interactions.

The co-ordination of all data compilation, evaluation and generation activities is done at the annual Data Centre Network meetings. The agenda of these meetings usually includes the following items:

- progress report on DCN activities and results accomplished in the previous year;
- discussion of current priorities in the A+M/PMI data needs and adjustment of data activity plans for the next year accordingly;
- co-ordination of the next year activity programmes of the Network data centres to achieve rationalization of efforts and optimum output;
- mutual assistance and collaboration in the execution of adopted working plans;
- discussions on data processing and exchange methodologies and ALADDIN system developments.

In the reporting period, the 10th and 11th Data Centre Network meetings were held in Vienna on 23-24 September 1991, and 15-16 June 1992, respectively. The summary reports of these meetings are published in the IAEA reports INDC(NDS)-259/N7 and INDC(NDS)-275, respectively. The work of the Data Centre Network has been coherent, well focussed on fusion data needs priorities, and highly productive. The spirit of co-operativeness within the Network and with the fusion community has also been high.

We note that, owing to the expansion of Data Centre Network membership in the recent years, the meetings of the Network have been reclassified in 1991 from Consultants' to Advisory Group Meetings on "Technical aspects of atomic and molecular data processing and exchange".

6.2. A+M and PMI Data Processing

The data processing activity of the A+M Data Unit consists of the following elements: (i) introduction of externally provided evaluated or recommended data into the ALADDIN system (i.e. ALADDIN data formatting); (ii) intercomparison of various sets of evaluated data for further critical assessments; (iii) parametrization of recommended data sets (i.e. constructing appropriate analytic-fit data representations); and (iv) processing the externally provided bibliographic input for the "International Bulletin on Atomic and Molecular Data for Fusion" into the accepted Agency format.

Most of the data processing work of the Data Unit in the reporting period was related to constructing analytic-fit representations to recommend data (e.g. for electronimpact excitation of He, and Be^{q+} and B^{q+} ions, the data base for the C and O plasma impurities, the H-beam atomic data base), and to the bibliographic data processing involved in the preparation of issues No. 42 - 45 of the Bulletin.

6.3. A+M and PMI Data Exchange

A+M and PMI data exchange between the IAEA A+M Data Unit and the A+M/PMI national data centres is a continuous process going both ways. The exchange of recommended and/or evaluated data uses all available means of information transfer, and most frequently is done by electronic mail. Bibliographic reference data are usually exchanged on diskettes. The data exchange process is not confined only to the members of the A+M/PMI Data Centre Network, but includes also a number of active data generating or data collecting groups (e.g. the Plasma Spectroscopy Group at Cadarache, the Radiation Transport Group at the Los Alamos National Lab., the Lebedev Physical Institute of the Russian Academy of Sciences in Moscow, etc.). This intense data exchange process provides the national data centres with the entire body of recommended/evaluated data information, so that they can act as data dissemination points for the major data users in their own countries (NIST and ORNL for USA, Kurchatov Institute for Russia, JAERI and NIFS for Japan, GAPHYOR for France, Belfast University for UK and CRAAMD for China).

7. <u>A+M/PMI_DATABASE_AND_ALADDIN_SYSTEM_MAINTENANCE_AND</u> <u>DEVELOPMENT</u>

7.1. Maintenance, Updating, and Development of A+M and PMI Databases

The maintenance and the continuing updating and development of the A+M and PMI recommended numerical databases is one of the major responsibilities of the A+M Data Unit. In the reporting period, extensive work has been done on updating the recommended database for carbon and oxygen plasma impurities, including generation of new analytic fits for all the reactions (more than hundred) in the database.

A similar work is now in progress on the A+M data for hydrogen-helium plasmas.

Apart from this activity, the staff of the Unit is also heavily involved in different joint projects with other experts' groups on the establishment of new evaluated and/or recommended numerical A+M/PMI databases (see Section 5), or in the further development of the existing ones (e.g. by adding new reactions, providing new, physically more acceptable parametrizations, etc.).

The most extensive databases currently stored in the ALADDIN database are given in <u>Attachment 4</u>.

7.2. ALADDIN System Maintenance and Development

Another major responsibility of the IAEA A+M Data Unit is to maintain and further develop the Agency's ALADDIN database system, which serves for storage, processing and exchange of all recommended or evaluated A+M, PMI and MATPROP data for fusion. The ALADDIN structure and interface developments in the reporting period include:

- (i) Definition of ALADDIN hierarchical and Boolean labelling schemes and dictionaries for formatting and introducing the material properties data in the system (in co-operation with several IAEA consultants).
- (ii) Initiation of the work on definition of ALADDIN hierarchical and labelling schemes for ALADDIN formatting of the spectroscopic data and their incorporation in the system (in collaboration with NIST, Gaithersburg and ORNL, Oak Ridge), including development of a conversion subroutine to convert the NIST recommended spectroscopic (now in ORACLE) into the ALADDIN format.
- (iii) Development of a new interface (written in C) for ALADDIN to enhance its search (menue driven interactive programme), processing (multiple access to files), graphics and editing capabilities. This effort was undertaken jointly with the Efremov Institute for Radio-Physical Aparatus, St. Petersburg (Dr. G. Yushko) and the staff of the Agency's Physics Section (Dr. V. Osorio). A new, C-version of ALADDIN is now under preparation, and this work is expected to be finished in the next few months. Although the present C-ALADDIN interface is written for PC's (DOS), the transition to UNIX workstations will also be possible.

