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Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion

Summary Report of a Joint IAEA-NFRI Technical Meeting

Daejeon Convention Center, Daejeon, Republic of Korea

4–7 September 2012

Prepared by

Hyun-Kyung Chung

December 2012

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Abstract

This report summarizes the proceedings of the Joint IAEA-NFRI Technical Meeting on "Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion" on 4-7 September 2012. Twenty five participants from 10 Member States and two from the IAEA attended the four-day meeting held at the Daejeon Convention Center in Daejeon, Republic of Korea hosted by the National Fusion Research Institute (NFRI) in conjunction with the 8th International Symposium on Standard Reference Data. The report includes discussions on the issues of the critical assessment of fundamental data required for fusion and plasma applications, meeting conclusions and recommendations. The abstracts of presentations presented in the meeting are attached in the Appendix.

December 2012

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1. Introduction

The Joint IAEA-NFRI Technical Meeting (TM) on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion was held in the Daejeon Convention Center, Daejeon, Republic of Korea from 4th to 7th September 2012 hosted by the National Fusion Research Institute (NFRI, Korea) in conjunction with the 8th International Symposium on Standard Reference Data organized by the Korean Research Institute of Standards and Sciences (KRISS, Korea).

The meeting objectives were to discuss the various aspects of the critical assessment and evaluation of atomic, molecular and plasma-material interaction data used in fusion and other plasma applications. This meeting is the 3rd of the series of meetings on data evaluation activities organized by the IAEA Atomic and Molecular (A+M) Data Unit in 2012 upon the recommendation of the IAEA Data Centre Network. The Unit organized the 1st Consultants' Meeting (CM) on "Procedures for Evaluation of Atomic, Molecular and Plasma-Material Interaction Data for Fusion" hosted by the National Institute of Fusion Science (NIFS, Japan) in 7-9 February and the 2nd CM on "Data Evaluation and the Establishment of a Standard Library of A+M/PMI Data for Fusion" in the IAEA Headquarters. The Unit aims that this meeting will bring the wider consensus and recommendations from the community of data producers for data evaluation and establishes the work plans towards the evaluated and recommended data sets by the community.

Twenty five people from 10 Member states and two people from the IAEA A+M Data Unit participated in the four day meeting. Unfortunately, Dr. Emile Biémont and Dr. Predrag Krstic could not attend at the last moment. The presentation of Dr. Krstic was given by Dr. Braams. The full list of participants with the affiliation information is available in Appendix 1.

The topics of the presentations and technical discussions of the meeting are as follows:
- Current Status of Evaluated Databases
- Data Evaluation Methods
- Error Propagation and Sensitivity Analysis
- Theoretical Data Evaluation and Uncertainty Estimates
- Experimental Data Evaluation and Semi-Empirical Fits
- Evaluation Activities of Data Centres

2. Proceedings of the Meeting

The meeting was opened by the scientific secretary Dr Hyun-Kyung Chung (A+M Data Unit, Nuclear Data Section).who introduced the local organizer Dr. Jung-Sik Yoon (NFRI) and the scientific advisory committee. It was followed by the opening address from Dr Myun Kwon, the director of National Fusion Research Institute (NFRI, Korea). He welcomed the participants to the meeting and the city of Daejeon and described the fusion activities at NFRI. The institute hosts the KSTAR (Korea Superconducting Tokamak Advanced Research) tokamak device as well as the Korean domestic agency of the ITER project (ITER KOREA). It has a long history of collaboration with ITER and IAEA. It was the host of the IAEA fusion energy conference in 2010 and has participated in the IAEA CRPs (coordinated research projects). Recently, the Data Center for Plasma Properties (DCPP) of NFRI joined the IAEA Data Centre Network (DCN) and actively collaborated in the data compilation and evaluation activities organized by the IAEA A+M data unit. The NFRI DCPP would like to broaden the collaboration with the IAEA with a formal agreement.

The IAEA A+M Data Unit Head Dr Bas Braams welcomed the participants to the meeting and thanked the director of NFRI and the local organizers for the generous support of the meeting. The meeting proceeded with the introduction of all participants in the meeting. There was a significant change in the agenda. Two speakers of the first day had to cancel the trip at the last minute due to the health problems and another speaker changed the flight due to the unexpected family business. Three presentations on the 3rd and the 4th day were moved to the 1st day. The modified agenda was adopted.

The objectives of the meeting were reviewed by Dr Braams. Fusion plasma modeling and experiments have always had much need for atomic, molecular and plasma-material interaction data: in the 1960s and 1970s, atomic data and plasma spectroscopy developed together. There are several series of meetings that bring together fusion plasma modelers and experimentalists and producers of A+M/PSI data. However, our meeting is different from them as this meeting is concerned with data evaluation and therefore with estimating uncertainties, error propagation and sensitivity to errors, and the development of a library of recommended data. The topics of presentations are the evaluation for electron-atom, electron-molecule and heavy particle collision processes and for plasma material interaction processes. All fusion modeling relies on calculated data because computation is the only way to obtain comprehensive data sets. Therefore an uncertainty estimate for theoretical data is of a special interest in this meeting. The discussion sessions are an integral part of the meeting and the report of these discussions and their conclusions is a very important goal of the meeting. In addition to the meeting report, a special issue of the Fusion Science and Technology journal (published by the American Nuclear Society) based on the proceedings of this meeting is planned.

The total of 24 presentations were given in six sessions: 1) Current Status of Evaluated Databases 2) Data Evaluation Methods 3) Error Propagation and Sensitivity Analysis 4) Theoretical Data Evaluation and Uncertainty Estimates 5) Experimental Data Evaluation and Semi-Empirical Fits and 6) Evaluation Activities of Data Centres. The summaries of presentations are given in the Section 3.

On the third day, all participants attended the 8th International Symposium on Standard Reference data organized by the Korean Research Institute of Standards and Sciences (KRISS). Dr Braams gave a presentation on the IAEA program towards standard library of atomic and molecular data for fusion and Dr Joo, a program director of the National Science Foundation (USA), gave a presentation on "Big Data, Data quality in Science and Technology: Headaches or Opportunities?". The importance of evaluated and critically assessed data in the development of technology was highlighted. The symposium ended with the presentation by Dr. Kang, a director of national center of standard reference data of KRISS on the National Standard Reference Data System in Korea and Its Future.

A chair was designated for each technical discussion session of five categories before the meeting. The role of a chair is to provide summaries of presentations during the session and lead the technical discussion session. After the two days of presentations, speakers gathered together to come up with the specific questions and topics for each technical discussion. The final discussion session was led by Dr Braams on the roadmap to an internationally agreed standard data library and the data evaluator's network. The summary of discussions is given in the Section 4.

3. Meeting Presentation

The summaries of presentations in six Workshop sessions are given here, and the abstracts are given in Appendix 3. A special presentation was given by Dr Choi of KRISS (Korea Research Institute of Standards and Science), who outlined the basic concepts and applications of measurement and uncertainty defined by Metrology. The definition and importance of traceability were described and the methods of evaluating uncertainties based on the GUM (Guide to the expression of Uncertainty in Measurement, 1993) were presented. The terminologies of error and uncertainty, often confused by physicists in assessing measurement results, were explained.

3.1 Current Status of Evaluated Databases

Dr Kramida outlined the general workflow of critical evaluation of data on atomic energy levels, wavelengths and transition probabilities preformed at the National Institute of Standards and Technology, USA (NIST). The evaluation procedure starts with selection of data sources from bibliographic databases and involves evaluation of wavelengths, intensities, and consistency of analysis, level optimization, derivation of ionization energies, theoretical interpretation of levels, and isoelectronic comparisons. Critical evaluation of transition probabilities involves the steps of checking critical factors, matching calculated transition probabilities with experimental energy levels, matching different calculations with each other, estimating uncertainties, selecting the best values, and checking for regularities. The lack of workforce in the field poses a potential risk to continuing the critical evaluation of atomic data at NIST.

Dr Landi presented a database for astrophysical plasmas, the 17 year old CHIANTI, which includes atomic data of the following processes: electron and proton collision excitation, photoexcitation, innershell and dielectronic processes, recombination and ionization. The database aims to be complete and accurate and the data evaluation is carried out in two-folds: 1) assess the data quality before adding in the databases and 2) compare the CHIANTI predictions with observations. The versions of the CHIANTI database are documented and updated regularly.

Prof Mason reviewed the status of databases for electron-atom and electron-molecule scattering data needed by many areas of science and technology. The electron scattering database is relatively good and reliable for atoms, however, the database for molecules is far from satisfactory. He outlined several basic pre-requisites for electron-molecule databases: 1) it should be comprehensive with a full list of experimental and, where applicable, theoretical results, 2) Any database should provide a critical review of the presented data, 3) Any database that aims to be adopted by an applied community should include a list of recommended values. He proposed the development of a database that the community has the ownership of (eMOL) which would work like a journal editorial board for data review and analysis.

3.2 Data Evaluation Methods

Prof Itikawa discussed the evaluation of evaluated data and shared his life-long experience in data evaluation. A few methods to evaluate the evaluated data were presented: 1) Test of the consistency of the total scattering cross-sections, 2) Comparison of calculated Swarm parameters with experimental values, and 3) Comparison of chemical modeling results using the reaction rate database with observation. He concluded that an application of available evaluated data sets could be a chance to evaluate itself. In this sense, the user feedback is very important in the evaluation of evaluated data.

Prof Kumar presented general criteria for selection of well-validated atomic data, which are applied to a few examples: 1) selection between absolute cross-sections and relative measurement, 2) selection between experimental data and theoretical computation, 3) selection of single data, 4) cross checking using two different techniques, 5) discretion in the selection of cross-section measurements at discrete impact energies, 6) selection between effusive molecular beams versus supersonic beams in collision experiments. An example of high temperature plasma spectroscopy was discussed.

Prof Cho shared his experiences in evaluation of standard reference data, particularly for total electron scattering cross sections of some plasma-relevant molecules. He described general criteria in evaluating standard reference data and presented results of reviewed molecules of water, halofluorocarbon, fluorocarbon and hydrocarbon. The conclusion is that the total cross-sections are far from satisfactory and reliable cross-section is required for reliable evaluation.

Prof Karwasz described some systematics in electron-atom and electron-molecule cross-sections. A database should host well-elaborated and comprehensive numerical data and should be established in the international context. He presented examples of evaluated data by constructing the database from the “bottom-up” with data of different experimental and theoretical techniques, different partial processes and different energy ranges, or by the “top-down” approach of searching for some semi-empirical or theoretical dependencies. Some simple relations such as additivity rules, dispersion relation for total cross-section, electron/positron convergence and resonances are explored. A few working hypothesis or systematic approaches for various processes are recommended.

