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IAEA Technical Meeting: Assess and Co-ordinate Modelling Needs and Data Providers

4-5 December 2003, IAEA Headquarters
Vienna, Austria

SUMMARY REPORT

Prepared by: R.E.H. Clark

May 2004

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

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Abstract

This report briefly describes the proceedings, conclusions and recommendations of the Technical Meeting to "Assess and Co-ordinate Modelling Needs and Data Providers", held on 4-5 December 2004. Eight international experts on atomic and molecular data related to fusion energy research activities participated in the meeting. Each participant reviewed the current status of their own speciality and current lines of research as well as anticipated needs in new data for nuclear fusion energy research. Current CRPs on related topics were reviewed. In light of current research activities and anticipated data needs for fusion, a detailed set of tasks appropriate for a new CRP was developed. This meeting completely fulfilled the specified goals.

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1. INTRODUCTION

The Technical Meeting to Assess and Co-ordinate Modelling Needs and Data Providers was held on 4-5 December, 2003 at IAEA Headquarters, Vienna. The purpose of this meeting was to review current status and research activities in a number of areas in Atomic and Molecular (A+M) data research and co-ordinate these research activities with anticipated data needs for nuclear fusion energy research. The outcome was expected to a specific proposal for a new CRP on providing such data needs in the form of a database suitable for use with modelling codes applied to fusion plasmas.

Eight experts on various aspects of A+M data participated in the meeting. Each participant gave a summary of current work in their field of expertise as well as active lines of research. Anticipated data needs in fusion were discussed and summarized. Finally, a detailed proposal for producing a specific database for fusion research was formulated, along with a number of proposed participants.

2. BRIEF MEETING PROCEEDINGS

The meeting was opened by the Scientific, Secretary, R. Clark, who welcomed the participants and introduced Dr. N. Ramamoorthy, Director of the Division of Physics and Chemistry. The strong support of the Agency and the Division to fusion activities was noted. It was also pointed out that fusion energy research has been advancing rapidly. The high probability of agreeing on a site for ITER in the next six months to a year was pointed out as one example. That strong possibility is likely to increase the activity in fusion related research, in particular in the atomic, molecular and plasma-surface interaction areas. It was emphasized that activities such as new CRPs are vital to continue to generate new data needed for the fusion research projects.

Following the introductions, the agenda (see Appendix 1) was reviewed and adopted by the participants. The meeting was attended by eight participants from outside the IAEA (see Appendix 2). During the course of the first day, each participant gave a summary presentation of current research activities. The first session was chaired by J. Tennyson.

The first presentation was from R. Celiberto on elementary processes and transport properties in H_2 plasmas. A published report now gives data for a large number of processes for hydrogen molecules and details the calculations behind the data.

J. Hogan summarized A+M data uses in relation to fusion devices. The data play a key role in plasma confinement optimisation, helium ash removal, impurity effects, tritium retention and other aspects of machine performance. Data are needed for a number of processes for many possible constituents of fusion devices.

M. Kimura described interactions of cold edge plasmas with H_2 and other impurity molecules. He detailed the methods of obtaining data for a number of processes and pointed out that there is limited data for processes from ground state inelastic processes and almost no data for excited states.

M. Larsson gave the final presentation of the first session. He described experimental techniques and reaction products in dissociative recombination of molecular ions. Some of

this research is needed for modelling combustion reactions, such as in jet engines, but can also be applied to fusion plasmas. Possible measurements include recombination cross sections, product branching ratios, excitation of atomic products and angular distributions. A significant list of molecules with some study undertaken was presented.

During the afternoon session chaired by R. Celiberto, the summaries of current research continued.

Y. Martynenko summarized a large scale computer modelling project. This project links together a number of existing codes, develops new codes and provides an interface to connect computing capabilities with remote access. He gave a summary of the current overall capabilities and the systems for which data are reasonably complete.

B. McLaughlin gave the next presentation on electron molecule collisions. He summarized the collision processes considered. Current work is underway on total, differential and momentum cross sections. He outlined the types of molecules for which data are needed in fusion research, and summarized R-matrix theory and capabilities. Several examples of applications were given, and work in progress was summarized.

