Past, Present and Future Activities of IAEA Atomic and Molecular Data Unit

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IAEA Atomic and Molecular (A+M) Data Unit to support for fusion program worldwide

We say that we will <u>put the sun into a box</u>. The idea is pretty. The problem is, we don't know <u>how to make the box</u>. -- Nobel prize winner Pierre-Gilles de Gennes Eusion research requires huge amounts of material data – AM/PSI data

- IAEA A+M Unit formed in 1977
- Review progress and achievements of <u>Atomic, molecular and</u> plasma-surface interaction (A+M/PSI) data for Fusion programme worldwide
- Stimulate international cooperation in measurement compilation and evaluation of A+M / PSI data to full



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Coordinated Research Projects http://www-amdis.iaea.org/CRP

Objectives:

- · Generation, compilation and evaluation of data for fusion applications
- Establishment of databases for AM/PSI data
- Development of new techniques related to data activities
- Joint research :

Unique Opportunity for Comprehensive and Synergistic Collaboration
 Experiment + Theory + Modeling + Fusion (ITER) Representatives from 10 to 15 institutes world-wide

Duration 3-5 years; 3 Meetings

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<u>Data and results:</u>
 Journal publications

- Technical Reports
- Numerical databases and libraries

Meetings and Publications (2003-2014)

- 88 meetings have been organized by the Unit for 12 years on average of 7.3/year. (TM, CM, RCM, Cooperation, WS)
- 76 INDC(NDS) reports have been published.
- 6 volumes of the series Atomic and Plasma-Material Interaction Data for Fusion ("Green Books") have been published for CRPs.
- 8 volumes of the series International Bulletin on AM Data for Fusion have been published.
- 4 Special issues have been published or arranged for journal publication from the CRP, meetings and workshops (CCN, SLSP, ICTP, Tungsten)
- A book was published : Nuclear Fusion Research: Understanding Plasma-Surface Interactions (edited by R.E.H. Clark and D.H. Reiter, Springer, 2005)

Outline

- Overview of IAEA A&M Data Unit Activities
- Data Evaluation Activities
- Future of IAEA A&M Data Unit Activities

Network Collaboration for AM/PSI Data for Fusion



CRP reflects the most current data needs in fusion research

2002-2006: <u>Tritium Inventory</u> in Fusion Reactors 2004-2008: Atomic and Molecular <u>Data for Plasma Modelling</u> 2005-2009: Atomic <u>Data for Heavy Element Impurities</u> in Fusion Reactors 2007-2011: <u>Data for Surface Composition</u> Dynamics Relevant to Erosion Processes 2008-2012: Characterization of Size, Composition and Origins of <u>Dust in Fusion</u> Devices

2009-2013: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions

2010-2014: <u>Spectroscopic and Collisional Data for Tungsten</u> from 1 eV to 20 keV 2011-2015: <u>Data for kinetic modelling of molecules of H and He and their isotopes</u> in fusion plasma

2012-2016: <u>Erosion and Tritium Retention for Beryllium</u> Plasma-Facing Materials 2013-2017: Plasma-Wall Interaction of <u>Tungsten and its Alloys in Fusion Devices</u> 2015-2019: Plasma-Material Interaction With <u>Reduced-Activation Steel Surfaces</u>

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Databases for data compilation and distribution

- ALADDIN: SQL based Numerical Database
- Atomic/Molecular Collisional Data, Plasma Surface Interaction Data
- Data traceable, evaluated or produced by experts
- AMBDAS: SQL based Bibliographic Database
 Spectroscopic and Collisional data as well as PSI data
 - Published in the International Bulletin
- GENIE: Search Engine among Databases
 - Radiative properties 9 databases
 - Collisional databases 6 databases
- XSAMS: XML Schema for A+M/PSI Data (guardian)
 SUP@VAMDC node (Virtual Atomic and Molecular Data Centre)
- A Knowledge base provides data information in a "context"

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Online Codes and Code Results for **Modeling Research**