3.3 Error Propagation and Sensitivity Analysis

The presentation on the role of fusion atomic databases in the internet environment prepared by Dr Krstic and given by Dr Braams outlines three components in error propagation and sensitivity analysis: 1) model validation defined to mean "substantiation that a computerized model within its domain of applicability possesses a satisfactory range of accuracy consistent with the intended application of the model", 2) model verification defined as "ensuring that the computer code of the computerized model and its implementation are correct" and 3) uncertainty quantification. He proposed that the only way towards trusted data for plasma-material interaction (PMI) is the integration of experimental and theoretical PMI research which includes Molecular Dynamics and Monte Carlo simulations with ion-surface scattering experiments, high-flux linear PMI experiments and toroidal confinement experiments.

Dr Reiter reviewed the evaluation of data in fusion edge transport codes. Edge codes use processed data (integrated, condensed and bundled) from a massive number of fundamental and raw data sets. The data processing is carried out by a toolbox, a collisional-radiative code, which can be used for sensitivity analysis. He proposed strategies to establish "evaluated reference data" for fusion applications based on those for rapidly developing plasma chemistry models.

Dr O'Mullane presented the approaches to accommodate uncertainty in ADAS which is a set of codes and data designed for spectroscopic and radiated power diagnostics and modeling of hot plasmas. Emphasis was made on the codes and models since the emission from fusion devices is not a direct representative of an isolated atomic system, but influenced by the collisional environment of ions and electrons. He outlined features of an authoritative and useful set of data for fusion and the future plans in ADAS with regards to the improvement of data quality.

Dr Ballance presented approaches to assess the uncertainties on atomic data with Monte-Carlo Calculations. Uncertainties are quantified as the difference between different theoretical approaches or determined from the sensitivity of the Monte Carlo R-matrix calculations to key input parameters. The latter approach, the sensitivity study, produces fully correlated uncertainties. The methods were applied for oxygen ions.

3.4 Theoretical Data Evaluation and Uncertainty Estimates

Dr Aggarwal outlined the problems and solutions in assessing uncertainties of atomic data. The problems include, number of states in the calculations, configuration interaction, energy or temperature range, relativistic effects, number of partial waves, pseudo states, resonances and radiation damping. Examples are shown to demonstrate the problems. Advices are made to data producers and data users.

Dr Liang presented an evaluation of electron impact excitation data along iso-electronic sequence. Motivated by astrophysical plasmas, R-matrix calculations are assessed for Li-like Ne-like and B-like sequences. For near neutral ions, calculations with pseudo-states included are recommended and for ions with Z~ 33-36, fully relativistic calculations are recommended. Large-scale R-matrix calculations are a better choice than distorted-wave and small-scale calculations for most ions of intermediate states.

Prof Takagi presented cross-sections on the processes induced by electron collisions with H_2^+, HeH^+ and their isotopes. Electron collisions with molecular ions are important in divertor regions and the state specific processes play an important role. Reliability of calculated data is checked by comparing with experiments though it is governed by the uncertainty of experiments or by the physical insights obtained with performing more complete calculations and checking convergence.

Dr Song evaluated the electron impact excitation data of n=2 and 3 states in Helium in order to explore the evaluation procedures. Data are collected from the literature and from both experimental and theoretical results. The evaluated data, using a newly-developed evaluation procedure, was compared with the existing evaluated data sets by de Heer (1992, 1998) and Ralchenko (2000). The uncertainties of evaluated data are calculated based on the GUM method. The results show that the evaluation is most difficult near threshold energies where the measured cross-sections are not available and calculated results disagree.

3.5 Experimental Data Evaluation and Semi-Empirical Fits

Prof Nakamura presented the work on electron swarm parameters which can evaluate and even provide cross-section data, since every possible scattering process of electrons is reflected in their collective behaviours. A small amount of molecular impurities can alter swarm parameters drastically and hence elastic momentum and vibrational cross-sections can be separately determined. An example of C_2H_4 molecules is shown.

Prof Buckman shared his experiences on the evaluation of atomic scattering data and the compilation and evaluation of low energy electron collisions with plasma processing gases. Examples of successful semi-empirical techniques were shown. He proposed guiding principles and outlined important elements in evaluation: 1) Need a clear set of guiding principles for data evaluation and presentation set by the "community", 2) involve teams of broad expertise where possible, 3) use trends or regularities in data, 4) use theory well benchmarked and 5) use semi-empirical approaches where necessary.

Dr Shevelko presented the new calculations of electron-loss and capture cross-sections of W and its ions colliding with H and He atoms. The isotope effect was found to be several orders of magnitude larger. He formulated 10 recommendations on the data evaluation: 1) The physics of the radiative or collisional characteristics, 2) asymptotic behaviour, 3) scaling laws for self-consistency, 4) semi-empirical formulae for prediction, 5) estimate of a real accuracy of the data from experiment or theory, 6) accuracy of theoretical data due to the approximations, 7) consistency in physical relations, 8) recommended cross-sections at the moment of evaluation, 9) fitting parameters and 10) getting absolutely new data.

Dr Imai described the work on the production and compilation of absolute cross-sections for fusion-relevant electron capture processes since 1988 and presented the absolute measurement of single electron capture cross-sections for W^+ and W^{2+} Ions. Anomalous energy dependence in the low-energy region has been observed for the first time, while no characteristic target isotope effect was observed in energies > 5 eV. Cross-sections showed deep dependence on target ionization potential, which is different for rare-gas and molecular gas targets. Cross-section scaling on ΔIP (Q-value) might be possible.

3.6 Evaluation Activities of Data Centres

Dr Yoon presented the current activities on data evaluation and compilation at Data Center for Plasma Properties in NFRI (National Fusion Research Institute, Daejeon, Korea). The DCPP started its operation for making databases by collecting and compiling data sets relevant to plasma applications. With the lack of data needed for applications identified, the centre expanded to produce needed data by experimental measurements. The centre actively pursues data evaluation activities in order to produce a database of a full set by compiling, producing data and collaborating with a larger group of international experts. He shared three evaluation principles: 1) how well data generation procedure is described, 2) how data follow the known physical laws and 3) how data compare to other measurements or calculations. The evaluated cross-sections were presented.

Prof Murakami described the atomic and molecular databases and data evaluation activities at NIFS (National Institute for Fusion Science, Toki, Japan). NIFS currently maintains approximately half a million numerical AM/PSI data, which are used as a tool for data evaluation by providing easy access for data comparison and storing the evaluated data. Working groups work on compilation of data with specific targets and the data evaluation activities have been carried out by domestic and international collaborations. Evaluated data are published as IPPJ-AM reports and NIFS-DATA reports (http://www.nifs.ac.jp/reports/nifsdata.html)

Prof Mason presented the SUP@VAMDC project, a follow-up to outline the next step of the highly successful project VAMDC (Virtual Atomic and Molecular Data Centre) development to provide a common portal 'single point entry' for atomic and molecular databases worldwide. It aims to establish the necessary coordination methodology by formulating the roadmap that will ultimately combine VAMDC with complimentary (e)-infrastructures organised by existing international bodies, committees and networks dealing with the production, evaluation and dissemination of A+M data.

Dr Chung described the IAEA atomic and molecular data unit activities in data evaluation, which led to a series of meetings on the subject. The motivation behind the recent initiatives in the Unit to establish the evaluated and recommended data libraries for fusion relevant data was presented as well as the conclusions and recommendation from a series of IAEA meetings. The future activities of the Unit for the internationally agreed standard data library, such as the world survey of currently used AM/PSI data for fusion applications or the compiled evaluated data libraries, were outlined.

4. Technical Discussions

Each presentation session consisted of 3 to 5 speakers and after presentations they had a panel discussion to decide the relevant questions to be addressed during the main discussion session with all the participants. The designated chair led the technical discussion session by summarizing the comments from the short panel discussions and by proposing questions. The questions, comments and ensuing discussions are summarized.

4.1 Evaluated Databases

Prof Murakami was a chair of the session and the members of the panel were Dr Kramida, Dr Landi and Prof Mason. They shared the experiences of developing and maintaining the databases of evaluated data sets, and particularly the concerns with the rest of participants. The questions, comments and suggestions are summarized.

- Do we need to have ***common workflow guidelines to evaluate data*** for the evaluated data library?
    - Advantages: It is easier to expand the evaluators' network including early career researchers (at least at the expertise level of postdocs). It introduces 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 with sscientific advisors and the editorial panels will be a great mechanism to produce the evaluated data library.
- How can we ***engage young generation (in early career) in the data evaluatio***n activities? It is important to enlighten the younger generation that the data evaluation is a critical part of their work and to find a way to make the data research more attractive for them.
    - We should educate the young generation scientists with the science community culture in the right way and get them think about how and where their data to be used.
    - We should prepare the materials on how to evaluate (or critically assess your data sets) for distribution to the community and engage them in the evaluators network to interact with senior people
    - We should develop a strategy in training of the "Critical Analysis Skills" not only for the young generation scientists but also for the students

    - Review papers from the evaluation work are beneficial for their careers
    - The IAEA workshop at ICTP is proposed to invite the senior evaluators as lecturers and conduct hands-on training for data evaluation, which can be published afterwards.
- It is important to ***influence the community*** to change its notion on data research activities.
    - First we should stop vocabularies of databases (DB) and use the terms of data researcher
    - Data evaluation activities will not be successful without training for young researchers and educating the science community culture in the right way
    - The materials on how to evaluate (or critically assess your data sets) should be distributed to educate the community more widely.
    - We should engage Journal publishers for the successful data evaluation activities.
    - Publication issues: There are many journals to publish evaluated data sets. However, young people need to publish their work in the journal of high “impact” factors. The review papers from the critical assessment of data will be the right vehicle.
- A benchmark test could be applied for spectra or other plasma properties using a set of “evaluated” atomic and molecular data to compare with experiments for checking the accuracy and the completeness. To do this test, applications such as CHIANTI and ADAS and “standard plasma model” are required.
- ***Evaluation activities should be performed by the community***
    - We need to build up the community consensus with an endorsement from the IAEA
    - Evaluation Options:
        1. Evaluation in a group of 4-5 panelists including young people like the editorial board for a journal. This option will facilitate the knowledge transfer to younger generation
        2. Self-Evaluation by the data producers with a deep knowledge in some cases. Theoretical data sets in particular may be better off with self-evaluation.
    - Establishment of the evaluation guidelines: If the community is involved in the evaluation, the guidelines should be established and updated systematically.
- Questions
    - Do we need communication and collaboration between data centers with the same kinds of database for allowing people to have access to the same data like the VAMDC portal and making common sense on data evaluation procedure?
      IAEA can play an important role to organize a workshop for communication.
    - Is it good to have a key database center for evaluating specific kinds of atomic data, i.e. NIST for energy levels, wavelengths, and transition probabilities, where there are experts on data evaluation and they have specified workflow on evaluation?
    - Do we estimate “uncertainties” especially for theoretical data through benchmark tests?

4.2 Evaluation Methods and Semi-Empirical Fits

Dr Yoon was a chair of the session and the members of the panel were Prof Itikawa, Prof Kumar, Prof Cho and Dr Song. They have published review papers on the evaluated data and shared their experiences of performing evaluation with the rest of participants. The questions, comments and suggestions are summarized.

