

Activities of A+M Data Unit of the IAEA CRPs and XML

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CRP: Co-ordinated Research Project

Joint Project with research effort on topic of interest to fusion:

- Representatives from 10 to 15 research institutions
- Duration of 3-5 years
- Research Coordination Meeting (RCM): periodic meeting at IAEA Headquarters

Goals:

- Data generation
- Compilation and assessment of data
- Data evaluation
- Establishment of databases

Data and results:

- Final results published in “**Atomic and Plasma-Material Interaction Data for Fusion**” (APID)
- Data included in ALADDIN: <http://www-amdis.iaea.org/ALADDIN/>



Active and Planned CRPs

Title	Duration
Atomic and molecular data for plasma modelling	2005-2009
Atomic data for high Z element impurities in fusion reactors	2005-2009
Data for surface composition dynamics relevant to erosion processes	2007-2012
Size, composition and origin of dust in Tokamaks.	<i>To be initiated in 2008</i>

CRP on A + M Data for Plasma Modelling 2005 - 2009

Overall objective

Gathering and generating new data relevant to modeling the edge region of plasmas relevant to nuclear fusion energy devices

- Cross sections, rate coefficients, branching ratios, and kinetic energies from various sources for hydrides (with isotopes) and hydrocarbons.
- Surface interactions, such as sticking and generation of hydride species

First outputs and outcomes

- New generated data
- Data used in the EIRENE code

Agenda

- Second RCM, 18-20 June 2007
- Final RCM, November 2008

CRP on Atomic Data for High Z elements impurities in Fusion Reactors

Overall objective

Two main areas addressed: edge and core regions.

Relevant elements heavier than Mg: noble gases (Ar, Kr and Xe), Si, Cl, Cr, Fe, Ni, Cu, Mo and W, for nearly all stages of ionization.

Processes:

- *Electronic collision*: excitation, ionisation, recombination including DR
- *Heavy particle collisions*: charge exchange and excitation (thermal and beam)
- *Radiative data*: transition probabilities, transition energies and energy levels, ranging from IR to X-rays

First outputs

Benchmark data for some important processes (transition probabilities, excitation and ionization cross sections, charge transfer and recombination)

Agenda

Second RCM, 26-28 September 2007

Final RCM, May 2009



CRP on Surface Composition Dynamics

2007-2012

Overall objective

- To collect and generate new data relevant to erosion dynamics in fusion reactors
- To better understand of the erosion processes and to find possible methods to control the erosion
- Investigated materials will be the most common in fusion reactor machines and mainly the ones foreseen for ITER: C, W, Be

Outcomes

- Experimental and theoretical Data on erosion processes
- Data on transport of atoms and molecules
- Data to be included in the plasma modelling codes like EIRENE

First RCM 17-19 October 2007

Size, composition and origin of dust in Tokamaks

Objectives

- To determine the size, composition and origin of dust in tokamaks

Recommendation

- Consider dust from a variety of elements such as C, W and Be
- Evaluate the role of dust in the tritium inventory and in safety issues

First RCM planned in 2008

Ending CRPs

Title	Duration
Tritium inventory in fusion machine	2001-2006
Atomic and Molecular Data for Fusion Diagnostics	2002-2006
Data for molecular processes in edge plasmas	2002-2006

CRP on Tritium Inventory in Fusion Reactors

Overall Outputs: New data relevant to the overall inventory of tritium in fusion reactors, with special emphasis on the interactions of tritium with plasma facing components and methods for tritium removal

- Removal of tritium is an important issue for ITER
- Investigated materials include carbon, tungsten and beryllium
- Effects of dopants, dependence on particle and heat load
- Flux and fluence dependence of chemical erosion, main issue in plasma modelling
- Still some questions on erosion sources
- Electron-simulated desorption, glow discharge and laser heating are all being investigated for tritium removal
- APID publication, volume 15 is in progress. Review paper to be published in Nuclear Fusion.

CRP on Data for Molecular Processes in Edge Plasmas

Overall Objective

To identify the specific molecular processes that are important to the plasma physics in the edge regions and to provide data for some of these processes

Outputs

- Most important molecular species were: molecular hydrogen with all possible isotope distributions, CO, CO₂, CH₄, C₂-C₃ group hydrocarbons, silicates, nitrogen compounds and H₂O
- Numerous data were produced for the following processes: ionisation, recombination, attachment, detachment, excitation, de-excitation, dissociation, charge transfer, chemical reactions, energy transfer and plasma wall interactions
- APID, volume 13 is in press. Available data are included into ALADDIN.