8. <u>A+M AND PMI DATA PUBLICATION AND DISSEMINATION</u>

8.1. The IAEA Series on "Atomic and Plasma-Material Interaction Data for Fusion"

This IAEA Series has been established in 1990 to provide a medium for publication of large sets of generated or evaluated A+M and PMI data relevant to fusion research and their rapid communication to the entire fusion community. This journal-level publication also serves for publishing reviews on the A+M and PMI data needs for specific research areas in fusion, data status assessments for specific classes of atomic or plasma-material interaction processes, and reviews on the wider A+M and PMI approximately supervised by an International Editorial Board, and technically produced by the "Nuclear Fusion" journal editorial staff.

Three volumes of this series have sofar been published, containing a large body of evaluated A+M and PMI data, detailed data assessment and data status and needs reviews, and sets of original data calculations and measurements.

- Vol. 1 of the series (September 1991) represents a data compendium for particle-surface and plasma-material interaction processes;
- Vol. 2 of the series (June 1992) contains a number of comprehensive data assessment reviews on the A+M collision processes in the fusion edge plasmas;
- Vol. 3 of the series (November 1992) contains recommended and/or evaluated data sets and data status reviews on the A+M collison processes involving He, Be and B atoms and ions;
- Vol. 4 of the series is planned to appear in 1993. It will contain evaluated/recommended sets of data for the thermo-physical and thermo-mechanical properties of fusion reactor plasma facing candidate materials, and a number of reviews on PMI data related issues of the fusion reactor design.

8.2. Data Compendia, Reviews and Journal Publications

The work on the establishment of evaluated/recommended A+M and PMI data bases has resulted in the publication (or preparation) of the following data compendia, reviews and journal publications:

- (i) *Compendia*
 - (1) Collision Processes of Metallic Ions in Fusion Plasmas (Ed. R.K. Janev), Physica Scr. T37 (1991)
 - (2) Atomic and Molecular Processes in Magnetic Fusion Edge Plasmas (Ed. R.K. Janev) (in preparation for Plenum Press)
 - (3) R.K. Janev, J.J. Smith "Recommended Cross Sections for Collision Processes of Hydrogen Ground-State and Excited Atoms with Electrons, Protons and Multiply Charged Ions" (in preparation for At. Data Nuc. Data Tables, and as an IAEA publication)
 - (4) Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion (Eds. R.K. Janev and H.W. Drawin), Elsevier Publ. Co., Amsterdam, 1993 (in preparation)

- (ii) *Reviews*
 - R.K. Janev Atomic physics issues in fusion reactor design Comments At. Mol. Phys. <u>25</u>, 83 (1991)
 - R.K. Janev, A. Miyahara
 Plasma-material interaction issues in fusion reactor design and status of the database
 At. Plasma-Mat. Int. Data Fusion, <u>1</u>, 123 (1991)
 - R.K. Janev
 Atomic processes in thermonuclear fusion plasmas.
 Chapter in: "Progress in Atomic and Molecular Physics", (Ed. C.D. Lin) World Scientific Publ. Co., Singapore 1993 (in press)
- (iii) Journal publications

In the reporting period, the IAEA A+M Data Unit's staff has published more than <u>15 publications</u> in international scientific journals containing A+M or PMI data relevant for fusion. Five of these publications <u>contain recommended</u> <u>A+M/PMI data</u>.

8.3. IAEA-NDS Publications of Recommended Data

Expanded versions of certain A+M/PMI data bases, supplemented by appropriate background physics comments, are sometimes also published as IAEA-NDS publications. In the reporting period, two such publications appeared:

- "Particle Reflection from Surfaces: A Recommended Database" (by E.W. Thomas, R.K. Janev and J.J. Smith) IAEA Report INDC(NDS)-249 (1992)
- (2) "Radiative Losses and Electron Cooling Rates for Carbon and Oxygen Plasma Impurities" (by R. Marchand, R.K. Janev and X. Bonnin) IAEA report INDC(NDS)-255 (1992)

8.4. Numerical Data Dissemination

The dissemination of evaluated or recommended numerical A+M and PMI data to fusion laboratories and research groups, as well as to the most active A+M/PMI physics groups, is done on a continuous basis. The recommended/evaluated

A+M/PMI databases available at the IAEA are being announced in each of the issues of the international bibliographic A+M data Bulletin, where the procedure for requesting and obtaining the data is explained.

All the recommended and evaluated A+M/PMI data are also stored at a number of national data centres (see Section 6.4.), from where data dissemination also takes place.

The ORNL A + M/PMI Data Centre is currently establishing a IBM RISK Workstation based ALADDIN database (identical to that stored at the IAEA) which will be accessible on-line by all users within the US Magnetic Fusion Programme.

9. INTERNATIONAL BULLETIN ON ATOMIC AND MOLECULAR DATA FOR FUSION

The International Bulletin on Atomic and Molecular Data for Fusion publishes semiannually selected bibliographic information on references containing A+M and particle-surface interaction data of interest to fusion research. References on spectroscopic A+M data are also included. The input for the Bulletin, prepared and edited by the A+M Data Unit, is provided by the NIST, ORNL, NIFS, Kurchatov Institute, and GAPHYOR data centres. The Bulletin is being distributed to over one thousand institutions, laboratories and individuals. Five issues of the Bulletin (Nos. 42 - 45) have been published and distributed in the reporting period. The delay in the replacement of the staff member responsible for the Bulletin publication has resulted in a similar delay in the publication of the Bulletin. The issues No. 42-45 have, therefore, been published in one volume.