- What should be the object of evaluation: should we evaluate data or the method (or theory)?
    - We have to concentrate on evaluating “data”.
- We need ***to define terminology and vocabulary used in evaluation activities***.
    - We may use the standard definitions of terminologies based on VIM (2007, BIPM, International Vocabulary of Metrology-Basic and general concepts and associated terms) which is widely adopted international organizations and societies.
    - Our communities should be informed by working with international organizations (IAEA, IUPAC, IUPAP) and by interacting with colleagues, writing reviews and publications and presenting in meetings.

- It is difficult to input uncertainty into the theoretical data: However, it may be possible to select reasonable data sets for evaluation.
- ***The procedure of evaluation towards a standard reference data*** have several steps:
    - Compilation: the relevant data sets should be collected
    - Evaluation of a single data set: each data set should be evaluated by an expert
    - Collection of valid data sets.
    - Decision on a single standard reference data
        - Not all data sets but only those required by the user community are needed to be evaluated for standard reference data sets
        - Establishing a complete data set needs a different approach in evaluation
        - It is possible that some may oppose to the idea of the single standard data.
- We should review all guidelines of data evaluation methods and ***establish a general guideline.***
    - Can a systematic method for validation can be established like workflow used by the NIST group for the spectroscopic data evaluation?
    - We agree that there is a merit to establish the systematic methods for validation.
        - The guidelines will evolve with time and experience.
        - We need collaborations from the Community.
        - Once the guidelines are established, the community will follow or we may make them follow.
    - An endorsement from an authority (such as IAEA, IUPAP, IUPAC) on the general guidelines will help its establishment and maintenance.
        - We need task forces for different fields of expertize.
- ***The scaling method*** used for evaluation
    - A semi-empirical fit is needed for validation, non-existing data and several other reasons. Unfortunately, it has been widely used without caution
    - The validity of semi-empirical fit should be included in the guidelines and the danger of its abusive uses should be warned to users.
    - The semi-empirical formula needs an evaluation as well.

4.3 Theoretical Data Evaluation and Uncertainty Estimates

Dr Aggarwal was a chair of the session and the members of the panel were Dr Liang and Prof Takagi. They shared their thoughts on evaluating theoretical data sets with the rest of participants. The questions, comments and suggestions are summarized.

- Currently we do not have ***the criteria of assessment for theoretical data sets***. There are a few elements to be reviewed:
    - Methods, size limitations of approximation should be reviewed.
    - One should reject those which appear to be suspicious or limited in range.
- The ***uncertainty estimates for theoretical data*** are needed for evaluation.
    - One should not try to give a straight recipe for assessing the uncertainties, however, there are still several to start with.
        - There are prescriptions for making uncertainty estimates such as energy grids for resonances and partial waves.
        - One may take a model to see a convergence (partial waves, coupled channels) and estimate uncertainties based on assumptions within the model.
    - Comparison with experiments for example, by taking the differences and extrapolating to the region of interest: this can be dangerous.
    - Different theories: if some theories are better than another, it may be given a benchmark status.
- There are many ***unpublished data sets***, especially for theoretical data sets. Should we include them in the evaluation?
    - Unpublished data sets are often needed for applications (unavoidable). In principle, they should not be prohibited, but strongly discouraged.
    - There are two types of unpublished data:

        - data from data centres and databases – it is the data centre's responsibility
        - data unverified by others – it is probably better not to use.
    - "Any data is better than no data" : it is a dangerous idea.
        - The user of unpublished data sets should be responsible.
        - The use of unpublished data should be flexible but with a lot of caution
    - One should keep in mind that people write the paper and get the credit for their work.
        - If a work goes into the database without a description (or publication), it will not be repeatable. If it is the case, it is not called a scientific result.
- We need to assess data and prioritize the ions for evaluation. Not all data needs to be assessed.
- The data should be assessed by a team of diverse backgrounds.
    - Producers and Users, Theorists and Experimentalists, Active or senior/retired scientists should be involved.
    - Teams should be small, impartial and have some experience.
- Questions:
    - Should authors be warned in case of an anomaly found by evaluators?
    - What are assessment criteria for theoretical data?
    - What importance should be given to authors' assessment of errors?

4.4 Experimental Data Evaluation

Prof Buckman was a chair of the session and the members of the panel were Prof Nakamura, Dr Shevelko, Dr Imai and Prof Karwasz. They shared their thoughts on evaluating experimental data sets with the rest of participants. The questions, comments and suggestions are summarized.

- How can we make ***the data assessment open and critical***, frank but fair?
    - If possible, the assessment should be carried out by a group of "established" experts with broad expertise
    - It is critical to have uncertainty estimates or an error assessment.
    - One should provide the clear assessment output for users
        - Should we tabulate data or are the graphical representations good enough?
        - We should present recommended values where possible.
        - A comparison with theory (perhaps) and an assessment of overall status of the field may be more needed.
- ***Experimental data evaluation***:
    - Evaluated data should be checked to be self-consistent.
    - Experimental techniques should be evaluated.
    - Reputation of the data producer should be considered (qualified and accepted)
    - One should identify anomalies in some experimental processes (ro-vibrational states or metastable states)
    - We should engage atomic physics community who provide relative measurements for cross-section measurements
    - Evaluation will lead to the understanding of the gaps of the field.
    - We should seek to establish "benchmarks" where possible:
        - The comparison between experiments and theory is important.
        - One should broaden assessment to include theory where possible or as a guiding hand. (Some cases, theories are more trusted)
        - Benchmarks will be accepted as heavier connotation than recommendation.
- What we should evaluate/assess:
    - We should focus on important areas – a poll from the community of users
    - It is more likely to get traction for activities
- Questions
    - Should we establish and accept instruments or methods as a standard?
    -

4.5 Error Propagation and Sensitivity Analysis

Dr Reiter was a chair of the session and the members of the panel were Dr Braams, Dr Balance and Dr O'Mullane. They shared their thoughts on the error propagation and sensitivity analysis with the rest of participants. The questions, comments and suggestions are summarized.

- There are three groups of uncertainties existent from the structure data to the Collisional-Radiative (CR) model results,
    - Uncertainty propagation from the A+M structure data to collisional data (or fundamental data) : Responsibility of Atomic and Molecular (A+M) experts
    - Uncertainty propagation from fundamental data to processed data (rate coefficients): Responsibility of Evaluators or Data centres
    - Uncertainty propagation from processed data to the CR results (population densities, effective rates, cooling rates etc): Responsibility of Data centres and user community
- There are two approaches presented to investigate the uncertainty propagation:
    - Uncertainty propagation using Monte Carlo simulations
    - Sensitivity analysis using the Linear Algebra
    - There seem to be separate issues of "Data" (uncertainty propagation from atomic structure to fundamental data) and "Data processing toolbox" (linear sensitivity analysis, or Monte Carlo simulations)
- Questions
    - At which level to specify "propagated errors" in a database?
        - Reduced population coefficients or effective rates
        - Individual rates (before Collisional-Radiative modeling)
        - Total or differential cross sections

5. Meeting Conclusions and Recommendations

The final discussion session was led by Dr Braams. This meeting was highly successful in drawing the consensus and recommendations for the future activities of the IAEA A+M data unit and the communities. Participants expressed high satisfaction of the meeting outcomes and great expectation for the coming events. The meeting conclusions, recommendations and action items are summarized.

5.1 Roadmap to the Establishment of Internationally Agreed Standard Data Library for AM/PSI Data Relevant to Fusion Applications

The roadmap developed in the earlier meetings was reviewed. Please see the Appendix for the longer version; here is a shortened version.

Phase 0: Inventorise the AM/PSI Data Collection used by Fusion/Plasma Community

Use a questionnaire addressed to active modellers and diagnosticians to identify precisely what data sets they use in their work and where they see the highest need for evaluation work. In connection with that, develop a network of high intensity A+M+PMI data users to provide and update the priority list of data needs for fusion applications.

Phase 1: Establishment of infrastructure towards evaluated data library

- IAEA Atomic and Molecular Unit: Development of database to host the standard data library
- Data Centres: Compilation of relevant data for evaluation
- Data Centres and Evaluators: Establishment of data evaluators' network
- Data Evaluators: Guidelines of evaluation methods
- Data Producers: Guidelines of uncertainty estimates

Phase 2: Establishment of evaluated data library

- IAEA: Establishment / maintenance of databases to host the evaluated data library
- Data Centres: Coordination of data evaluators' network activities
- Data Evaluators: Evaluation of data sets
- Data Producers: Guidelines of scaling laws / fit expressions
- Data Users: Development of data format compatible to applications

Phase 3: Establishment and maintenance of standard data library

- IAEA: Establishment / maintenance of databases to host the standard data library
- Data Evaluators and Data Centres: Coordination of Technical Committees
- Data Producers: Feedback on data sets (production of missing data, data improvement)
- Data Users: Feedback on data sets

5.2 Developing an Evaluators Network

Key people have been identified in the meeting and nominated by the communications after the meeting: The following people are designated to be the contact point to organize a network of researchers who will perform the evaluation activities of specific processes. Each network will be responsible for establishing an editorial board and the technical guidelines for evaluation. The IAEA A+M Data Unit will coordinate the network of evaluators with the IAEA Data Centre Network (DCN).

- In general: IAEA Data Centres (I. Murakami, J.-S. Yoon, M.-Y. Song), Y. Itikawa
- Atomic structure and spectroscopy: A. Kramida, E. Landi
- Photon scattering: C. Ballance
- Molecular structure and spectroscopy: J. Tennyson
- Electron-atom scattering: E. Landi, K. Bartschat, C. Ballance
- Electron-molecule scattering: Karwasz, S. Buckman, N. Mason
- Heavy particle scattering: I. Tolstikhina, M. Imai, V. Shevelko
- Plasma-Material interaction:

5.3 Guidelines for Uncertainty Assessment of Theoretical Data (how to proceed)

The uncertainty estimates and the guidelines of the critical assessment of theoretical data sets have been the hot topics of discussion in the previous meetings. It is an extremely difficult task in itself and it was equally difficult to gain the consensus on how to proceed with this task. Nevertheless, theoreticians such as scattering theorists do have an idea of the uncertainty estimates of their own data but do not merely write down in practice. It is important to change the culture if theoretical data sets without uncertainty estimates are not included in critical evaluations.

For scattering data maybe we should aim for "ideas" or "suggestions" rather than "guidelines". The same division into topical areas applies as for the evaluators network, except that for the uncertainty assessment it makes sense to lump electron-atom and electron-molecule scattering together into one topic, electron scattering. So all the theorists named in the previous section are also suitable people for developing guidelines (ideas, suggestions) for uncertainty assessment of theoretical data. We can ask additional people to join that are active in computation but that may not have the interest to join an evaluators' network; they can still provide advice about assessing uncertainties.

It would be very helpful to organize a workshop some time that is entirely focussed on uncertainty assessment of theoretical data. It could be done in connection with SUP@VAMDC and/or eMol.