Average Approximation <u>http://www-amdis.iaea.org/AAEXCITE/</u>

- A code for electron impact excitation cross sections of ions Heavy particle collisions http://www-amdis.iaea.org/HEAVY/
- A code for calculation of cross sections for excitation, ionization and charge exchange for bare nucleus on hydrogenic target
- Effective Ionization/Recombination Rates http://www-amdis.iaea.org/RATES/
 Results from collisional radiative calculations of plasmas
- LANL code results http://www-amdis.iaea.org/LANL
- Complete data sets of for Argon, Chlorine and Silicon atoms (~ 2GB) Average Charge States in a wide range of plasma conditions
- FAC code results <u>http://www-amdis.iaea.org/FAC</u>
- FLYFAC based on CFACDB
- A package of codes to solve collisional-radiative model based FAC data 🛞 IAEA



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Community Role: Consensus Building

- An evaluation of data is a critical part of research (PRA policy).
- Disseminate materials to train students and researchers with the "Critical Analysis Skills"
- Disseminate the standard definitions of terminologies adopted by international organizations (IAEA, IUPAC, IUPAP, BIPM, etc)
- The community consensus with an endorsement from the IAEA or other international authorities
 - Group Evaluation: 4-5 panelists like the editorial board for a journal with the broad backgrounds (experimentalists, theoreticians, producers and users)
 - Establishment of the evaluation guidelines: will evolve with time and experience with broad collaborations from the community

Define Terminology: Uncertainty Approach It's NOT AN ERROR but AN UNCERTAINTY

- · Terminology in metrology adopted by international communities (IAEA, IUPAC, IUPAP, BIPM, ISO, WHO, FAO, etc)
- Conceptual Changes of <u>Values and Uncertainties</u>

<u>**True Value**</u> (Error Approach, ~ 1984) \rightarrow A measure of the possible *error* in the estimated value of the measurand as provided by the result of a measurement

<u>rred Value (</u>Uncertainty Approach) \rightarrow Parameter that characterizes the dispersion of the quantity value that are being attributed to a

IAEA AMD Unit Home Page (AMDIS)

http://www-amdis.iaea.org



Coordination Meetings for Evaluation

http://www-amdis.iaea.org/DCN/Evaluation/ CM on Procedures for Evaluation of AM/PMI Data for Fusion
 Current status & future coordination (Japan) CM on Data Evaluation & Establishment of a Standard Library of AM/PMI Data for Fusion (IAEA) TM on Data Evaluation for AM/PSI Processes in Fusion (Korea) TM on International Code Centre Network · General Guidelines for Uncertainty Assessments of Theoretical Data CM on Evaluation of Data for Collisions of Electrons with Nitrogen Molecule and Nitrogen Molecular Ion

Joint IAEA-ITAMP TM on Uncertainty Assessment for Theoretical Atomic Molecular

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Data Evaluation Projects

eMOL project

- · Project to develop methodology for analysing, validating and recommending electron molecule collision data sets
- · Assembled like a journal board. Current "Board" is 43 people.
- Each evaluation is a small group project by 4-7 people
- Aim to provide recommended datasets self-consistent and complete
- (entire energy range, all processes). The first evaluation e-H₂O (May 2013) one joint day with IAEA TM.
- NFRI group evaluation
- e-Methane collisional data evaluation
- IAEA Consultant meetings
- CM on Beryllium atomic collisional data planned
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Theoretical cross-sections without uncertainty estimates



without physical measurements?

IAEA-ITAMP TM : Uncertainty Assessment for **Theoretical Atomic and Molecular Scattering Data**

- Bring together a number of people who are working on electron collisions with atoms, ions, and molecules, heavyparticle collisions, and electronic structure of atoms and molecules (~ 25 Participants)
- Come up with reasonable uncertainty estimates for calculations using the various methods of collision physics: perturbative, nonperturbative, time-independent, timedependent, semi-classical, etc.
- Output \rightarrow Guidelines for estimating uncertainties of theoretical atomic and molecular data

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Critical Assessment for Modeling of Physical Processes (optimized based design)

- Verification. The process of determining how accurately a computer program ("code") correctly solves the equations of the mathematical model.
- Validation. The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model
- Uncertainty quantification (UQ). The process of quantifying uncertainties associated with model calculations of true, physical QOIs, with the goals of accounting for all sources of uncertainty and quantifying the contributions of specific sources to the overall uncertainty.