IAEA PROGRAMMES

ON

ATOMIC AND PLASMA - MATERIAL INTERACTION

DATA FOR FUSION

IAEA A+M DATA UNIT

NUCLEAR DATA SECTION DIVISION OF PHYSICAL AND CHEMICAL SCIENCES

OBJECTIVES AND RELEVANCE

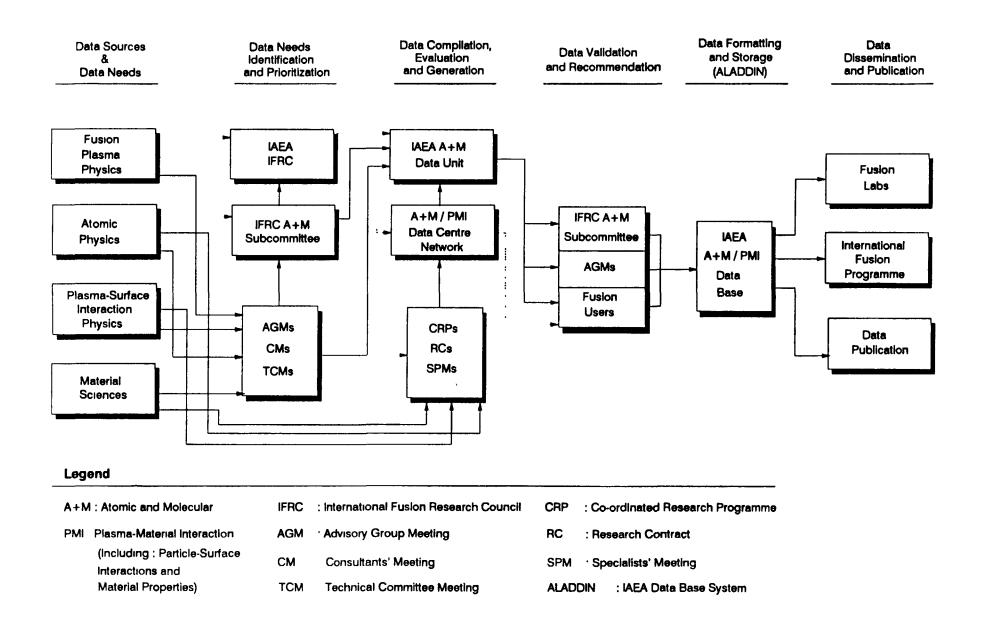
PROGRAMME OBJECTIVES

- * ESTABLISH AN INTERNATIONAL BANK OF RECOMMENDED ATOMIC, PLASMA-WALL INTERACTION AND MATERIAL PROPERTIES DATA FOR FUSION ENERGY RESEARCH AND REACTOR DESIGN;
- * CO-ORDINATE AND INTEGRATE THE WORLD'S EFFORTS IN PROVIDING THE FUSION PROGRAMME WITH EVALUATED DATA;
- * DISSEMINATE THE DATA INFORMATION TO NATIONAL FUSION LABORATORIES, INTERNATIONAL FUSION PROJECTS AND OTHER USERS IN THE AGENCY'S MEMBER STATES.

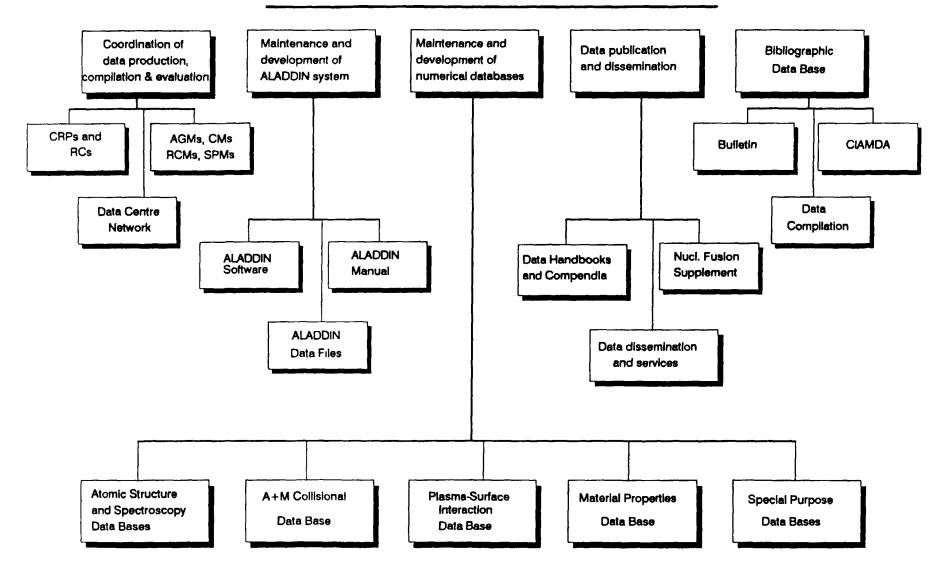
FUSION RELEVANCE

- * SELECTION OF PLASMA FACING REACTOR MATERIALS;
- * OPTIMIZATION OF REACTOR IMPURITY CONTROL SYSTEM;
- * OPTIMIZATION OF REACTOR POWER AND PARTICLE EXHAUST SYSTEM;
- * PLASMA ENERGY BALANCE AND RADIATION LOSSES;
- * OPTIMIZATION OF PLASMA HEATING NEUTRAL BEAM SYSTEM;
- * PLASMA MODELLING;
- * PLASMA DIAGNOSTICS.

