The IAEA Programme towards a standard library of atomic and molecular data for fusion

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Daejeon, Korea, 06 September 2012
Outline

1. About the International Atomic Energy Agency and our place in it; some other IAEA work on standards and reference data.

2. About fusion energy development and the role of atomic, molecular and plasma-material interaction (A+M+PMI) processes.

3. The IAEA programme towards a standard library of A+M data for fusion.
1. About the IAEA

Founded in 1957 as the “Atoms for Peace” organization of the United Nations.
About the IAEA…

The International Atomic Energy Agency

- is a science and technology-based organization in the United Nations family that serves as the global focal point for nuclear cooperation;
- assists its Member States in using nuclear science and technology for various peaceful purposes and facilitates the transfer of such technology and knowledge to developing Member States;
- develops nuclear safety standards and promotes the achievement and maintenance of high levels of safety in applications of nuclear energy, as well as the protection of human health and the environment against ionizing radiation;
- verifies through its inspection system that States comply with their commitments, under the Non-Proliferation Treaty and other non-proliferation agreements, to use nuclear material and facilities only for peaceful purposes.
About the IAEA...

Mainly in the news because of inspections

IAEA establishes Iran Task Force
Las Vegas Sun - Sep 4, 2012
Dated Wednesday, the International Atomic Energy Agency statement says the unit will concentrate on implementing IAEA agreements with...

International: Soltaniyeh: Iran Continues N. Activities under IAEA Supervision Fars News Agency
Blog: Mideast IAEA reports Iran has doubled enrichment capacity Foreign Policy (blog)
IAEA Report Shows Iran Reduced Its Breakout Capacity Truth-Out
Report: IAEA's findings may move up plans for Ynetnews
all 1659 news articles »

With latest IAEA report in hand, UN chief slams Iran for lack of...
MinnPost.com - 22 hours ago
Even as the Non-Aligned Movement (NAM) today backed Iran's nuclear program in its final statement from the Tehran summit, the United Nations chief and a...
International: IAEA Envoy: NAM Presidency to Intensify Support for Iran's Peaceful... Fars News Agency
IAEA report: Iran blocking access as it doubles number of... CBS News
Iran rejects IAEA nuclear report as "political move" Reuters
The Seattle Times - About - News & Issues - Jerusalem Post
all 2502 news articles »
About the IAEA...

Our work belongs to Nuclear Applications
About the Department of NA

http://www-naweb.iaea.org/

Many interests:

- Food and agriculture (cooperation with FAO)
- Human health
- Programme of Action for Cancer Therapy (joint programme with WHO)
- Environment
- Water resources
- Radioisotope production and radiation technology
- Nuclear science
Work on Standards and References has special interest to the IAEA. E.g., the Agency supplies reference materials characterized for presence of

- Radionuclides
- Trace elements and methyl mercury
- Organic contaminants
- Stable isotopes

Examples: Vienna Standard Mean Ocean Water 2 (precise radionuclide composition); standard natural materials characterized for C14; many other.
The IAEA/WHO SSDL Network

The IAEA/WHO Network of Secondary Standards Dosimetry Laboratories (SSDL Network) was established in 1976 as a joint project between the IAEA and the World Health Organization (WHO). At present, it includes 80 laboratories and six (6) SSDL national organizations in 67 Member States, of which over half are developing countries.
Within Nuclear Applications there are several activities in Nuclear Science:

- Nuclear, atomic and molecular data;
- Research reactors and their effective management;
- Accelerators, nuclear spectrometry and allied instrumentation;
- Nuclear fusion and plasma physics.
# About the Department of NA...

Work on nuclear data libraries:


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<td>Experimental nuclear reaction data</td>
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<td>Evaluated nuclear reaction libraries</td>
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<td>reference parameters for nuclear model calculations</td>
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<td>Beam monitor reactions</td>
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<td>Neutron cross-sections, 2006, Decay data, 2005</td>
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About the Department of NA...

Some of the nuclear data libraries at IAEA:

- **EXFOR**: Experimental nuclear reaction data
- **ENDF**: Evaluated nuclear reaction libraries
- **ENSDF**: Evaluated nuclear structure and decay data
- **XUNDL**: Experimental Unevaluated Nuclear Data List
- **FENDL**: Fusion Evaluated Nuclear Data Library
- **IBANDL**: Ion Beam Analysis Nuclear Data Library

These libraries are developed through a network of national data centres coordinated by the International Nuclear Data Committee (INDC) and through technical meetings and consultancies. Some (EXFOR) have a history of 40+ years.
2. About Fusion Energy
About Fusion Energy...

Research was declassified at the 2nd “Atoms for Peace” conference, Geneva, 1958.

Brief (10 seconds) demonstrations of the principle in JET (Joint European Torus, UK) and TFTR (Tokamak Fusion Test Reactor, Princeton, USA).

Korea Superconducting Tokamak Advanced Research (KSTAR) is here at National Fusion Research Institute.

Next step device ITER (Latin: “The way”) is under construction in Cadarache, France; parties are the EU, India, Russia, China, South Korea, Japan and the United States.
About Fusion Energy…

ITER is big:

- 23000 tons mass;
- 840 m³ plasma volume;
- 500 MW fusion power (goal);
- $1.5 \times 10^8$ K (15 keV) central temperature;
- Cryostat 29.3m × 28.6m (h×w)
About Fusion Energy…

Image of a plasma discharge (Asdex Upgrade, Germany)
Fusion plasma involves atomic, molecular and plasma-material interaction processes.