D. Reiter gave an overview of the situation faced by a modeller of fusion plasmas. He described the different parts of the plasma from the core to the edge and the important parameters in each area and the main processes affecting the different regions. He outlined the importance of molecular processes in the edge region and noted that the molecular processes can have a big impact on the plasma characteristics in the edge, therefore making the quality of the data an important issue. He noted that different databases lead to noticeably different answers and that some databases in use are clearly obsolete. He gave a summary of his view of current database needs.

J. Tennyson gave the final presentation of the first day. He described electron molecule collision calculations using the R-matrix method. He listed the processes that are important at low energies, meaning below the ionization limit in the R-matrix context. He gave a review of the method and the codes available for diatomic and polyatomic molecules. He noted that electron dissociation of H_2 is important for fusion, and compared calculated cross sections with experiment.

3. RECOMMENDATIONS AND CONCLUSIONS

The morning session of the second day was devoted to summarizing the current status of research. B. McLaughlin chaired the session. The first portion of the discussion focussed on formulating a list of the major topics. After considerable reflection, the following list was adopted:

[1] complete data set for molecular hydrogen and ions and cation

[2] general issue of hydrocarbons including ions – basic molecular rates

[3] edge impurities (atomic processes) low charge states W, B, Be, N, O, Ne, Ar, Kr, C, Si; include radiative processes and charge exchange

[4] Be compounds

[5] ambient tritium removal, plasma interaction with surface, molecules emitted

These topics were discussed in turn to summarize the current status and specific data needs within each area, resulting in the following summary of the current status and data needs under each topic:

[1] For n=2 there are some data available in detail, for higher n states, there is not. State resolved data are needed. Data for n=3 are needed for spectroscopy. Also require data on charge exchange for ground state vibrationally resolved, autoionization, isotopes, H_3, H_3+, ion-molecule collisions.

[2] Possibility would be to collect and evaluate data from various sources. Data are needed for all possible channels. Data for cross sections, branching ratios, kinetic energies of products are needed. Electron temperatures from 1 to 10 eV are most important, but may need to go up to 100 eV. Data for the methane family are also important, CH_3, CH_4, CH_5. Surface and volume processes need to be included, also with H → D. A CRP on hydride compounds should be considered.

[3] Ionization, recombination, excitation, H+ collisions, electron capture are important processes. Charge exchange data exist for C, but very little else. Electron excitation and ionisation data exist for light elements. W is of high priority. There are few data for W, scaling formulas used.

[4] Be_xH_y and isotopes, BeO and their ions: currently there is very little available. It may be possible to generate data on these systems.

[5] Tritium removal is a surface topic.

The afternoon session focussed on formulating a specific proposal for a new CRP from the list of topics identified as important. After much discussion and weighing the needs for modelling against what reasonably could be accomplished in a CRP, the following proposal was developed:

Collect and evaluate cross sections, rate coefficients, branching ratios, and kinetic energies from various sources for hydrides and isotopes. Estimates should be made of vibrational relaxation times in the hydride complexes. Gaps in existing data should be identified and filled to the greatest extent possible. Data are needed for all possible break-up channels. Electron temperatures from 1 to 10 eV are most important, as well as an asymptotic extension to high energies. The methane family is the most important case including all the break-up products. Acetylene should be considered as well. BeH_y and their isotopomers as well as their ions should also be addressed. At present there is very little collisional/radiative data available, but it should be possible to generate data on these systems. Information on surface interactions, such as sticking and generation of hydride species is important. The result of this CRP will be a systematic database formatted in a suitable manner for use in plasma edge modelling codes.

The final portion of the afternoon session was used to develop the following list of potential participants in the proposed CRP:

Potential Participants:

Dr. Ursel Fantz
Lehrstuhl für Experimentelle Plasmaphysik
Institut für Physik
Universitätstr. 1
D-86135 Augsburg, GERMANY
Tel.: +49-821-598-3310
Fax: +49-821-598-3302
E-mail: fantz@physik.uni-augsburg.de

Dr. Wolfgang Jacob
Centre for Interdisciplinary Plasma Science
Max-Planck-Institut für Plasmaphysik
EURATOM Association
P.O. Box 1533
Boltzmannstr. 2
D-85748 Garching, GERMANY
Tel.: +49-89-3299-2618
Fax: +49-89-3299-1149
E-mail: wolfgang.jacob@ipp.mpg.de