NSF Division of Mathematics and encourage interdisciplinary scientists and mathematicians on the topic of uncertainty quantification, verification and validation, risk assessment, and

CRP (2015-2019): Plasma-Material Interaction With Reduced-Activation Steel Surfaces

CRP Objective:

- · Support an assessment if steel can replace beryllium or tungsten for the first wall in DEMO or a reactor.
- Topics:
 - · Sputtering and erosion due to exposure to plasma
 - · retention and transport of tritium in a steel surface.
 - Not a topic: Steel as a structural material.
- First meeting in 2015.

Planned Databases : Dust particles in collaboration with IPP-Garching and NFRI (Hong)

- · Serious safety and operational issues: radioactive tritiated co-deposits of nano- to micrometer size.
- Dust with high impact velocities up to several km/s which can easily damage the first wall or diagnostics.

Monitor in-vessel dusts: spatial locations of the origins of dust creation and its frequency, dust velocity distribution, quantitative measurements of amount of dusts created during a run day as well as in a campaign

Database of physical, chemical properties of in-vessel dusts: Size, shape, chemical composition of dusts



Data evaluation Plasma-Material Interaction Data FUTURE DIRECTION OF IAEA **AM DATA UNIT ACTIVITIES**

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Bayesian Update for Data Evaluation and Uncertainty Assignment

Bayes Theorem (1763):

 $p(\underline{x}|\underline{\sigma}|M) = p(\underline{\sigma}|\underline{x}M) \quad p(\underline{x}|M) \mid p(\underline{\sigma}|M)$ posterior = likelihood x prior / evidence

 $p(\underline{x}|\underline{\sigma} M)$: Aposteriori distribution, $p(\underline{x}|M)$: Prior distribution

Example: observable f(x)=a+bx+cx² Simulated experimental data given by $f(y)=(a+by+cy^2)(1+a^{t}r) + \Delta \tau(y)$ where *r* is a uniform random variable *d* is the width of the random interval $\Delta \tau(\mathbf{y})$ is a systematic erro

H. Leeb et al. Consistent Procedure for Nuclear Data Evaluation Based on Modeling,



<u>σ</u> : Set of experimental Data

1: The mean va dashed) of the fr FIG.

CRP (2016-2020): Data for Charge Transfer **Processes for Neutral Beams in Fusion Plasma**

CRP Objective:

- Inventorize, develop and evaluate data for charge
- transfer between neutral beam atoms and plasma ions.
- Provide database to support modelling and diagnostics.
- Topics:
 - · Processes for diagnostic neutral beams and for heating beams; Neutral atoms H, D, T, He, Li, Ne and Ar.
 - · Charge transfer processes in core plasma and in the neutral beam source.
 - · Cross sections and associated photon emission.
- First meeting expected in 2016

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International cooperation planned

- International Workshop on Models and Data for Plasmamaterial Interaction in Fusion Devices, May 2015
 - A follow-up of the hugely successful ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices in 3-7 November 2014
- Workshop on Uncertainty Quantification in Physics and Chemistry, Summer 2015
 - Organized by the Institute for Advanced Computational Science, Stony Brook University
- BIPM Workshop on Measurement Uncertainty, June 2015
 - Revision of the Guide to the expression of uncertainty in measurement (GUM) and discussion on its impact on various metrological aspects



Nuclear Data Sheets, 109 (2008) 2762

 $p(\underline{\sigma} \mid \underline{x}M)$: Likelihood function gives the probability distribution of the data $\underline{\sigma}\,$ for a model M with parameters





Summary

- IAEA AM Data Unit Activities continue the established program over 37 years.
- Currently data evaluation activities are main focus.
- Efforts towards the Internationally agreed standard data library
- More meetings on data evaluation activities planned
- IAEA AM Data Unit Activities are heading in two directions:
 - Coordination of international cooperation in data evaluation
 - Coordination of international cooperation to produce plasmamaterial interaction data for ITER and DEMO