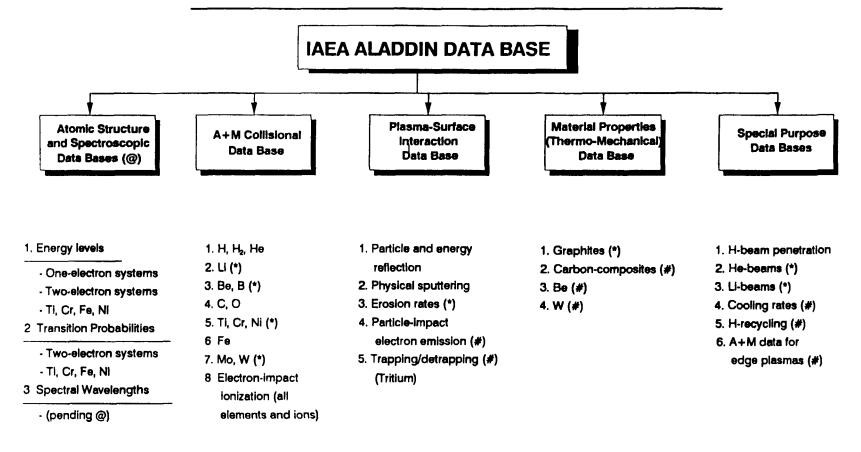
FUSION A+M / PMI DATABASE ESTABLISHMENT: INTERACTIVE ELEMENTS AND INFORMATION FLOW



IAEA A+M DATA UNIT ACTIVITIES



IAEA A+M/PMI NUMERICAL DATA BASES



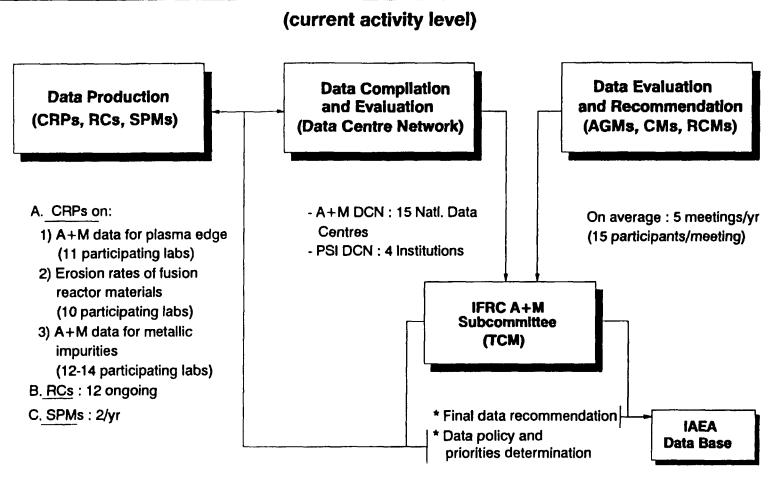
Legend :

@ Most of these databases are maintained at NIST (Washington)

and VNIIFTRI (Mendeleevo)

* Work in progress

Initiated or planned



CO-ORDINATION OF DATA PRODUCTION, COMPILATION AND EVALUATION

Legend :

DCN - Data Centre NetworkSPM - Specialists' MeetingTCM - Technical Committee MeetingPSI - Particle Surface InteractionAGM - Advisory Group MeetingCRP - Co-ordinated Research ProgrammeCM - Consultants' MeetingRC - Research ContractRCM - Research Co-ordination Meeting

DATA PUBLICATION AND DISSEMINATION

Data Handbooks and Compendia

Nucl. Fusion A+M/PMI Supplement

- @ Compendium on PSI data for Fusion
- (Nucl. Fus. Spec. issue, 1984) @ Compendium on A+M Data for Iron lons
- (Nucl Fus. Spec. Issue, 1988)
- @ Compendium on A+M Data for C and O lons
 - (Physica Scr. Topic. Issue, 1989)
- Compendium on A+M Data for Metallic Impurities
 - (Physica Scr. Topic. Issue, 1991)
- Handbook on A+M Data for H-beams in plasmas (IAEA, 1991)
- # Handbook on A+M data for He-beams in plasmas
- (IAEA, 1992) # Compendium on A+M data
- for Li-beam diagnostic
- (IAEA TecDoc, 1992)

(Regular journal-level publication, issued once per year)
Vol. 1 : PMI data (1990)
Vol. 2 : A+M data for plasma edge (1991)
Vol. 3 : He,Be,B-data (1992)