5.4 Which Systems are the Priorities for Evaluation?

In the discussion we looked for one electron-atom system, one electron-molecule system and one heavy particle collision system. After some discussion these three were favoured.

- Electron scattering on Be^{q+}. Currently, enough data are available and the system is of interest.
- Electron scattering on CH_4.
- Charge exchange and electron loss for H on Be^{q+}.

Some other systems were considered and then found to be not so suitable. The scattering on Be is great since we expect to have at least two good data sets; the scattering on W would be much more difficult to assess. For electron-molecule collisions we considered hydrogenic systems but decided that so many data are available that CH_4 would be easier (and also relevant). For heavy particle collisions again we choose H+Be because we expect several good data sets. We keep in mind that as people are asked to participate in the evaluation other system may be favoured.

5.5 Action Items

Finally, the action items were decided and assigned to participants. Here is the list of action items and the person in charge.

- Circulate meeting notes towards the meeting report – Chung
- Work on submission for Fusion Science and Technology (FST) – All
- Inventorise datasets that are now used by fusion plasma modellers (questionnaire) – Chung
- Sketch out guidelines/ideas/suggestions for uncertainty assessment of theoretical data – Braams
- Organize a workshop (SUP@VAMDC): Mason
- NFRI to organize a data evaluation group for demonstration – Yoon and Song
  - The group will demonstrate the evaluation procedure by the editorial board.
  - The group will establish general guidelines for evaluation criteria, evaluation process
  - The group will demonstrate the evaluation process from the scratch to the final product as discussed in the meeting
- The ITER project will require standard reference data (SRD) for A+M processes used in the design and we need to get ready – Reiter

5.6 Broader Action Items

Action items to be performed in the longer term were defined for broader activities to be fulfilled by all participants.

- Community role
  - Disseminate the concepts of VIM3 (International Vocabulary of Metrology) , GUM (Guide to the expression of Uncertainty in Measurement) and “critical assessment skills”
  - Engage groups who have negative views on evaluation
  - Engage younger generation in the process
  - Work with the colleagues of the community
- Publications should change the culture about data research
  - Policies of the PRA and other journals have been changing to include the critical assessment of uncertainties.
- Assess the needs of user communities

    - Some may want uncertainty assessments but not necessarily the best quality of the data
- Collaboration between SUP@VAMDC and International Atomic Energy Agency on the following:
    - Define a set of problems.
    - Issues to address in the roadmap.
    - What does it mean by data evaluation?
    - Do people want recommended values?

Joint IAEA-NFRI Technical Meeting on
"Data Evaluation for Atomic, Molecular and Plasma-material Interaction Processes in Fusion"

4–7 September 2012, Daejeon, South Korea

Scientific Secretary: Ms Hyun-Kyung Chung

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Joint IAEA-NFRI Technical Meeting on
"Data Evaluation for Atomic, Molecular and Plasma-material Interaction Processes in Fusion"

4–7 September 2012, Daejeon, South Korea

Scientific Secretary: Ms Hyun-Kyung Chung

Agenda

September 4th, Tuesday (DCC Room 205, 2nd Floor)

09:00 Reception
09:30 Welcome Address (NFRI)
Introduction of Participants/Adoption of Agenda
Review of Meeting Objectives (Braams)"

Session 1: Current Status of Evaluated Databases (Chair: I. Murakami)

10:00 Kramida: Critical Evaluation of Data on Atomic Energy Levels, Wavelengths, and Transition Probabilities
10:30 *Coffee*
10:45 Landi: CHIANTI - an atomic database for astrophysical plasmas
11:15 Choi: Measurement and Uncertainty
11:45 Yoon: Development of Standard Reference Data on A+M for Plasma at NFRI
12:15 *Lunch*

Session 2: Data Evaluation Methods (Chair: M. O'Mullane)

13:45 Itikawa: Evaluation of the evaluated data
14:15 Kumar: Criteria for Selection of Well-Validated Atomic Data
15:00 Cho: The experiences in evaluation of Standard Reference Data
15:30 *Coffee*
15:45 Karwasz: Some Systematics in Electron – Atom and Electron – Molecule Cross sections

Session 3: Error Propagation and Sensitivity Analysis (Chair: S. Buckman)

16:15 Reiter: Evaluation of data in fusion edge transport codes
16:45 Chung: The IAEA Data Centre Network : Data Evaluation Activities

September 5th, Wednesday (Room 205)

09:00 O'Mullane: Accommodating uncertainty in ADAS models and data
09:30 Ballance: The generation and propagation of uncertainties on atomic data

Session 4: Theoretical Data Evaluation and Uncertainty Estimates (Chair: N. Mason)

10:00 Aggarwal: Asessement of atomic data: problems and solutions
10:45 *Coffee*

11:00 Liang: Evaluation of electron-impact excitation data along iso-electronic sequences
11:30 Takagi: Cross Sections on the Processes Induced by Electron Collisions with H2+, HeH+, and Their Isotopes
12:00 Song: Evaluation of the electron impact excitation of n=2,3 states in Helium
12:30 *Lunch*

Session 5: Experimental Data Evaluation and Semi-Empirical Fits (Chair: G. Karwasz)

14:00 Nakamura:Electron Swarm Parameters and Electron Collision Cross Sections
14:30 Buckman: Low Energy Electron Collisions with Plasma Processing Gases - Data Compilations and Evaluations
15:00 Shevelko: Electron-loss and capture cross sections of W ions colliding with H and He atoms
15:30 *Coffee*
15:45 Imai: Target dependence of single electron capture cross sections for W+ and W2+ ions
16:15 Krstic: Role of the Fusion Atomic Databases in Internet Environment
16:45 Group discussions for Technical Discussions

September 6th, Thursday (Room 101)

The 8th International Symposium on Standard Reference Data

10:00 Opening: Kang, D. I. (President, KRISS) Seo (President, KATS, MKE)
Kwon (SNL, Chair, NCSRD SC)
10:30 Braams (IAEA) : The IAEA program towards standard library of atomic and molecular data for fusion
11:00 Joo (Program Director, NSF) :Big Data, Data Quality in Science and Technology: Headaches or Opportunities?
11:30 Kang, K. H. (Director, NCSRD, KRISS) : National SRD System and Its Future
12:00 *Lunch*

Session 6. Evaluation Activities of Data Centres (Chair: Braams)

13:30 Mason: The electron scattering data base - Is it fit for purpose ?
14:00 Murakami: Atomic and Molecular Databases and Data Evaluation Activities at NIFS
14:30 Mason: SUP@VAMDC Uniting the international atomic and molecular data community
15:00 *Coffee*
15:15 Technical Discussions (Murakami) :Current Status of Evaluated Databases

September 7th, Friday (Room 205)

09:00 Technical Discussions (Reiter) : Error Propagation and sensitivity analysis
10:00 Technical Discussions (Aggarwal) : Uncertainty Estimates
11:00 *Coffee*
11:15 Technical Discussions (Buckman) : Experimental Data Evaluation
12:15 Lunch
13:30 Technical Discussions (Yoon) : Data Evaluation Methods and Semi-Empirical Fits
14:30 Technical Discussions (Braams): Review of the Roadmap to the Internationally Agreed Standard Data Library, Establishment of Evaluator's Network
15:30 *Coffee*
15:45 All (Chung): Conclusions and Recommendations

Abstracts of Presentations

The abstracts are given below for the meeting presentations available at http://www-amdis.iaea.org/ .

Critical Evaluation of Data on Atomic Energy Levels, Wavelengths, and Transition Probabilities

A. Kramida

All modern concepts of implementation of thermonuclear fusion for energy production involve high-temperature plasmas confined by different methods. These plasmas generally contain impurities of multiple chemical elements in various stages of ionization. These impurities can be used to control and diagnose the plasma conditions. In both cases, extensive kinetic modeling is required in order to produce a predictable response of plasma parameters to changes in impurity contents and extract the plasma parameters from observed spectra. This implies that a large quantity of atomic data must be precisely known. One of the primary goals of the Atomic Spectroscopy Data Center of the National Institute of Standards and Technology (NIST) is to provide such critically evaluated data to the fusion research community. I will describe the methods we are using in this compilation process. Our procedure begins with an exhaustive review of the literature for relevant data. This process makes use of our online bibliographic databases. The critical assessment of atomic wavelengths and their energy-level classifications is based on level schemes and theoretical interpretations that have survived examinations for consistency (experimental, isoelectronic, theoretical). Reliable line classifications are thus a primary output of our evaluations of the laboratory data and analysis. We include leading eigenvector percentages for the energy levels, where available, and references to theoretical calculations in our level compilations. These give an immediate indication whether large deviations from, for example, Russell-Saunders multiplet intensities can be expected and serve as a guide to the theoretical literature. Calculations are used to help discriminate between possible contradictory line classifications. Our critical assessment of atomic transition probabilities follows a well-developed systematic approach. This is a key element of our work, since practically all calculated data – the great majority of our available transition probability data – do not include uncertainty estimates. In our approach, a uniform critical assessment of the data provides the basis for data selection and assignment of numerical uncertainties. All data are reviewed with respect to the following four primary criteria: 1) the author's evaluation and numerical estimate of the uncertainties, 2) the degree of agreement of the results with other reliable data, 3) the author's consideration of critical factors (such as cascading in lifetime experiments or self-absorption in emission experiments) affecting the results, and 4) the degree of fit of the results into established systematic trends, or the reasons for possible deviations. In special cases, additional criteria may be used, such as comparisons of calculated and observed relative intensities of spectral lines. On the basis of this assessment the most reliable data are selected. Finally, the data are characterized with respect to their uncertainties on a scale from AA (less than 1%) to E (greater than 50%). A detailed description of our assessment procedure is given in Wiese et al. J. Phys.Chem. Ref. Data Mon. 7 (1996).

CHIANTI - an atomic database for astrophysical plasmas

Enrico Landi

The CHIANTI spectral code consists of an atomic database and a suite of computer programs to calculate the optically thin spectrum of astrophysical objects and carry out spectroscopic plasma diagnostics. The database includes atomic energy levels, wavelengths, radiative transition probabilities, collision excitation rate coefficients, ionization and recombination rate coefficients, as well as data to calculate free-free, free-bound and two-photon continuum emission. All CHIANTI data are critically evaluated in two different ways: by comparing individual atomic data and rates with other calculations and laboratory measurements, and by comparing predicted spectral line intensities with observed spectra from the laboratory (when available) and from astrophysical sources.

In this talk, I will introduce the main features of CHIANTI, discuss its current status in light of current and future atomic data needs, describe the past and ongoing activities to benchmark and validate CHIANTI atomic data and rates, and outline future developments of the database.

The electron scattering data base - Is it fit for purpose ?