Atomic and Molecular Data for Fusion Diagnostics

Objective

To identify the needs for A+M data for the diagnostics of core and edge plasmas and for the diagnostics of the velocity distribution of fusion alpha particles.

Outputs

- A variety of cross-sections, required for spectral observations near the strike zone and divertor region, have been measured and calculated
- Cross-section data for both electron and proton impact, required for helium beam diagnostics, have been generated
- Data have been produced for use in the determination of species from light elements such as helium, boron and hydrocarbons, as well as heavy elements such as tungsten
- Data on spectral properties were generated to assist greatly in spectral analysis of plasma emissions
- X-ray emissions from impact on surfaces have been addressed
- Data have been generated for use in hydrogen charge exchange spectroscopy for determination of the flow and temperature of impurities in the divertor region
- APID, volume 14 is in press. Available data are included into ALADDIN.

Computing Developments

Web

- Numerical database ALADDIN
- Bibliographic database AMBDAS
- Web search engine GENIE
- Tools for cross section calculations

XML format for A+M/PSI Data

OPEN ADAS: IAEA-ADAS joint project



Web calculation tools

IAEA

- Cross sections of bare nuclei on hydrogenic ions
<http://www-amdis.iaea.org/HEAVY/>
New process : ionization, Pablo Fainstein and Alain Dubois
- *Average approximation for electron impact excitation of atomic ions*
<http://www-amdis.iaea.org/AVERAGE/>
- *Results from collisional radiative calculations of plasmas are available, as carried out with the Los Alamos modelling codes*
<http://www-amdis.iaea.org/RATES/>

LANL

- Los Alamos atomic physics codes: an interface is available to run several Los Alamos atomic physics codes to calculate atomic structure and electron impact excitation and ionization cross sections (fine structure levels and configuration average)
<http://aphysics2.lanl.gov/tempweb/>

IAEA International Workshop on Challenges in Plasma Spectroscopy for Future Fusion Research Machines

20-22 February 2008, Jaipur, India

http://bitmesra.ac.in/iaea_cps08/index.htm

Joint International workshop

- Birla Institute of Technology (BIT)
- Plasma Science Society of India (PSSI)
- International Atomic Energy Agency (IAEA)

Topics

- Fusion plasma diagnostics using radiations covering infrared to X-ray region
- Development of high performance instrumentation for spectroscopy and detection
- Active diagnostics using atomic beams and lasers
- Imaging techniques
- Simulation and modelling for interpretation of spectra
- Collisional-radiative and impurity transport modeling
- Generation of new Atomic and Molecular data relevant to fusion research

Registration and abstract deadline: 30 October 2007



Distribution List Daff

Daff (Data for fusion), daff@lists.iaea.org

Distribution list to disseminate information on Atomic and Molecular, Particle Surface Interaction (AM/PSI) data relevant to the fusion energy research

176 members, as of October 2007

List administrated by A+M Data Unit



New standards for AM/PSI Data Exchange and XML

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AM/PSI Data Exchange and XML

Need for new methods

- ❑ Old methods (e.g., ALADDIN) are outdated
- ❑ Data exchange is presently determined by internet technologies (IT), where new techniques are permanently developed
- ❑ Structured data, consistency, relationships

AM/PSI Data Exchange and XML

Main idea

- To teach different *databases* and *applications* to speak the **same language**

Tool of choice

- eXtensible Markup Language (XML)
- Metalanguage: tool for development of languages

Example: atomic energy level

□ HTML: `something`

□ One can define new tags, e.g.:

■ `<energy units="eV">2.306</energy>`

must be a
real number

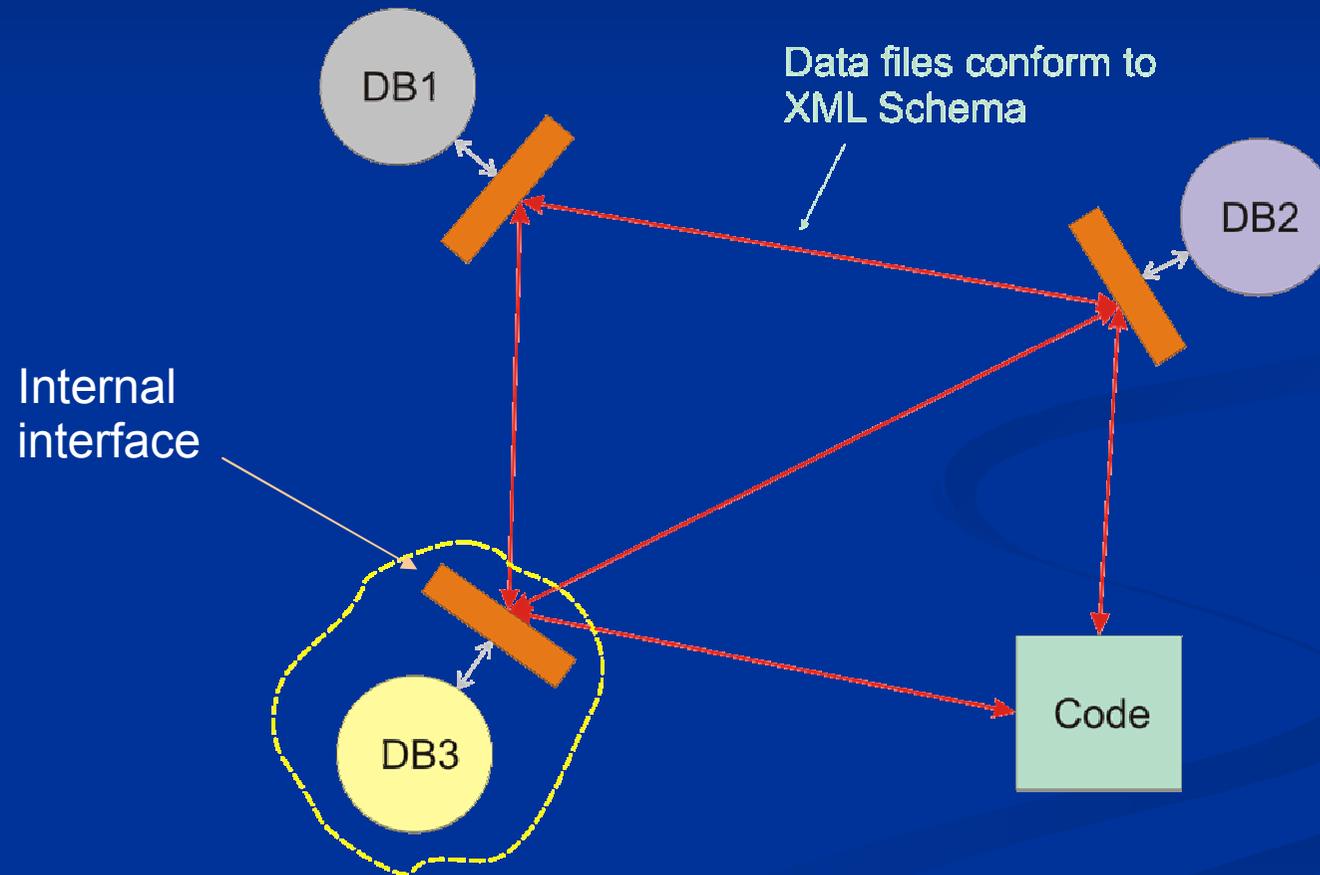
■ `<total_J>1.5</total_J>`

must be a non-negative
integer or half-integer

■ `<total_L>1</total_L>`

must be a
non-negative integer

Data Exchange Strategy



Development Issues

- Technical meetings twice a year
 - IAEA, NIST, ORNL, Observatoire de Paris
- Collaboration with NFRC (Korea), CRAAMD (China) and NIFS (Japan)
- NIST Workshop, May 2007
- Presentations:
 - Iron Project Meeting, August 2007, Yu. Ralchenko
 - IVOA, China, August 2007, M-L. Dubernet
- Schema, version 0.1, June 2008
- Development of DB interfaces
 - NIST ASD
 - IAEA ALADDIN
- Presentation and panel discussion at ICAMDATA, 28-31 October 2008, Beijing, China

IAEA, Vienna International Centre, Atomic and Molecular Data Unit

<http://www-amdis.iaea.org/>