Dr. Detlev Reiter
Institut für Laser und Plasmaphysik
Heinrich-Heine-Universität Düsseldorf
Universitätsstrasse 1
D-40225 Düsseldorf, GERMANY
Tel.: +49-211-81-12867
Fax: +49-211-81-13718
E-mail: detlev.reiter@laserphy.uni-duesseldorf.de

Dr. Andreas Wolf
Bo 335
Max-Planck-Institut für Kernphysik
Postfach 103980
D-69029 Heidelberg, GERMANY
Tel.: +49-6221-516-503
E-mail: a.wolf@mpi-hd.mpg.de

Prof. M. Capitelli
Centro di Studio per la Chimica de Plasmi
Departmento di Chimica
Universita di Bari
I-70126 Bari, ITALY
Tel.: +39-80-544-2088
Fax: +39-80-544-2024
E-mail: m.capitelli@area.ba.cnr.it

Dr. R.K. Janev
Macedonian Academy of Sciences and Arts
Bulevar K. Misirkov, 2
P.O. Box 428
91000 Skopje, MACEDONIA
Tel.: +389-91-114200
Fax: +389-91-114685
E-mail: rjanev@manu.edu.mk

Dr. Mats Larsson
Department of Physics
Stockholm University
SE-106 91 Stockholm, SWEDEN
Tel.: +46-8-5537-8647
Fax: +46-8-5537-8601
E-mail: mats.larsson@physto.se

Dr. Brendan M. McLaughlin
Dept of Applied Mathematics and
Theoretical Physics
The Queen's University of Belfast
Belfast, BT7 1NN
Northern Ireland
UNITED KINGDOM
Tel.: +44-28-90273369
Fax: +44-28-90239182
E-mail: b.mclaughlin@qub.ac.uk

Dr. Jonathan Tennyson
Department of Physics & Astronomy
University College London
Gower Street
London, WC1E 6BT
UNITED KINGDOM
Tel.: +44-20-7679-7809
Fax: +44-20-7679-7145
E-mail: j.tennyson@ucl.ac.uk

Dr. Alan Garscadden
1950 5th Street
Wright-Pattersan AFB
OH 45433
U.S.A.
Tel.: +1-937-255-2246
E-mail: alan.garscadden@wpafb.af.mil

Dr. John Hogan
Oak Ridge National Laboratory
MS 8072
P.O. Box 2009
Oak Ridge, Tennessee 37831-8072
U.S.A.
Tel.: +1-865-574-1349
Fax: +1-865-576-7926
E-mail: hoganjt@ornl.gov

Dr. D.N. Ruzic
University of Illinois
Department of Nuclear Engineering
103 S. Goodwin
Urbana, IL 61801
U.S.A.
Tel.: +1-217-333-0332
Fax: +1-217-333-2906
E-mail: druzic@uiuc.edu

Dr. David R. Schultz
Oak Ridge National Laboratory
MS-6372, Bldg. 6003
P.O. Box 2008
Oak Ridge, TN 37831-6372
U.S.A.
Tel.: +1-865-5769461
Fax: +1-865-5744745
E-mail: schultzd@ornl.gov

Dr. Albert Viggiano
19 Stone Road
Arlington, MA 02474
U.S.A.
Tel.: +1-937-255-2246
E-mail: albert.viggiano@hanscom.af.mil

In conclusion, the Technical Meeting completely achieved the goals of reviewing the current status of a number of A+M research areas and co-ordinated those research activities with data needs for fusion energy research. A very specific proposal for a new CRP was formulated and potential participants identified. Upon the formulation of the list of potential participants, the meeting was adjourned.