N J Mason

Electron induced reactions in both the gaseous and condensed phases initiate and drive many of the basic physical and chemical processes in science and technology with applications from industrial plasmas to radiation damage in living tissue. For example, in contrast to previous hypotheses, collisions of very low energy secondary electrons with the components of DNA molecules (or to the water around them) has been shown to be a crucial process in inducing radiation damage in the DNA of living systems. Understanding electron interactions with larger biomolecules is therefore providing new insights to radiation damage and thence the development of new, alternative radiotherapies. In the technological field electron induced reactions underpin most of the multibillion dollar modern semiconductor industry since it is those reactive fragments produced by electron impact of etchant gases that react directly with the silicon substrate. Studies on electron scattering from molecules capable of improving the etch rate of surfaces are leading to development of new (environmentally cleaner) plasma technologies. Electron induced processes are also of extraordinary importance for determination of structure and chemical reactivity of species adsorbed on surfaces.

Such research and technology is intricately linked to our knowledge of the key interactions between electosn and atoms and molecules and thus we require a database for characterizing electron interactions with atomic and molecular species. However the compilation of the electron collsion data required is rarely a coherent, planned research programme instead it is a parasitic process. Indeed today it is rare for researchers to be funded to measure fundamental collision processes since these are no longer regarded in themselves as 'cutting edge' research rather the field has developed to explore more exotic phenomena such as cold atoms; nanotechnology and chemical control.

The fundamental research community, the providers of such data, therefore need to assemble, update and police a set of approved databases. This is no longer as complicated as it was a decade ago. Most publications are accessible online and most authors place their data on home pages and in archives, Hence compiling databases is easier than it was in the past for example by using the General Internet Search Engine for Atomic Data (GENIE) developed as part of the International Atomic Energy Agency facility. In this talk I will review the current status of the electron scattering databases, how they are assembled and updated and thus whether they are 'fit for purpose' or if not how they may be developed to meet the challenges of the 21st century Science and technology. I will contend that ultitalte it is or the communityu to develop a method for archiving and recommending sets of electron scatterign data and propose methods by which this can and will be done.

Finally it should be noted that the greatest challenge to the community is to maintain the infrastructure (including people) that will allow the fundamental data to be collected. This in turn challenges the wider scientific community to recognize that their fields rely upon such data. A united applied and fundamental research community must then confront the funders of research (government and industrial) to ensure that such data compilation, evaluation and curation must be supported and sustained.

Evaluation of the evaluated data

Yukikazu Itikawa

In a wide variety of fields of science and technology, collision cross sections or reaction rates play a fundamental role. Reliable data on those quantities are needed there. To satisfy those requirements, various activities have been attempted to compile data and develop databases. The most important and most difficult part of the activity is the evaluation of the compiled data to establish a reliable database. There are no standard ways of data evaluation. The resulting recommended data are often different from each other depending on who evaluate the data. It is desirable, therefore, to evaluate the evaluated (or recommended) data. Here I will introduce three examples of such attempts of evaluation of evaluated data. They are

(1) A consistency check through the relation of the total scattering cross section and the cross sections of individual processes.
(2) Calculation of swarm parameters (transport coefficients) to compare with experiment.
(3) Applications in practical modeling

The first two examples are concerned with the cross section for electron-molecule collisions and based on my own works. The third example, taken from an activity of interstellar chemical modelling, is the evaluation of a set of chemical reaction rates.

Criteria for Selection of Well-Validated Atomic Data

Vijay Kumar

There are a large number of papers, theoretical and experimental, published on different aspects of Atomic and Molecular Physics. These include the measurement and computation of oscillator strengths, radiative lifetimes, line shapes, line shifts, energy levels, ionization energies etc. for neutral and ionized atoms. Also, more than adequate data is available on electron and photon impact of molecules leading to many processes like excitation, dissociation, ionization and dissociative ionization, electron attachment, photo-ionization, photo-dissociation etc. All these data are needed to give a better understanding and insight regarding the different phenomena occurring at different sites and also help in putting forward better explanations and mechanisms.

But all these data need to be validated for accuracy in spite of the fact that the latest developments in science and technology are now capable of producing better results with higher resolution and sensitivity. However, all data still cannot be considered as the benchmark data which may be used further without ambiguity by different scientists in different fields.

It is the foremost duty of the scientific community to well-validate different atomic and molecular data. But unfortunately, it is not being done systematically as the criteria for rejection of data followed in the process have not been used in a consistent manner. That is why we have to ascertain and fix these criteria once for all.

Any data leading to relative measurements normalized using other standard data should not be considered for evaluation. Only absolute measurements should be included for validation. Measurements or computations which are obtained at a few electron or photon energies and not in the continuous range of energies should also be avoided even though new innovative approach may have been used to obtain the required data. Measurement/computation of cross section if made by two different techniques can be used as a cross-check on one another and on theory. Sometimes, only single set of data is available for a given parameter. Such data may only be considered if repeatability is ensured. It is strongly believed that the experimental data should be preferred to one obtained by theoretical computation. This is mostly true for polyatomic molecules where target wave function cannot be represented unambiguously. Cross checking experimental data could also be useful if carried out choosing some standard values provided by theory.

In some experiments, accuracy is claimed to a large number of decimal places. It should be ascertained by checking different parameters used in the experimental system such as resolution of the projectile beam, the instrumental accuracy for measuring the number of atomic or molecular species involved in the collision etc. Otherwise, the claim for higher accuracy should not be entertained.

It should be made sure that the new technologies are used in the experiment to bring drastic improvement in the measurement of different atomic/molecular parameters. Where ever the atomic lines or molecular bands are observed as emission features due to projectile-target collisions, the absolute cross sections can be obtained only when the emission intensities are measured absolutely using standard radiometric techniques.

The experiences in evaluation of Standard Reference Data

H. Cho

Electron-molecule scattering cross sections are vital in modelling and characterising the various plasmas.

To serve industrial and scientific communities, South Korean government set up Stanard Reference Data Centers including a plasma data center. The status of the available cross sections of electron-molecule scattering, difficulties and problems in evaluating cross section data, and some suggestions will be presented, based on the author's experiences in evaluation of standard reference data relevant to the plasma applications.

The specific examples of evaluation criteria and evaluated data will also be discussed.

Some Systematics in Electron – Atom and Electron – Molecule Cross sections

Grzegorz P. Karwasz

Numerous data bases for electron – atom and electron – molecule scattering have been created within national (eg. French, Japanese) and international (EU, IAEA, NIST etc. programmes). The overall collection of data is impressive. What still lacks is some comparison, in search of analogies and differences among total and partial cross sections, in broad energy ranges.

For some processes knowledge of partial cross sections seems to be sufficient. Electron –*ionization* cross sections based on the analytical formulae using energies of the electron binding developed by Kim and Rudd [1] covers a number of targets and is available on-line up to high energies at NIST. On the opposite end of the energy scale the *electron-attachment* cross sections obtained from Rydberg-atom quenching [2] and pulse-radiolysis microwave measurements [3] seem to reach theoretical maximum limits for some targets (like halo-methanes, see [4]). Synchrotron - based electron sources opened new perspectives in the zero energy limit for *elastic scattering* for as important targets, like H2O [5] and noble gases [6].

In the few eV range, where *resonances* appear in elastic, electron attachment and vibrational excitation channels, critical comparisons with swarm data proved to be stringent tests for the choice of recommended data, see for ex. [7] for NO. Modified effective range theory, recently solved analytically, shows to be applicable to *elastic cross section* in targets like N2 from zero up to a few eV. However, inverting the scattering potential needed for extrapolations is very sensible to the choice of reference integral cross sections, see for ex. [8]. An improvement can be obtained by using *differential cross sections*, now available from new laboratories.

There remain two energy/ partial cross section ranges: 1) elastic data at *intermediate* and high energies and 2) *electronic excitation* and/or *dissociation* into neutrals cross sections. Both are difficult to estimate theoretically and tedious for measurements. Some scaling rules for elastic/ inelastic partitioning like that observed for noble gases vs. methane, silane, germane series [9] could be developed. The *total cross sections* in the intermediate energy range also allow for some scaling [10]. The remaining difference between total cross sections (corrected for forward scattering [11]) and known partial cross sections (elastic, ionization) would account for *other inelastic channels*. Geophysics of polar aurora is an additional check [12].

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Role of the Fusion Atomic Databases in the Internet Environment

P.S. Krstić

Most of the original atomic collision data used by the researchers in boundary plasma and in the plasma-material interface (PMI) are currently easily and instantenuously accessible using world wide web, from both scientific publications and institutional databases. However, critical evaluations of the data with respect to their quality, applicability in a desired range of parameters and extendibility of the data beyond their measured or calculated range are widely absent, and is certainly a desired activity which would signifficantly upgrade the role of the data centers to a higher level. Even more rare are the recommended data sets, developed by the critical evaluation and comparison of large number of available experimental and theoretical data, which passed the strict process of verification, validation and uncertainty quantification (UA). Such recommendations require close collaboration of the theoretical and experimental physicsts as well as mathematical and computational scientists. On the other hand, UA or error assesment of the data with respect to the plasma response is another critical set of information, a feddback of the data users, which is readily missing, and requires a mutual interaction of the data users and producers. The national and international funding restrictions for the atomic data production and the data dissemination are one of the main reasons for the poor activity in this field. The IAEA Atomic and Molecular data unit has played an important coordination role in the efforts of the national data centers, and its activity in the recommendation of hydrogen and helium atomic data in the Aladdin database was noticable in the past. After more than a decade the updates and extensions to the new recommendations for the plasma boundary and PMI data are a must.

Prominent example which well illustrates the importance of the data evaluation and recommendation, as well as verification, validation and UQ is the design of the plasma-material interface. The traditional trial-and-error approach to PMI for future fusion devices by successively refitting the walls of toroidal plasma devices with different materials and component designs is becoming prohibitively slow and expensive because of the increasing device size, curved toroidal geometry, access restrictions, and complex programmatic priorities. A comprehensive UQ effort is very valuable for this research since one has to couple multiple codes to span the partially overlaping but disparate time and length scales involved in PMI. In addition, it was established that the details of the surface microstructure play a large role in both qualitative and quantitative outcome of the targeted cross sections and yields in the particle-surface interactions, promoting importance of statistical sampling of local variations in surface microstructure in studies of the PMI processes.

Evaluation of data in fusion edge transport codes

D.Reiter[a], B. Küppers[a], R.K.Janev [b]

Atomic, molecular and plasma surface interaction data (AMS data) are key ingredients in fusion edge plasma transport codes. These codes are indispensible tools both for interpretation of current magnetic fusion experiments, in particular for the plasma domain near exposed components of the furnace chamber. But they are also used to guide reactor design of particle (ash) and heat removal components (so called divertors) from future fusion power plants. In magnetic fusion research the issue of atomic, molecular and PMI data used in transport codes is often regarded as being largely “in hand”, and the focus is often on transport terms rather than on the collision integrals in the kinetic equations. However, in particular the favorable plasma states of so called “divertor detachment”, which are currently regarded as the divertor operational regime for the ITER fusion reactor and possible also for the first fusion power plants, show a chemical richness and sometimes even dominance over transport issues not otherwise encountered in magnetic fusion. In order to allow evaluation of AMS data in fusion edge transport codes (and their further improvements) the only way seems to be via public exposure of AMS data as activated in any particular code application.