Data Dissemination and Services

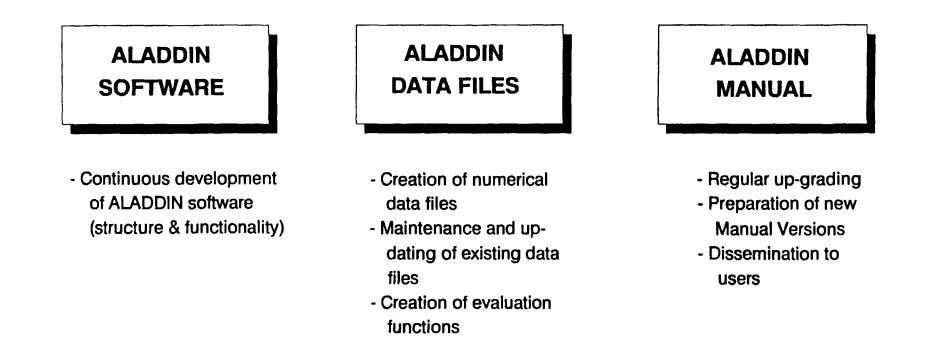
- Ø Dissemination of numerical data in computer-readable form and in book format on a regular basis
- @ Dissemination of data and publications on request

Legend :

- @ Work already performed
- * Work in progress
- # Work initiated or planned

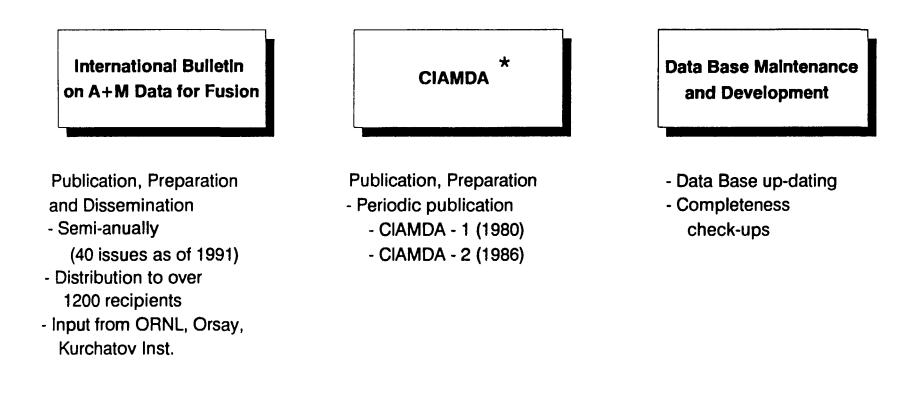
- A+M Atomic and Molecular PSI - Particle Surface Interaction
- PMI Plasma Material Interaction

MAINTENANCE AND DEVELOPMENT OF ALADDIN^{*} SYSTEM



* ALADDIN is the IAEA computerized system for storage, management and exchange of all numerical data bases for fusion, maintained by the A+M Data Unit

IAEA A+M BIBLIOGRAPHIC DATA BASE FOR FUSION



* Computerized Index of Atomic and Molecular Data for Fusion

Draft

PROPOSAL FOR CO-ORDINATED R & D PROGRAMME TASKS FOR ITER

1. Introduction

At the request of the International Fusion Research Council the Atomic and Molecular (A + M) Data Unit of the I A E A has, for more than 15 years, been co-ordinating the world wide efforts on compilation, evaluation and generation of A + M data for fusion. Five years ago this unit also established a similar activity in the area of plasma-material interactions (PMI). In recent years, both the ITER activities and the results of current tokamak experiments have further emphasised the importance of A + M and PMI processes. Whilst it has long been established that (A + M) processes play diverse and significant roles in fusion discharges and in their associated diagnostic tools the ITER studies have directed particular attention to processes related to divertor performance, the impact of plasma facing materials upon plasma condtions, the exhaust of helium ash and the various applications of neutral beams.

In order to meet the specific needs of ITER during the CDA phase the A + M Unit provided the the ITER Physics Team with a recommended atomic data base for determination of neutral beam attenuation in ITER plasma (thereby allowing the determination of the required beam energy). In the post - ITER CDA period the Unit has initiated the establishment of a similar data base for ITER He-Beam alpha particle diagnostics. The purpose of this Proposal is to extend the activity of the Unit to the specific and highly important needs of the plasma edge region.

2. The Role of the A + M Data Unit

In the organisational context of fusion physics, A + M processes are unusual insofar as expertise and activities in this field lie predominantly outside the fusion community. This has impeded the ready formulation and co-ordination A + M R & D tasks for ITER. Furthermore there are to varying degrees disparities in the data used by the partners of ITER, and in order to improve precision and to ensure consistency amongst the predictions of ITER performance, it is highly desirable that internationally recommended data be used. The A + M Data Unit is in a unique position to eliminate both of these weaknesses due to its world wide links and its interaction with both the fusion and the A+ M communities.

The Unit co-ordinates the work of about 15 national A + M data centres (A + MData Centre Network) and maintains an international data bank of recommended A + Mand PMI data for fusion. For enhancing the generation of A + M and PMI data relevant to fusion, the IAEA currently conducts three major Co-ordinated Research Programmes (CRP's) with involvement of more than 30 world leading laboratories in the areas of atomic and plasma wall interaction physics, and sponsors about ten additional research projects in support of these programmes. The A + M and PMI data activity of the IAEA is strongly correlated with the data needs of the fusion programme through continuous direct interaction with fusion research laboratories and through the advisory supervision of the Subcommittee on Atomic and Molecular Data for Fusion of the IFRC.

For the ITER related R & D tasks proposed below, there already exists in the A + M and PMI data bases a significant amount of evaluated data which will be considerbaly augmented during the next few years by the results from the on-going CRP's and by the data compilation/evaluation activity of the A + M Data Centre Network (A + M DCN). The motivation of this proposal is therefore to ensure that the IAEA data base and the associated potential for data generation can be efficiently coupled to the specific needs of ITER.