- Atomic processes in hot plasma: ionization, recombination, charge transfer, line radiation. Main species H (D, T), minor species may include He, C, N, O, Ne, Ar, Fe, Mo, W,…

- Molecular processes near wall: vibrational excitation, ionization, dissociation, recombination. Main species: H₂, H₂⁺, H₃⁺, H⁺; minor species may include He⁺, HeH⁺, LiH⁺, BeH⁺, BH⁺, CₓHᵧ⁺, …

- Plasma wall interaction processes: sputtering (of wall material), trapping (of plasma material), redeposition (of eroded material), …
About Fusion Energy…

Work on Fusion energy development within IAEA/NA: Physics Section programme on Nuclear Fusion Research.

- Biennial Fusion Energy Conference (Daejeon, 2010)
- Journal *Nuclear Fusion* (Published by IOP)
- Technical Meetings, Coordinated Research Projects

Nuclear Data Section has Atomic and Molecular Data Unit.

- Databases ALADDIN, AMBDAS and others; search engine GENIE; wiki-style knowledge base
- Technical Meetings, Coordinated Research Projects

NDS also has the

- FENDL: Fusion Evaluated Nuclear Data Library
A+M Data Unit at IAEA

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

“Atomic and Molecular Data”

• Really A+M+PMI: atomic, molecular and plasma-material interaction data
• Data for magnetic confinement fusion energy

Activities of the Unit

• Maintain numerical and bibliographical databases and knowledge base
• Organize coordinated research projects
• Organize technical and other meetings
Atomic and Molecular Data Unit Activities

The Atomic and Molecular Data Unit operates within the Nuclear Data Section of the International Atomic Energy Agency, Vienna, Austria. The primary objective of the Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other plasma science and technology applications.

- Databases on Atomic and Molecular Data for Fusion.
  - Atom, Molecule Plasma Surface Data
  - ALADDIN Numerical Database
  - AMDBAS Bibliographic Database
  - GENIE Atomic Data Search Engine
  - OPEN ADAS Database Search
  - Revbin Data Base Levels Triplet D
  - FC Factors & A-values of H2 & Isotopes

- Online Computing Capabilities
  - Code Centres Portal
  - LANL Atomic Physics
  - FLYCHK Non-LTE Kinetics
  - Heavy Particles Collisions
  - Averaged e-Impact Cross-section
  - Effective e-Ionization Rates
  - ATOM-AKM e-Collision Data

- Knowledge Base for Atomic, Molecular and Plasma-Material Interaction Data for Fusion

Our Unit achieves its objectives by coordinating the activities of the International Atomic and Molecular Data Center Network (DCN) and Code Center Network (CCN), initiation and conducting international Coordinated Research Projects (CRP), organization of various types of Expert Meetings, publication of technical reports on meetings and research activities and using other forms (research contracts, research agreements, consultancies) for stimulation of the generation, collection and critical assessment of the required atomic, molecular (A+M) and plasma-material interaction (PMI) data information.

The activity of Our Unit is supervised and biennially reviewed by the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC A+M Subcommittee), an advisory body to the Agency’s Director General.
A+M Data Unit at IAEA...

ALADDIN
Numerical database maintained by the IAEA Nuclear Data Section A+M Data Unit

Atomic and Molecular Data
- Electron Collisions
- Photon Collisions
- Heavy Particle Collisions

Particle-Surface Interactions
- Erosion, Sputtering, Sublimation
- Reflection
- Trapping, Penetration

http://www-amdis.iaea.org/ALADDIN/
The IAEA Programme on A+M Data

“The IAEA Programme towards a standard library of atomic and molecular data for fusion” (1978-2012).

**Start**: Active programme of data gathering, data evaluation; “best” data or recommended data entered into the ALADDIN database at IAEA.

**Later**: Less interest (worldwide) in data evaluation. IAEA activities support data development, data exchange issues, not data evaluation or recommendation.

**Status**: IAEA database is out-of-date. It has recommended and best data from the 1980s, 1990s; not best data today.

**Present objective**: Re-invigorate data evaluation work, with the aim to provide an assessed and recommended library of A+M+PMI data for fusion.
Towards a standard library...

- Build up an infrastructure for evaluation (including a library of un-evaluated data). *We work with NFRI (DCPP) on this.*
- Develop guidelines for evaluation; especially uncertainty assignment for calculated data.
- Build up a data evaluators network with good ties to the fusion modelling and diagnostics community.
- Inventorise which data sets are used in fusion energy research and which areas are most in need of evaluation.
- Inventorise and reconsider previous evaluated data sets. These activities are valuable long before the goal is reached to have a recommended standard library of A+M+PMI data.
This week: “Joint IAEA-NFRI Technical Meeting on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion”.

Organized with generous support from the National Fusion Research Institute (NFRI, Daejeon).

Technical Sessions (Focused on Reaction Data)

- Evaluation Methods and Experiences
- Current Evaluated Databases
- Error Propagation and Sensitivity Analysis
- Theoretical Data Evaluation
- Experimental Data Evaluation
- Data Centres Network Activities

Valuable and important step towards the standard library.
Concluding remarks

- Atomic, molecular and plasma-material interaction processes are extremely important in fusion plasma and the production of data for A+M+PMI processes is a world-wide effort.
- The IAEA aims to support fusion development through the provision of evaluated and recommended data for A+M+PMI processes.
- Scientific challenge: uncertainty assessment for calculated collision data.
The IAEA Programme on A+M Data…

• Scientific challenge: uncertainty assessment for calculated collision data.
• Organizational challenge: database management with widely distributed sources.
• Social challenge: Strengthening an evaluators network with focus on A+M data for fusion.

Thank you for your attention!