For this puropse the online data analysis tool HYDKIN (www.hydkin.de) is developed and maintained at FZJ. The goal of this online “toolbox” is threefold:

a) processing of the “as unprocessed as possible” raw atomic data (typically: cross sections vs. collision energy) into condensed data as needed in transport codes (e.g.: rate coefficients, or collisional radiative “effective” rate coefficients based on quasi steady state assumptions for some of the species, etc.

b) public exposure of atomic and molecular data as finally active in particular code applications, including also their extrapolation beyond the tabulated or fitted range, as encountered during the code runs,

c) spectral analysis of the collision-radiative rate matrix of the system, providing both identification of possibly underlying reduced chemistry models as well as closed form sensitivity coefficients for all rates and species.

The status of the HYDKIN toolbox, its underlying cross section database, its interface to the EIRENE kinetic (Monte Carlo) Boltzmann solver, and results from a sensitivity analysis for the example of hydrocarbon fragmentation in fusion divertor plasmas is discussed.

Accommodating uncertainty in ADAS models and data

M. G. O'Mullanea, N. R. Badnella, A Giuntaa, F. Guzmana, L. Mencheroa and H. P. Summersa

The Atomic Data and Analysis Structure (ADAS) is an interconnected set of computer codes and data collections for modelling the radiating properties of ions and atoms in plasmas and for assisting in the analysis and interpretation of spectral measurements. Fundamental atomic data is mediated via collisional-radiative population models to produce the effective coefficients for practical use in impurity transport modelling, influx estimation, beam stopping efficiency and active charge exchange quantification. Away from the coronal picture, the simple connection between fundamental processes and the derived population or emissivity is lost. Instead these coefficients become dependent on many fundamental processes with unknown weightings.

The challenge is threefold: to develop methods for assigning an uncertainty to the fundamental data, to propagate these through the population models and to enable techniques to utilize within plasmas models atomic data that comes with an accompanying error surface.

Pure atomic properties, such as energy levels and some transition probabilities, are measurable and are known to high precision. However most of the fundamental data required for fusion work, such as excitation and state selective charge transfer cross sections, ionisation and recombination rates (for both electron and ion drivers) remain the result of theoretical calculations and this is not likely to change. The envelope of variation between different methods and calculations is the simplest approach to ascribing an error and is useful in identifying both the principal contributors to the final quantity of interest and to assess its domain of influence. A more refined approach, based on variation of the control parameters of the fundamental ab initio codes, is adopted for this smaller set of significant cross sections.

The error for the derived quantities is computed via a statistical sampling methodology assuming an error distribution within the ascribed uncertainty range of the fundamental inputs, thus generating a manifold of population solutions of which the half-width of the fit is taken as the error in the derived quantity.

Illustrative examples will be given to show how the uncertainty in fundamental data is manifested in the error in the widely used diagnostic charge exchange lines, in the equilibrium fractional abundance and radiated power of silicon and the shine through variation in a 2% carbon plasma. Applying errors in impurity transport codes is at an early stage and non-linear effects may prove to be important.

The ADAS database stores data in well defined ADAS Data Format (adf) files (of which there are approximately 50) and these data files are numerical tabulations over appropriate independent parameters such as energy, temperature or electron density. Enabling an error capability is a simple extension of storing an accompanying error file for each data file with the overall goal to have such matching error files for each dataset of the ADAS and OPEN-ADAS databases.

The generation and propagation of uncertainties on atomic data

C.P. Ballance[a], M.C. Witthoeft[b], S.D. Loch[a], and M.S. Pindzola[a]

The need for meaningful uncertainties on atomic data has been identified as a critical issue for fusion plasma modeling. It would allow one to determine the range of values on photon emissivities, plasma transport coefficients and impurity abundances due to uncertainties on the atomic data.

We propose two objective methods to quantify meaningful uncertainties on electron-impact excitation, ionization and recombination rate coefficients. The first we refer to as *baseline uncertainty* which provides an estimate of the range of likely rate coefficients to be found in the literature, leading to a generous estimate of the uncertainties on observable quantities. The second method we call *method sensitivity* which is more involved, but provides a systematic calculation of the likely uncertainties within the state-of-the-art method of each data type (e.g. electron excitation). This method includes effects such as correlation between the various atomic processes in the collisional-radiative modeling, and an appropriate distribution function for the range of atomic rate coefficients.

As a preliminary study, illustrating the use of baseline uncertainty data, we show results for O6+. Uncertainties on O6+ diagnostic line ratios are generated from a Monte-Carlo set of collisional-radiative calculations.

ASESSMENT OF ATOMIC DATA: PROBLEMS AND SOLUTIONS

K. M. Aggarwal and F. P. Keenan

Atomic data, namely energy levels, radiative rates (A- values), and effective collision strengths, which are obtained from the electron impact collision strengths, are required for a range of ions for the analysis and modelling of a variety of astrophysical and laboratory plasmas. Experimental energy levels for several ions are available on the NIST website, in particular for low-lying levels. For some ions, critically evaluated theoretical results are also available, but often the range available on the NIST website is limited. Therefore, in modelling applications there is sometimes no choice but to adopt unassessed theoretical results. However, discrepancies for energy levels, in both orderings and magnitude, are often noted among different calculations. Some of these discrepancies will be shown during the meeting, reasons for these discussed, and suggestions offered for the assessment of accuracy.

Similar results for collision strengths are also available for many ions of interest, but often either the available data are limited (to only a few transitions and/or to a few energies) or lack accuracy, particularly for the effective collision strengths (Υ). This is because calculations for Υ are computationally intensive, with resonances in the thresholds region needing to be resolved in a fine energy mesh, in practice at thousands of energies depending on the ion. These closed-channel (Feshbach) resonances often significantly contribute to the determination of Υ, particularly for lighter ions and at low temperatures. However, their contribution is also significant for many heavier ions, such as Kr, Mo and Gd, and at the high temperatures ($\geq 10^6$ K) found in fusion plasmas. Nevertheless, calculations are available in the literature for many of the required ions. However, the accuracy of the available results is often suspect, because different calculations using similar methods/codes sometimes differ by up to two orders of magnitude for some transitions, such as in He-like and Li-like ions. Reasons for discrepancies, large and small, among different calculations for both allowed and forbidden transitions, can be many, such as: inadequacy of configuration interaction, limited range of partial waves and/or the energy range, limited inclusion (or exclusion) of relativistic effects, or errors in the adopted version of the code. Examples of such discrepancies will be shown, reasons explained, and suggestions offered for avoiding large errors, so that comparatively more accurate data can be generated for the benefit of user fusion community.

Evaluation of electron-impact excitation data along iso-electronic sequences

G.Y. Liang, N.R. Badnell, G. Zhao

The advent of high-quality high-resolution laboratory and astrophysical X-ray and EUV spectra requires correspondingly accurate electron-atom/ion interaction data (including electron-impact excitation, EIE) to utilize fully their potential diagnostic modelling capability for celestial objects. A program — the Atomic Processes for Astrophysical Plasmas network — was setup in the UK to generate accurate atomic data (including electron-impact excitation) along iso-electronic sequences and to assess the reliability of the final product. These data and their evalution method are also applicable for the magnetic fusion community.

The intermediate-coupling framework transformation (ICFT) *R*-matrix approach [1] was used to calculate EIE data. The R-matrix method efficiently includes resonances usually omitted by the distorted-wave method. The ICFT variant is less resource (time/memory) demanding than the full Breit-Pauli *R*-matrix method, without reduction of accuracy. So far, calculations for the He-like, Li-like, F-like, Ne-like and Na-like iso-electronic sequences [2, and references therein] have been completed and an assessment of the resultant data has been carried-out. Calculations for another three iso-electronic sequences (including Be-like, B-like and Mg-like) and some urgently important ions are planned in the 2nd APAP program.

A detailed accuracy assessment was done for four/five/six selected ions spanning the iso-electronic sequence and which poses insight into the behaviour of the whole sequence of ions. For each ion, we adopt the following procedures: (1) firstly, the target structure was assessed by comparing the calculated level energies with available experimental data and previous calculations with different methods. (2) secondly, weighted oscillator strengths or line strengths or radiative decay rates were compared with various available theoretical works for several transitions. Usually a 'survey' comparison with another database has been done for all available transitions by way a scatter plot. (3) thirdly, direct comparison for the excitation (effective) collision strength is done with available measurements or with previous published data. A 'survey' comparison with another database is usually presented to investigate the widespread of consistency or inconsistency among the different calculations. In conclusion, the resultant excitation data along the iso-electronic sequences were assessed to be reliable and were incorporated into astrophysical and fusion database/modelling codes, such as CHIANTI, ADAS, AtomDB etc.

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Cross Sections on the Processes Induced by Electron Collisions with H_2^+, HeH^+, and Their Isotopes

H. Takagi

The collision processes of molecular ions and electrons play an important role in the divertor plasma such as molecular assisted recombination. Besides the main process of dissociative recombination (DR), dissociative excitation (DE) and rotational-vibrational transition of molecular ion affect the distribution of molecular and atomic states in plasma. The cross sections (CSs) of those processes, in principle, strongly depend on the electronic, rotational, and vibrational states. Plasma simulation also requires the data on the electronic state distribution of dissociated products. Those CSs should be state-specific both for initial states and for final states.

Almost all of available experimental data are on the DR of which initial vibrational-rotational state are confined to the ground state or mixture. Theoretical calculation could give state specific CS for various states. Thus, the accuracy of calculated CS could be check by comparing with the experiment for some limited states of limited molecular species. Roughly speaking, recent calculation on the DR of H_2^+ and HD^+ agree with experiment within about 20% difference for the rotationally and vibrationally ground state ions at the collision energies below 0.2 eV. The isotope effect could be accurately estimated by theoretical calculations. That means the calculated CSs of D_2^+, HT^+, DT^+, and T_2^+ have accuracy equal to H_2^+ [1].

We need to investigate the physics to estimate the accuracy of calculations since the check by experiment is limited. The theoretical calculations of those processes are composed of two parts; one is (a) electron scattering by a fixed-nuclear molecular ion, the other is (b) dynamics including nuclear motion. The accuracy of part (a) depends how complete electronic basis functions are adopted in the variational or close coupling calculations like R-matrix method: the basis functions for (1) partial waves of incident electrons and for (2) excited states of collision complex. By investigating a convergence with various these two types of electronic basis functions, we could estimate the accuracy. A converged calculation of the low energy DR of HeH^+ could be achieved (collaboration with M. Tashiro). For the high energy, we should investigate the convergence on type (2) basis functions. On H_2^+, we need check the convergence both type (1) and type (2) even for low energy collisions. The accuracy for very high rotational and vibrational states could be secured if enough basis functions are adopted. Theoretical calculation shows that the rotational motion is not important at the collision energy higher than 1 eV. It is empirically known that the multichannel quantum defect theory (MQDT) for the dynamics (part (b)) gives more reliable cross sections than the perturbation theory. The MQDT, however, could not secure the accuracy quantitatively. The off-the-energy-shell contribution deeply affects the CS. The effect becomes about one order of magnitude (1000%) for the DR of H_2^+. This work was supported by the JAEA.