3. Proposed R & D Programme Tasks

Task 1: Radiative Cooling of the Plasma Edge

<u>Objective</u>: To provide accurate information on the radiative cooling capabilities of the scrape-off and divertor regions for various impurity compositions and plasma edge conditions.

Task duration: 3 years

<u>Task_description</u> :	Collect, evaluate and generate (when necessary) all the radiative and collisional atomic data for a collisional-radiative treatment of plasma edge impurity radiation (Be, B, C, O, Ti, Fe, Cr, Ni, Mo and W), including also He, H_2 and hydrocarbon molecules. Establish computer programme packages for radiative cooling rate calculations (with recommended atomic data implemented) under various plasma ionization regimes, impurity transport conditions and impurity influxes. Provide a comprehensive data base for the impurity radiative power loss functions and for the plasma edge radiative cooling in a broad range of ITER relevant plasma conditions.
Available base for the task:	The collisional data bases for He, Be, B, C, O and Fe impurities are virtually complete and stored in the Agency's ALADDIN data base system. The ongoing IAEA CRP on "Atomic data for medium- and high-Z impurities" is expected to generate the recommended data bases for Ti, Cr, Ni, Mo and W by 1994. Information on impurity influxes can be obtained from another

reactor materials".

ongoing IAEA CRP on "Plasma-interaction induced erosion of fusion

	Impurity transport and ionization balance codes with provisions for impurity radiative cooling calculations already exist in fusion laboratories. Implementation of recommended atomic data for C, O and Fe in these codes has already been initiated in several fusion laboratories (Princeton, Cadarache, JET, Varennes).
Additional work required for task <u>accomplishment</u> :	Completion of the radiative and collisional data bases for the low ionization stages of high-Z impurities (Ni, Mo, W) will require both stronger focussing in the existing IAEA CRP on impurities and inclusion of new contributors to the task. Significant additional efforts will be required to document the processes involving excited states (needed for the collisional-radiative plasma model). Implementation of all the available and expected new atomic data information in the impurity radiation codes is also a labor intensive task. For predictions of radiative cooling capabilities of entire edge plasma (including molecular related radiation and dissociative cooling), coupling of impurity and neutral transport codes must be achieved.

Task 2: Particle Recycling and Helium Exhaust

Objective: Development of comprehensive multidimensional computer codes for the impurity and neutral particle transport in the scrape-off and divertor plasmas for modelling the hydrogen and impurity recycling in the plasma edge and the helium exhaust from the reactor.

Task duration: 3-4 years

- **Task description:** Establish complete data bases for the atomic processes involving hydrogen (atomic and molecular forms), helium and the major plasma edge impurities (including molecular impurities) and for the particle-surface interaction processes for the candidate plasma facing materials. Implement this information into:
 - (1) Multidimensional Monte Carlo codes of neutral transport,
 - (2) Codes for analytical treatment of neutral transport (both of these linked to 2-D impurity ion and background plasma transport coeds),
 - (3) Erosion/redeposition codes for plasma facing components,
 - (4) Possibly codes for particle transport in the plasma core.

Available base for the task: Recommended collisional atomic data bases for H, H₂ and He and major edge impurities (Be(?), B(?), C, O, Fe) are virtually complete. More data should become available from the ongoing IAEA CRP's on "A+M data for fusion edge plasmas" (ending 1994) and "Atomic data for medium- and high-Z impurities" (ending 1995). Data on some particle-surface interaction processes have already been collected and evaluated (backscattering, physical sputtering), while for other impurity generating processes they are expected from the CRP on "Plasmainteraction induced erosion of fusion reactor materials" (ending 1995).

> There already exist in fusion laboratories neutral transport codes based on 3-D Monte Carlo and as well as analytical treatments. There are also codes for erosion/redeposition and for the transport of impurity ions and background plasma. Coupling between these codes has been initiated to varying degrees.

Additional work Important new information has to be collected, evaluated and/or required for task generated for the elastic ion-neutral scattering, for the angular and accomplishment: energy distributions of reaction products in ionization and dissociation processes, and for all processes involving molecular impurities (such as hydrocarbons) which is necessary for the neutral transport modelling. Generation of all this information is outside the capacity of the ongoing IAEA programmes. Due to current uncertainties in the choice of plasma facing reactor materials, generation of new data on impurity release from later specified materials will certainly be necessary. Under all circumstances, the effects of surface roughness, surface oxide layers on backscattering should be better characterized, as well as the impurity release at elevated material temperatures and under high neutron fluences. Implementation of all the available (recommended) and expected new data information in the neutral and impurity transport and erosion/redeposition codes, as well as the mutual coupling of all relevant codes, is also a significant effort.

Task 3: Data Bases for Optimization of Neutral Beam Heating and Diagnostic Systems

Sub-task 3A: Data Base for the D-beam heating and diagnostic systems;

Sub-task 3B: Data Base for the He-beam alpha particle diagnostic system.

Objectives: Optimization of ion production, ion neutralization and neutral beam penetration efficiencies of the D- and He-beam heating and diagnostic systems. Determine the range of required beam parameters (energy, intensity, shape) for adequate fulfilment of injected beam functions (provision of required heating power and current drive, plasma parameters profile control, adequate diagnostic signals).

