Database and Data Evaluation Activities by the IAEA A+M Data Unit

Bas Braams and Hyun Chung

Second Research Coordination Meeting of the CRP on A+M Data for Hydrogen and Helium in Fusion Plasma

Vienna, 3-5 July 2013
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
  - AME/DAS Bibliographic Database
  - GENIE Atomic Data Search Engine
  - OPEN ADAS Database Search
  - Rovibronic Energy Levels
  - Triplet D3
  - FC Factors & A-values of H & 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's 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.
Data Evaluation

Our task: To provide internationally recommended and validated data for A+M+PMI/PSI processes relevant to fusion.

Before recommendation comes evaluation.

Evaluation has multiple facets: documentation, traceability, data integrity, domain of validity, quantification of uncertainty.

Uncertainty assessment is well established for experimental data; needs work for theoretical data.
Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

- If the authors claim high accuracy, or improvements on the accuracy of previous work.
- If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.
- If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

A presentation by G. W. F. Drake shows that the policy is effective for papers on structure and spectra; not yet for papers on scattering.
Define Terminology: Uncertainty Approach

It’s NOT AN ERROR but AN UNCERTAINTY

- Terminology in metrology
  - VIM (Vocabulaire International de Métrologie, Bureau Int. des Poids et Mesures) 2007
  - GUM (guide to the expression of uncertainty in measurement) 2008

- Measurement and uncertainty
  - The objective of a measurement is to determine the value of the measurand (GUM)
  - In general, a measurement has imperfections that give rise to an error in its result.
  - Error 1 = Measurement result – True value (Error approach)
    - True value: value consistent with the definition of a given particular quantity
  - Error 2 = Measured value – Reference value (Uncertainty approach)
    - Reference value (Assigned value): The reference quantity value can be a true quantity value of the measurand, in which case measurement error is unknowable, or an appropriate, known quantity value such as a conventional quantity value or a specified target quantity value to be realized in a production process.
Nuclear Data Evaluation (Following R. Capote)

Evaluated cross sections and covariance matrices

Experimental Input
- Inter and intra experiment correlations
- Experimental cross sections

Prior Knowledge
- Model Defects
- Parameter Uncertainties
- Model cross sections

From D. Neudecker, S. Gundacker, H. Leeb et al., ND2010, Jeju Isl., Korea
Nuclear Data Evaluation (Following R. Capote)

Typical situation; optimize model parameters, GLSQ
Unified Monte Carlo (Bayes + Metropolis)


\[
p(\sigma) = C \times \mathcal{L}(y_E, V_E | \sigma) \times p_0(\sigma | \sigma_C, V_C)
\]

\[
p_0(\sigma | \sigma_C, V_C) \sim \exp\{-(\frac{1}{2})[(\sigma - \sigma_C)^T \cdot (V_C)^{-1} \cdot (\sigma - \sigma_C)]\}
\]

\[
\mathcal{L}(y_E, V_E | \sigma) \sim \exp\{-(\frac{1}{2})[(y - y_E)^T \cdot (V_E)^{-1} \cdot (y - y_E)]\}, \quad y = f(\sigma)
\]

\(y_E, V_E\): measured quantities with “n” elements

\(y_C, V_C\): calculated using nuclear models with “m” elements
Selection of experimental data

Cross Section (barns)

Incident Energy (MeV)
Nuclear Data Evaluation (Following R. Capote)

A real evaluation

$^{55}\text{Mn}(n,\gamma)$
Fusion Science and Technology

CONTENTS / MAY 2013—VOL. 63, NO. 3

Selected papers from
IAEA-NFRI TECHNICAL MEETING ON DATA EVALUATION FOR ATOMIC, MOLECULAR AND PLASMA-MATERIAL INTERACTION PROCESSES IN FUSION
September 4–7, 2012
Daejeon, Republic of Korea

Preface / H. Chung, B. J. Braams
TECHNICAL PAPERS

313 Critical Evaluation of Data on Atomic Energy Levels, Wavelengths, and Transition Probabilities / Alexander Kramida

324 CHIANTI: An Atomic Database for Astrophysical Plasmas / E. Landi, K. P. Dere, P. R. Young, G. Del Zanna, H. E. Mason

333 Evaluation of the Evaluated Cross-Section Data for Atomic and Molecular Collisions / Y. Itikawa

338 Some Systematics in Electron Scattering Cross Sections / Grzegorz Karwasz, Kamil Fedus


363 Assessment of Atomic Data: Problems and Solutions / Kanti M. Aggarwal, Francis P. Keenan


378 Electron Swarm Parameters and Electron Collision Cross Sections / Yoshiharu Nakamura

385 Atomic Scattering Data and Their Evaluation: Strategies for Obtaining Complete Cross-Section Sets for Electron Collision Processes / Stephen J. Buckman, Michael J. Brunger, Kurunathan Ratnavelu
392 Target Dependence of Single-Electron-Capture Cross Sections for Slow Be, B, C, Fe, Ni, and W Ions Colliding with Atomic and Molecular Targets / M. Imai, Y. Iriki, A. Itoh

(CONTINUED)

CONTENTS / MAY 2013—VOL. 63, NO. 3

(CONTINUED)

400 Atomic and Molecular Databases and Data Evaluation Activities at the National Institute for Fusion Science / Izumi Murakami, Daiji Kato, Masatoshi Kato, Hiroyuki A. Sakaue

406 Cross Sections of the Processes Induced by Electron Collisions with \( H_2^+ \), HeH\(^+\), and Their Isotopes / Hidekazu Takagi

413 IAEA Coordinated Activities on Evaluation of Atomic, Molecular, and Plasma-Surface Interaction Data for Fusion Applications / H.-K. Chung, B. J. Braams
Other activities

Planning a meeting joint with ITAMP, 2014: “Uncertainty propagation in calculated scattering data” (or similar title).

Ongoing cooperation with NFRI and with a European EMOL network (N. J. Mason) on data evaluation.
Conclusion

There is new interest in data evaluation as a more systematic activity.

Uncertainty assessment is a challenge for theoretical data, especially cross section data; methods need to be developed and/or demonstrated for our A+M data.

The IAEA A+M Data Unit seeks to encourage and support this work through its meetings.
Common Workflow Guidelines for Evaluation of Collisional data

Workflow of critical evaluation of data on wavelengths and energy levels (NIST)

Advantages:
- Easier to expand the evaluators’ network including early career researchers.
- Introduce more rigorous procedures for evaluation and increases the dependability of the evaluation.

Disadvantages:
- The quality of evaluation critically depends on the experiences of the evaluators.
- It is possible that different people may reach at different conclusions using the same guidelines and the results may not be reproducible.

Solutions:
- Collaborations can help reducing the disadvantages.
- Evaluation activities by scientific advisors and editorial panels will be a great mechanism to produce the evaluated data library.