Appendix 1

IAEA Technical Meeting:
"Assess and Co-ordinate Modelling Needs and Data Providers"

4-5 December 2003, IAEA Headquarters
Vienna, Austria

MEETING AGENDA

Thursday, 4 December **Meeting Room: A-10-38**

09:30 - 09:45	Dr. Ramamoorthy R.E.H. Clark	Welcoming remarks Adoption of agenda

Session 1: Reports on current status

Chairman: J. Tennyson

09:45 - 10:15	R. Celiberto
10:15 - 10:45	J. Hogan
10:45 - 11:15	***Coffee Break***
11:15 - 11:45	M. Kimura
11:45 - 12:15	M. Larsson
12:15 - 14:00	***Lunch***

Session 2: Reports on current status II

Chairman: R. Celiberto

14:00 - 14:30	Y. Martynenko
14:30 - 15:00	B. McLaughlin
1500 - 15:30	***Coffee Break***
15:30 - 16:00	D. Reiter
16:00 - 16:30	J. Tennyson

Friday, December 5

Session 3: Summary of current status and needs for new database

Chairman: B. McLaughlin

09:00 - 10:30 Summary of current status of available databases.

10:30 - 11:00 ***Coffee Break***

Session 3: Continued

11:00 - 12:00 Discussion of overall need for new data.

12:00 - 13:30 ***Lunch***

Session 4: Planning for generation of new database

Chairman: D. Reiter

13:30 - 15:00 All participants: Discussion of scope of new CRP to fit those needs. Formulation of statement of goals of new CRP. Formulation of list of participants for new CRP.

15:00 - 15:30 ***Coffee Break***

Session 4: Continued

15:30 - 17:00 All participants: Formulation of conclusions of the TM with specific recommendations for new CRP.

17:00 - ***Adjournment of Meeting***

Appendix 2

IAEA Technical Meeting:
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LIST OF PARTICIPANTS

Dr. Detlev Reiter
Institut für Laser und Plasmaphysik
Heinrich-Heine-Universität Düsseldorf
Universitätsstrasse 1
D-40225 Düsseldorf
GERMANY
Tel.: +49-211-81-12867
Fax: +49-211-81-13718
E-mail: detlev.reiter@laserphy.uni-duesseldorf.de

Dr. Roberto Celiberto
Dipartimento di Ingegneria Civile
ed Ambientale
Politecnico di Bari
Via Orabona 4
I-70125 Bari
ITALY
Tel.: +39-80-596-4244
Fax: +39-80-596-4229
E-mail: r.celiberto@poliba.it

Prof. Mineo Kimura, Ph.D.
Professor of Physics
Yamaguchi University
Ube, Yamaguchi 755-8611
JAPAN
Tel/Fax: +81-836-85-9805
E-mail: mineo@rikaxp.riken.go.jp

Dr. Yuri Martynenko
Scientific Research Centre
"Kurchatov Institute"
Ploshchad I.V. Kurchatova
Moscow D-182, 123 182
RUSSIAN FEDERATION
Tel.: +7-095-196-7041
Fax: +7-095-9430073
E-mail: martyn@nfi.kiae.du

Dr. Mats Larsson
Department of Physics
Stockholm University
SE-106 91 Stockholm
SWEDEN
Tel.: +46-8-5537-8647
Fax: +46-8-5537-8601
E-mail: mats.larsson@physto.se

Dr. John Hogan
Oak Ridge National Laboratory
MS 8072
P.O. Box 2009
Oak Ridge, Tennessee 37831-8072
U.S.A.
Tel.: +1-865-574-1349
Fax: +1-865-576-7926
E-mail: hoganjt@ornl.gov

Dr. Brendan M. McLaughlin
Dept of Applied Mathematics and
Theoretical Physics
The Queen's University of Belfast
Belfast, BT7 1NN
Northern Ireland
UNITED KINGDOM
Tel.: +44-28-90273369
Fax: +44-28-90239182
E-mail: b.mclaughlin@qub.ac.uk

Dr. Jonathan Tennyson
Department of Physics & Astronomy
University College London
Gower Street
London, WC1E 6BT
UNITED KINGDOM
Tel.: +44-20-7679-7809
Fax: +44-20-7679-7145
E-mail: j.tennyson@ucl.ac.uk

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1)26007
telephone: (43-1)2600-21710

Online: TELNET or FTP: iaeand.iaea.org
username: IAEANDS for interactive Nuclear Data Information System
usernames: ANONYMOUS for FTP file transfer;
FENDL2 for FTP file transfer of FENDL-2.0;
RIPL for FTP file transfer of RIPL.
NDSONL for FTP access to files sent to NDIS “open” area.
Web: http://www-nds.iaea.org