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Evaluation of the electron impact excitation of n=2,3 states in Helium

M. Y. Song, H. C. Chor, D. C. Kwon, S. Y. Jung, S. H. Hwang, J. H. Park, W. S. Chang, H. U. Chang

A collision processes involving helium by electron impact are fundamental to the investigation of few electron interactions in atom and molecule. Knowledge of such collision processes is important not only for the understanding of the collision dynamics but also for laboratory and astrophysical plasma and fusion plasma. There are huge amounts of cross section data of helium by electron impact excitation. Evaluation of helium data already had done by de Heer et. al and Y. Ralchenko et. al, But they didn’t show uncertainty of recommended data. We would like to decide appropriate evaluation method through the available electron impact processes. This work will be started to understand a previous evaluation studies. First step to start, we collected published collision data until 2010 using NIFS database, KISTI database, and AMBDASD Bibliography. And we reviewed these articles and evaluated the electron impact excitation cross sections for the transition of the n=2, 3 states in Helium atoms and calculated uncertainty. Finally we compered our evaluated data and pervious evaluated data

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Electron Swarm Parameters and Electron Collision Cross Sections

Yoshiharu Nakamura

Electron collision cross section data for atoms and molecules and electron swarm data in respective gases are important for quantitative modeling of related plasmas. This fact and wide application of plasmas in various fields boos data collection and evaluation activities worldwide.

We have been measuring electron swarm parameters (drift velocity, longitudinal diffusion coefficient, ionization/attachment coefficients, and so on) over a wide *E/N* range (where *E* is the electric field and *N* the gas number density) in a number of gases. We also derived a set of electron collision cross sections for each gas so that the set was consistent with our experimental swarm data. Our speciality in studying molecular target is to measure swarm parameters not only in the pure molecular gas but also in dilute molecular gas-argon gas mixtures, the mix rations of the molecule are 0.5-5.0%. The swarm parameters in pure molecular gas depend primarily on the elastic momentum transfer cross section of the molecule and its vibrational excitation cross sections. Those in the mixtures, on the other hand, depend mainly on the elastic momentum transfer cross section of major argon atom and the vibrational cross sections of minor admixed molecule. Alternative use of swarm parameters in pure molecular gas and those in the mixtures enable us to derive the momentum transfer cross section and vibrational cross sections for the molecule separately. Combination of the Ramsauer-Townsend minimum of argon atom and sharp structures in vibrational cross sections of the molecule frequently gives rise prominent *E/N* dependences in swarm parameters, which can be used to determine the position and magnitude of resonances in the vibrational excitation cross sections. Detailed accounts of the procedure, including estimated uncertainty in our electron swarm data and also in the resultant set of electron collision cross sections, will be given in the presentation by referring to our recent results. Stress will be placed on the necessity of cooperation among swarm, beam and theory groups.

Low Energy Electron Collisions with Plasma Processing Gases – Data Compilations and Evaluations

J.-S. Yoon[1], M.-Y. Song[1], H. Kato[2], M. Hoshino[2], H. Tanaka[2], M.J. Brunger[3], H. Cho[4] and S.J. Buckman[5]

Gaseous electronics—the term which is loosely applied to describe low temperature discharge physics—is a broad and diverse area of research and development which encompasses both established and emerging technologies. These include semiconductor production, lighting, propulsion, environmental remediation, and materials processing, to name just a few.

Absolute electron-impact cross sections for molecular targets, including their radicals, are important in applications of gaseous electronics, such as the development of plasma reactors and testing various plasma processing gases. Low-energy electron collision data for these gases are in some cases quite sparse and only limited cross section data are available. In this work, elastic cross sections for electron collisions with a number of molecules relevant to plasma processing are reviewed. Elastic cross sections are essential for the absolute scale conversion of inelastic cross sections, as well as for testing computational methods. In this work data has been collected and reviewed for elastic differential, integral, and momentum transfer cross sections and, for each molecule, recommended values of the various cross sections are provided. The project encompasses data for more than 15 molecules and several radicals and selected examples will be presented in this presentation to illustrate the state of field.

We also highlight the comparison, where possible, with theoretical estimates of these cross sections. The strong rationale for this is that in many cases theory may be the only avenue to obtain cross sections, for reactive collisions for example, and elastic scattering measurements can provide a handy and accurate tool for benchmarking theory.

Electron-loss and capture cross sections of W ions colliding with H and He atoms

V.P. Shevelko[a], I.Yu. Tolstikhina[a] , M.-Y. Song[b], and J.-S. Yoon[b]

Electron-loss and charge-exchange cross sections of tungsten ions colliding with H and He atoms are calculated in the energy range of 1 keV/u – 10 MeV/u using DEPOSIT, RICODE and CAPTURE codes based on the classical energy-deposition model and the first Born approximation. The data obtained can be used for plasma modeling and interpretation of future experiments at fusion devices using tungsten as a material for the plasma facing components (PFC). The details of calculations are presented in [1]. The data for charge-exchange cross sections for highly charged W ions are in good agreement with semi-empirical formula [2].

The data for these charge-changing cross sections were evaluated on the basis of their dependencies on collision energy, and atomic structure of colliding particles such as ionization potentials, ion charge, nuclear charge of the target atom and others. It was also very useful and important to obtain some *semi-empirical formulae*, for example, for electron loss cross sections obtained in [3]. This formula was evaluated on the basis of available experimental data and numerical calculations performed for a large number of colliding systems and in a wide energy range. Such formulae are required to get self-consistent data and to predict the charge-changing cross sections for an arbitrary colliding partners.

Figure 1 shows an example of the calculated cross sections for H gas target.

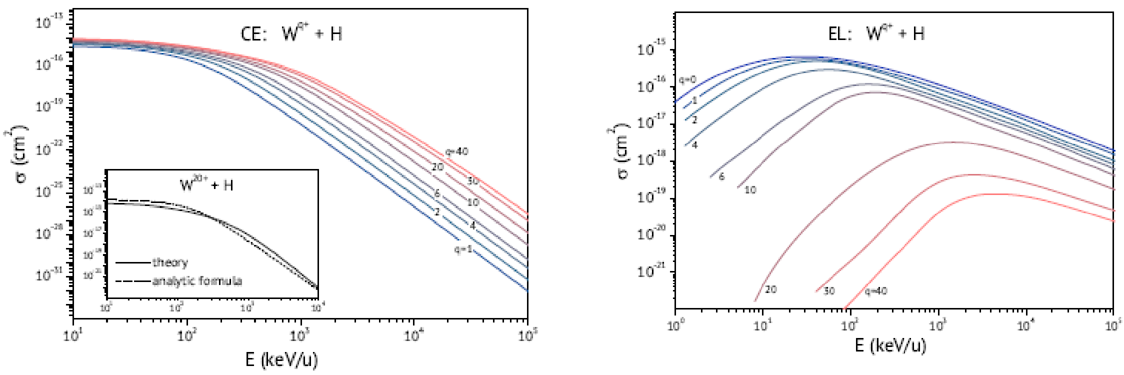

Fig. 1. Calculated charge-exchange (CE) and electron-loss (EL) cross sections of W^{q+} ions colliding with H atoms. In the left figure, calculated CE cross sections for W^{30+} +H collisions are compared with semi-empirical formula [2].

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Target dependence of single electron capture cross sections for W^+ and W^{2+} ions

M. Imai, Y. Ohta, and A. Itoh

Single electron capture cross sections for W^+ and W^{2+} ions colliding with He, Ne, Ar, Kr, H_2, D_2, N_2, CH_4, C_2H_6, and C_3H_8 gas targets were derived experimentally in low energy region of 5.0 – 15 keV. The measured cross sections show clear dependence on the ionization potential (IP) of the targets. The observed IP dependence is, however, much far steeper than previously proposed IP scalings, $IP^{-2.76}$, $IP^{-2.0}$, and $IP^{-1.59}$, by Müller and Salzborn [1], Kusakabe *et al*. [2], and Yamada *et al*. [3], respectively, to reproduce electron capture cross sections for low-energy highly-charged ions. Other scaling properties concerning data evaluation for the present cross sections will be discussed as a case-study of estimating uncertainties of datasets being derived for the first time. Our compilation on electron capture and loss cross sections for heavy particle collisions will be introduced as well with data evaluation efforts based on the compilation.

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Development of Standard Reference Data on A+M Data for Plasma at National Fusion Research Institute

Jung-Sik Yoon and DCPP members

The study of atomic and molecular (A+M) physics using electron, ion and neutral have been an active area of experimental and theoretical research for several years. Since, the interactions with various atomic and molecular target play an important role in many areas, such as nuclear fusion, semiconductor manufacturing, lighting, propulsion, environmental remediation and material processing. In addition, as interest has increased in the interaction between low-temperature plasmas and materials, the role of modeling and simulation of processing plasmas has become important in understanding the effects of charged particles and radicals in plasma applications.

In order to store, retrieve and digest vast quantities of A+M have been of great interest since the need of such a scientific and technical data are explosively increased with a remarkable growth of industry. Also, the demands of reliable and accurate well evaluated data have been greatly increased. Thus, Korea government have archived and distrivuted data which are evaluated on accuracy and reliability and authorized. Also, established National Center for Standard Reference Data (NCSRD) and specilized Data Center in order to develop and distribute Standard Reference Data (SRD).

In this presentation, we briefly introduce the overall data evaluation system of SRD and the development and distribution of SRD for A+M data for plasma.

Atomic and Molecular Databases and Data Evaluation Activities at NIFS

I. Murakami, D. Kato, M. Kato, H. A. Sakaue

The National Institute for Fusion Science (NIFS) has constructed atomic and molecular numerical databases for collision systems and makes them available via the internet at http://dbshino.nifs.ac.jp/ since 1997. Data compilation was started in the 1970s at the Institute of Plasma Physics, Nagoya University and has a long history. Working groups have been organized to compile and evaluate atomic and molecular collision data and plasma-wall interaction data. Now the NIFS database system has AMDIS (cross sections and rate coefficients of electron collision processes for atoms; 465,991 records as of May 10, 2012), CHART (cross sections of heavy particle collision processes for atoms; 7,054 records), AMDIS-Molecule (cross sections and rate coefficients of electron collision processes for molecules; 1,766 records), CHART-Molecule (cross sections and rate coefficients of heavy-particle collisions for molecules; 1,999 records), SPUTY (sputtering yields for solids; 1,241 records), and BACKS (backscattering coefficients of solid surface; 396 records). The databases are retrievable and numerical data can be shown as a graph or a table. Each data record contains bibliographic information as well as numerical data.