Task duration: 2-3 years

- **Task description:** Establish recommended data bases for the volume and surface processes in D⁻ and He-ion sources, for the processes in the beam line and neutralizer cells and for determination of beam penetration in reactor plasmas, with due inclusion of multistep processes and taking metastable He-beam fractions into consideration. Development of comprehensive computer codes for modelling the ion production efficiency as function of ion source plasma and surface materials conditions, for modelling the neutralization efficiency of neutralizer cells and for modelling the beam penetration in the plasma, heating rates, induced current drive profiles, on-set of Alfvén instabilities and effects on impurity generation.
- Available base for the task: Recommended atomic data bases for energetic (Mev/amu) D- and He-beams penetration in reactor-grade plasmas have already been established and stored in the IAEA ALADDIN data base. The data base for medium energy He probing beam (≤ 60 keV/amu) is still incomplete, particularly for collisions involving excited He-states and impurities. There exists a significant body of information which so far has not been critically evaluated, and data on important processes are still missing (see below). Computer codes for modelling of volume and surface interaction kinetics in negative ion sources and for neutral beam penetration into fusion plasmas already exist, but their further development is necessary (see below).

Additional work required for task accomplishment: Completion of the He probing beam data base by additional information on heavy-particle excitation collisions and proton induced transitions between excited states. Development of a He-beam penetration code which distinguishes the singlet and triplet beam states and includes their mixing. Critical evaluation of the available data for volume processes in the negative ion source and generation of new data information where it is missing. Of critical importance for the negative ion production efficiency are the processes of vibrationally excited H_2 and H_2^+ with other constituents of the ion source plasma, with the ion source walls (at various wall temperatures) and with the deliberately added impurities (Cs) in the ion source plasma. Depending on the choice of the neutralization scheme and the working gas in the neutralizer cell, a detailed knowledge of the collisional kinetics in the cell is required to determine the metastable fractions in the beam (which may critically influence the beam penetration).

4. Task Complementarity and Overlaps

Many parts of the above three tasks are complementary and the corresponding atomic data bases overlap to a great extent. Thus, the collisional data bases for impurities and impurity generating processes are essentially the same for impurity radiation and recycling problems, the data base for neutral particle transport and hydrogen recycling overlaps to a high degree with that for the kinetics in the negative ion sources, and there is also a complementarity on the energy scale for the processes involving neutral helium in the He-beam penetration and He-exhaust data bases. There are also similar overlaps in the computer programme packages for calculation of the plasma edge radiative cooling rates and particle recycling. These circumstances will help to minimize the efforts required for the establishment of atomic and particle-surface interaction data bases and computer code packages for all three proposed tasks.

5. Task Implementation

To implement the above proposed programmes, a <u>task group</u> should be formed for each of them consisting of 8-10 leading researchers from the ITER parties together with direct representation from the appropriate ITER design teams. These groups would meet anually in order to co-ordinate research, review the programmes, prepare interim reports and ensure close compliance with the needs of the ITER design groups. The work of these task groups will be supported by the three ongoing IAEA CRP's and by the IAEA co-ordinated A+M Data Centre Network. Further support to the work of the task groups should be ensured by attaching to each of them one or two individual IAEA-sponsored Research Contracts. The specific tasks of the IAEA A+M Data Unit in the programme implementation would be:

- a) to co-ordinate the work within each of the task groups and to organize the support to their efforts from the related ongoing IAEA CRP's and the international A+M Data Centre Network;
- b) to participate directly in the establishment of the required atomic and particle-surface interaction data bases through specific data generation and evaluation contributions (particularly when completion of certain data bases is required);
- c) to assemble the available recommended and newly generated/evaluated data and prepare appropriately formatted computer data files for direct introduction into the fusion application (modelling) codes;
- d) to provide an over-all co-ordination of the work within all three programmes (thus minimizing the over-all effort) and maintain close collaborative contacts with the corresponding ITER design groups.

ATTACHMENT 3

Members of A+M and PMI Data Centre Network

	Centre or A+M/PMI Unit	Key Person/Head
(1)	IAEA A+M Data Unit Vienna (Austria)	R.K. Janev
(2)	Chinese NDC/A+M Unit Institute of Atomic Energy Beijing (China)	Yao Jinzhang
(3)	CRAAMD Institute of Applied Physics and Computational Mathematics Beijing (China)	Sun Yongsheng
(4)	GAPHYOR Univ. Paris XI Orsay (France)	J.L. Delcroix
(5)	ENEA NDC/A+M Unit Bologna (Italy)	E. Menapace
(6)	JAERI NDC/A+M Unit Tokai-mura, Naka-gun (Japan)	T. Shirai
(7)	NIFS A+M/PMI Data Centre Nagoya (Japan)	H. Tawara
(8)	Kurchatov Institute/A+M Data Centre Moscow (Russian Federation)	V.A. Abramov
(9)	Obninsk NDC/A+M Unit Obninsk (Russian Federation)	V. Piksaikin
(10)	VNIIFTRI A+M Data Centre Mendeleevo (Russian Federation)	A.Ya. Faenov
(11)	Efremov Inst. PMI Data Centre St. Petersburg (Russian Federation)	V. Barabash

(12)	Belfast Queen's University A+M Data Centre Belfast (UK)	F.J. Smith
(13)	ORNL A+M/PMI Data Centre Oak Ridge, Tennessee (USA)	D.R. Schultz
(14)	NIST A+M Data Centre Gaithersburg (USA	W.L. Wiese
(15)	JILA Data Information Centre Boulder, Colorado (USA)	T. Broad
(16)	IPP Garching PMI Group Garching (Germany)	W. Eckstein