The NIFS databases are used to compare data to evaluate, and evaluated data are also stored in the databases. Evaluated data sets are published as reports in IPPJ-AM series (1977-1989) and NIFS-DATA series (1990 – present). Critical data evaluation was done for electron-impact excitation cross sections (e.g. C and O ions [1] and N-like ions [2]), electron-impact ionization cross sections (e.g. hydrocarbons [3]), and charge exchange cross sections (e.g. Li3+ and H [4]). Asymptotic behavior of cross sections at high collision energy was considered to determine analytic formulae for fitting data, and data were fitted to such analytic formulae. Even though reliable energy (temperature) ranges are limited, it is useful to express evaluated data with fitting formulae. Such evaluated data expressed with fitting formulae and parameters are important and useful for plasma simulations and modelings in fusion plasma research. Such evaluation has been done only for limited collision systems. We also selected data sets of electron-impact collision rate coefficients for Fe ions among existing theoretical calculations as recommended data sets for spectral modelings [5]. For the selection, we examined calculation method, number of configurations and ranges of collision energy and partial waves considered in the calculations, and availability of data sets. Such selection is one of evaluation methods for collision processes which experimental measurements are rare or do not exist. It is important to establish an international collaboration system on data evaluation to evaluate data for many collision systems with systematic way. It is also necessary to have an independent database of evaluated data for easy use for users.

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SUP@VAMDC : Uniting the international atomic and molecular data community

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Atomic and molecular (A+M) data are of critical importance across a wide range of applications such as astrophysics, atmospheric physics, fusion, environmental sciences, combustion chemistry, health and clinical science including radiotherapy and underpin a range of industries ranging from technological plasmas to lighting. Accordingly in the past decade the wider research community has appreciated the need to collate and make available the A+M data that describes fundamental atomic and molecular processes recognising how access to such data is central to achieving scientific breakthroughs across a range of disciplines. However such increasing demands by the research community for large amounts of A+M data present major challenges to the expert research teams in Europe, the USA, Asia and elsewhere that measure, derive and collate such data as demand outstrips supply. The interface between the producers of A+M data and the wide body of users of that data has therefore been a major bottleneck, slowing discovery and hence slowing economic growth. The VAMDC e-infrastructure (www.vamdc.eu) was developed to remove this bottleneck by designing/implementing interoperable protocols among a wide range of disparate databases A+M databases and providing a single portal through which users can access A+M data whilst providing data providers and compilers a large dissemination platform for their work. To date VAMDC has been mainly confined to those partners providing the databases for the shared platform and thence their established users.

The concept of the SUP@VAMDC programme is to establish the necessary coordination methodology required to formulate the roadmap that will ultimately combine VAMDC with complimentary infrastructures organised by existing international bodies/committees/networks dealing with the production, evaluation and dissemination of A+M data ultimately leading to a global e-infrastructure for the assembly, curation and access of the immense amounts of atomic and molecular data that will underpin the development of the scientific knowledge base that will be required to meet (and overcome) the great scientific challenges of the early 21st century (e.g climate change, space exploration, human health and. crucially, the continued technological advances that will drive the global economy).

SUP@VAMDC will therefore develop a strategy that will allow A+M databases/data centres (especially those outside the EU) to adapt their pre-existing structures to those fashioned by the VAMDC e-infrastructure whilst providing the mechanisms and tools for new data centres/databases to be developed such that they are immediately compatible with the recently developed VAMDC platform extending their reach and thence facilitating the adoption of such data centres/databases amongst a wider range of user communities spanning across academia, higher education, citizens and industry. Furthermore SUP@VAMDC will explore both the necessity for, and practicality of, an open e-infrastructure - Open VAMDC – that will takes a product based on e-science technology and primarily used by its established users, and transforms it into a worldwide product shared across communities from academia to citizens, with the inherent opportunities for training and exploitation that such a product brings.

The IAEA Data Centre Network – Data Evaluation Activities

H.-K. Chung and B. J. Braams

The Atomic and Molecular (A+M) Data Unit of the International Atomic Energy Agency works to establish databases and a knowledge base of atomic, molecular and plasma-surface interaction (PSI) processes that are important for fusion energy research. Activities for database development include IAEA Coordinated Research Projects (CRP), Technical Meetings, Consultant Meetings and a number of collaborations. New data produced through these activities is published in journals and in IAEA reports and is included in the numerical database ALADDIN that is freely accessible to all fusion researchers.

Since 1978 the A+M Data Unit has supported the International Atomic and Molecular Data Centre Network (DCN) where a number of institutions coordinate the production, exchange, compilation, dissemination and evaluation of fusion relevant data. Until recently, data centre activities were focused on producing, compiling and disseminating new data sets in response to demands for non-existing data from the fusion community. With the rapid advances in computing capabilities and in on-line search functions theoretical data sets are being generated and accessed with more ease. As a result, there have been increasing requests from the user community for evaluation of the quality of available data sets, and at their most recent meeting the DCN acknowledged the great need to increase data evaluation activities.

The DCN meeting and a subsequent smaller Consultancy meeting (at NIFS in Feb 2012) identified important issues that must be addressed to support data evaluation and, in the longer run, the development of a comprehensive internationally recommended standard library for A+M (+PSI) data for fusion. One key issue is the assessment of uncertainty of theoretical data when, as is very often the case, direct comparison with experimental data is not possible. (Theoretical cross-section data may be finely resolved with respect to incoming and outgoing states whereas measured cross-sections are often under-resolved on both sides.) In addition to such scientific issues there are practical issues of the provision of measured and calculated unevaluated data in a format that facilitates comparison and the assignment of uncertainties. The development of a standard library of evaluated data requires also a library, or at least a common format and convenient means of exchange, of unevaluated data. The initial effort by the IAEA A+M Data Unit and the DCN towards the development of a standard library is focussed on A+M collision cross section data. Plasma-surface interaction data are the other important component of the work of the A+M Data Unit and the DCN, and evaluation is much needed for such data too, but many more variables are involved both in experiment and in computation.

In the present meeting the recommendations and conclusions of the Data Centre Network meeting and the Consultancy meeting on data evaluation activities will be presented and the long-term goal to establish the IAEA standard library of fusion relevant atomic, molecular and plasma-material interaction data will be discussed.

Roadmap to the Establishment of Internationally Agreed Standard Data Library for AM/PSI Data Relevant to Fusion Applications

Phase 0: Inventorise the AM/PSI Data Collection used by Fusion/Plasma Community

Priority list of critical data needs and data sets currently used by data users

- There are a variety of A&M/PSI data sets required for fusion applications.
- A users' network of intensity data applications should be established to provide and update the priority list of critical data needs for fusion applications.
    - Draft of the present data sets used by data user community
    - Absolute grand canonical list of presently used data sets
    - What is the most critical and urgent need?
    - Reiter, Costner, Jet, Zagorski?, Borodin, 10 (Europe) 5 (US), 5(Far east)—30 people
    - What is the A+M/PSI data set used for fusion applications.
    - World Draft AM/PSI Data Collection
        - Questionnaires (ITM)
        - Working group formation
        - Reconcile, remediate and upgrade/expand/complete data library
    - Standard Data Format: Easy Data Access

Phase 1: Establishment of infrastructure for evaluated data library

IAEA Atomic and Molecular Unit: Development of database to host the standard data library

- It is understood that the IAEA A+M data unit will host two databases: 1) the internationally agreed standard (recommended) data library and 2) the evaluated data library.
- The standard data library is the final goal which gives a single recommended data set as the best data of the given process at the time of determination.
- The evaluated data library is the intermediate database where evaluated data sets are collected before standardization (recommendation) and there may be more than one evaluated data set for the given process. The version of data sets can be traced through the evaluated data library.
    - There may be another class of datasets, which was previously recommended.
    - Any interactions with providers of data sets used for evaluated & recommended data sets
    - Evaluated data is a data set reviewed by an expert.
- The data format and the maintenance of databases should be determined as the first step.
    - XSAMS-Lite may be useful for output tools/export tools
    - Full XSAMS should be used for data description
- The unit should make efforts to emphasize the importance of data evaluation activities to the member states for more support at the government level.

Data Centres: Compilation of relevant data for evaluation

- It was suggested that there should be a unified database available for evaluators.
    - NIFS
    - ADAS(Open)
    - NFRI
    - VAMDC?? – bilateral agreement?

- A meeting should be organized to discuss the location of the database, the coordination of data collection, the decision of data format for this data storage.
    - Theoretical data needs to include code descriptions

Data Centres and Evaluators: Establishment of data evaluators' network

- Data evaluator's network should be established to coordinate effectively evaluation activities in the community level.
- The network will train younger generation and facilitate the knowledge transfer from seasoned evaluators.
    - Collisional-radiative model descriptions
    - Processed data description (documents?)
    - If there is only one set, how would you evaluate it? – guidelines needed (threshold behaviours, asymptotic behaviours, simpler model comparison, semi-empirical fit comparison…)

Data Evaluators: Guidelines of evaluation methods

- Evaluation methods should be agreed among data evaluators and standardized.
- Meetings should be organized for evaluators to discuss the guidelines of evaluation methods for each category of processes.

Data Producers: Guidelines of uncertainty estimates

- There is a need of internationally agreed standards for theoretical data uncertainties.
- Meetings should be organized to draw a consensus among data producers and to find the methods to determine the uncertainties.

Phase 2: Establishment of evaluated data library

IAEA: Establishment / maintenance of databases to host the evaluated data library

- IAEA will host the database to contain the evaluated data sets in coordination with data centres and evaluators.
- IAEA will organize meetings for evaluation activities

Data Centres: Coordination of data evaluators' network activities

- The designated committee of the network will work with evaluators to assign an evaluation task to the corresponding expert.
- The committee will collect evaluated data sets in the evaluation data library and will publish the volume of evaluated data sets.

Data Evaluators: Evaluation of data sets

- Designated evaluators will evaluate data sets and maintain/improve the guidelines of evaluation methods
- Evaluators will review the previously evaluated data sets on regular basis

Data Producers: Guidelines of scaling laws / fit expressions

- Evaluated data sets need to be extended to ranges where no data sets are available.
- Data producers, especially of theoretical data will be able to provide the scaling laws or physically consistent fit expressions.

Data Users: Development of data format compatible to applications

- Evaluated data sets will be used for modeling and the common data format will make it easier to transfer data sets from the evaluated library to the modeling code.

Phase 3: Establishment and maintenance of standard data library

IAEA: Establishment / maintenance of databases to host the standard data library

- IAEA will host the database to contain the standard data sets in coordination with data centres and evaluators.
- IAEA will organize meetings for evaluation activities

Data Evaluators and Data Centres: Coordination of Technical Committees

- Data centres and evaluators will work together to form technical committees to recommend the evaluated data as the internationally agreed standard data.

Data Producers: Feedback on data sets (production of missing data, data improvement)

- The standard data library will provide an overview of the quality of the data required for fusion and data producers may provide a feedback on data sets.

Data Users: Feedback on data sets

- Data users will update the data lists required for plasma applications and may give the feedback about the quality of the standard data sets after applications to modeling work

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