ATTACHMENT 4

ALADDIN Formatted Recommended and/or Evaluated Data

A. A+M Collisional Databases

- "Atomic and Molecular Data for Fusion, Part I Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions", K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston and F.J. Smith, Culham Laboratory Report CLM-R216, Abingdon, Oxfordshire, United Kingdom (1982); J. Phys. Chem. Ref. Data <u>12</u>, 891 (1983).
- "Recommended Data on Excitation of Carbon and Oxygen Ions by Electron Collisions", Y. Itikawa, S. Hara, T. Kato, S. Nakazaki, M.S. Pindzola, D.H. Crandall, IPPJ-AM-27 report series of the Institute of Plasma Physics, Nagoya, Japan (1983); At. Data Nucl. Data Tables (ADNDT) <u>33</u>, 149 (1985).
- "Recommended Data on Atomic Collision Processes Involving Iron and its Ions", C. Bottcher, D.C. Griffin, H.T. Hunter, R.K. Janev, A.E. Kingston, M.A. Lennon, R.A. Phaneuf, M.S. Pindzola, S.M. Younger, Nucl. Fusion, Special Supplement, (1987).
- "Collisions of Carbon and Oxygen Ions with Electrons, H, H₂, and He, Atomic Data for Controlled Fusion Research, Vol. V", R.A. Phaneuf, R.K. Janev, M.S. Pindzola (Editors), Report ORNL-6090/V5, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA (1987).
- "Atomic and Molecular Data for Fusion, Part II Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions: Fluorine to Nickel", M.A. Lennon, K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, M.J. Murray, F.J. Smith, Report UKEA, Culham Laboratory, Abingdon, OX14 3DB, Oxfordshire, UK (1986); J. Phys. Chem. Ref. Data <u>17</u>, 1285 (1988).
- "Recommended Data for Excitation Rate Coefficients of Helium Atoms and Heliumlike Ions by Electron Impact", T. Kato and S. Nakazaki, IPPJ-AM-58 report series of the Institute of Plasma Physics, Nagoya, Japan (1988). At. Data. Nucl. Data Tables (ADNDT), 42, 313 (1989).
- 7. "Atomic and Molecular Data for Fusion, Part III. Recommended Cross Sections and Rates for Electron Ionization of Atoms and Ions: Copper to Uranium", K.L. Bell et al, Culham Report, CLM-R294, Abingdon, Oxfordshire, UK, (1989).
- 8. "Elementary Processes in Hydrogen-Helium Plasmas", R.K. Janev, W.D. Langer, K. Evans Jr., D.E. Post Jr., Springer-Verlag (1987).

- 9. "Collisions of H, H₂, He and Li Atoms and Ions with Atoms and Molecules, Atomic Data for Controlled Fusion Research, Vol. I", C.F. Barnett (Editor), Report ORNL-6086/VI, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA.
- "Collisional Processes of Hydrocarbons in Hydrogen Plasmas", A.B. Ehrhardt, W.D. Langer, Report PPPL-2477, Plasma Physics Laboratory, Princeton University, Princeton, USA (1988).
- 11. "Recommended Cross Sections for Collision Processes of Hydrogen Ground-State and Excited Atoms with Electrons, Protons and Multiply Charged Ions", R.K. Janev, J.J. Smith (1992; publication in preparation).
- 12. "Electron-Impact Excitation and Ionization of Helium Atoms" (T. Kato, R.K. Janev, At. Plasma-Mat. Int. Data Fusion, <u>3</u>, 33 (1992).
- "Recommended Cross Sections for State-Selective Electron Capture in Collisions of C⁶⁺ and O⁸⁺ Ions with Atomic Hydrogen" (R.K. Janev, R.A. Phaneuf, H. Tawara, T. Shirai; ADNDT-1992 submitted).
- 14. "Evauated Cross Sections for Collision Processes of Li Atoms with Electrons and Protons" (F. Aumayr, R.K. Janev, J.J. Smith et al; 1992; publication in preparation).

B. Particle-Surface Interaction Databases

- 1. "Energy dependence of Ion-Induced Sputtering Yields of Monatomic Solids in the Low Energy Region", N. Matsunami, Y. Yamamura, N. Itoh, H. Tawara, T. Kawamura, IPPJ-AM-52, Institute of Plasma Physics, Nagoya, Japan (1987).
- "Energy Dependence of the Yields of Ion-Induced Sputtering of Monatomic Solids", N. Matsunami, Y. Yamamura, Y. Itikawa, N. Itoh, Y. Kazumata, S. Miyagawer, K. Morita, R. Strimizu, H. Tawara, Report IPPJ-AM-32, Institute of Plasma Physics, Nagoya, Japan (1988).
- 3. "Particle Reflection from Surfaces: A Recommended Database" (E.W. Thomas, R.K. Janev, J.J. Smith; 1992; IAEA Rep. INDC(NDS)-249).
- 4. "Recommended Data for Physical Sputtering" (E.W. Thomas, R.K. Janev, J.J. Smith, Yughui Qin, J. Botero, 1993; publication in preparation).

C. Material Properties Database

1. "Thermophysical and Thermomechanical Properties of Beryllium" (V.R. Barabash, E. Prokofiev, et al, 1993; publication in preparation).