



**IAEA**

International Atomic Energy Agency

INDC(NDS)- 0580  
Distr. LP,NE,SK

# **INDC International Nuclear Data Committee**

## **International Code Centres Network**

### **Summary Report of the Technical Meeting**

IAEA Headquarters, Vienna, Austria

27–28 September 2010

Prepared by

H-K. Chung

International Atomic Energy Agency, Vienna, Austria

January 2011

Selected INDC documents may be downloaded in electronic form from  
*[http://www-nds.iaea.org/indc\\_sel.html](http://www-nds.iaea.org/indc_sel.html)* or sent as an e-mail attachment.  
Requests for hardcopy or e-mail transmittal should be directed to [services@iaeand.iaea.org](mailto:services@iaeand.iaea.org)

or to:

Nuclear Data Section  
International Atomic Energy Agency  
PO Box 100  
Vienna International Centre  
A-1400 Vienna  
Austria

Printed by the IAEA in Austria

January 2011

## **International Code Centres Network**

### **Summary Report of the Technical Meeting**

IAEA Headquarters, Vienna, Austria

27–28 September 2011

Prepared by

H-K. Chung

International Atomic Energy Agency, Vienna, Austria

#### **Abstract**

Fifteen international experts on computational aspects of atomic, molecular and particle surface interaction data for fusion energy research participated in the 2<sup>nd</sup> technical meeting of the International Code Centres Network. Participants reported their research on data production and computational capabilities at their institutions. Experts in the field of plasma modeling of magnetic fusion research joined this meeting to present the data needs and bring the perspective of data users. The interaction and discussion among data producers and data users in this two-day meeting led to an agreement that the scope and function of Code Centres Network should be reformulated to serve the needs of fusion community in more effective way.

January 2011



## TABLE OF CONTENTS

1.	Introduction.....	7
2.	Presentations and Proceedings.....	7
3.	Discussions and Recommendations.....	11
4.	Summary.....	12

### Appendices

1:	List of Participants.....	13
2:	Agenda.....	15
3:	Abstracts and Summaries.....	17



## 1. Introduction

The 2<sup>nd</sup> Technical Meeting to discuss the activities of an “International Code Centres Network” was held on 27-28 September 2010 at IAEA Headquarters, Vienna and was joined by all the attendants of the 1<sup>st</sup> meeting except for D. Stotler (PPPL). Participants reviewed research activities and computational tools of atomic, molecular and particle surface interaction (AM/PSI) data relevant to the fusion research community. As suggested in the previous meeting, new participants were invited to the network, M. Klapisch of HULLAC atomic physics codes and R. Schneider of SDTrimSP plasma-surface interaction physics code. Participants of the meeting on “Data Needs for Plasma Modeling” held on 29-30 September 2010 was invited to this meeting to their work on the plasma modeling of magnetic fusion research and its data needs, and offered a perspective from users of AM/PSI data (see Appendix 1 for participants’ list).

After presentations, participants discussed current data needs for the fusion research and the future direction of the “International Code Centres Network” (CCN). The interaction between data users and data producers was found extremely useful on both sides as data users had a chance to obtain information on both the computational capabilities and limits of available data and data producers to obtain information on the current needs directly from data users. Data users expressed the importance of evaluated and recommended data sets in the modeling. They also expressed the lack of information on the uncertainties of available data and hence the concerns over unevaluated data sets generated by inexperienced users of online codes. Other methods to distribute numerical data sets were discussed and finally, the scope of the CCN was suggested to be reformulated to enhance the collaboration between data producers and data users as well as among the data producers themselves.

## 2. Presentations and Proceedings

R. Forrest as Section Head of the Nuclear Data Section welcomed the participants on behalf of the IAEA. He acknowledged that the Code Centre Network (CCN) is rather new while it can become one of the key activities of the Unit. He emphasized that the importance of role of code development in assisting fusion energy research by complementing the database development and wished participants the productive meeting. B.J. Braams as Unit Head of the Atomic and Molecular Data Unit reviewed the proposed agenda, which was accepted without change (see Appendix 2 for agenda).

During the first and the half of the second day, participants gave a summary presentation of relevant research activities within their institutes (see Appendix 3) and code centre activities such as online activities or code/data sharing activities. Discussions then took place on the progress of recommendations and resolutions of the last meeting and the future functions of the CCN.

D. Coster of Max-Planck-Institut für Plasmaphysik reviewed the activities of ITM-TF (Integrated Tokamak Modeling-Task Force) and the use of atomic, molecular, nuclear and surface/solids data in European codes. Requirements, challenges and immediate needs in the data used for the modeling were described. Data should be robust, comprehensive, easy to use, efficient and able to address special needs. The version control, expert validations, standardized input and output are important for data modules used in the integrated tokamak modeling. The list was provided for missing or not verified data sets and immediate needs. Isotope-resolved atomic and plasma-surface interaction data and differential cross-sections are among the immediate needs. Current activities to incorporating atomic, molecular and plasma-surface interaction data sets in the ITM database were described.

D. Elder of University of Toronto, Canada, reviewed the plasma modeling codes relevant to fusion research, the OEDGE code suite. The OEDGE code suite used for modeling the behavior of the edge plasma of magnetic fusion devices is composed of several elements, an Onion Skin Model (OSM), the EIRENE Monte Carlo code and the DIVIMP Monte Carlo plasma impurity code. Results of simulations are compared to spectral measurements, plasma condition measurements by Thomson scattering and probes and other diagnostics. The OEDGE uses a broad range of atomic, molecular and surface data at a relatively processed level. He described the data requirements for these codes;

ionization and recombination rate data for hydrogen as well as all charge states of the impurity species, rate data for hydrogen molecules and the line emission data for both hydrogen and impurity species. The surface sputtering data for both impurity species as well as hydrocarbon molecules are required (see Appendix 3 for more details).

R. Schneider of Ernst-Moritz-Arndt University Greifswald, Germany, reviewed the tools and strategies for the description of plasma-wall interaction. The complex and different nature of the physics requires a combination of methods and the real structure of the material is important. Molecular dynamic simulations and simpler models can complement each other and more fundamental understanding of model systems are needed for validation. He described several version of the code TRIM which calculates the sputtering of a surface exposed to a flux of energetic ions. The TRIM code calculates the sputtering yield of a projectile of an ion of a volatile (recycling) element comparable to experimental results. If the projectile is a solid-state (non-recycling) ion, the dynamic change of surface by projectile implantation is important and can be treated with 1D-TRIM (TRIDYN, later SDTrimSP). As the surface roughness may increase the sputtering yield by as much as a factor of 5, the calculation is extended to 2D and 3D grids in lateral dimensions for rough surface problem. An example of a Si pitch grating exposed to 6 keV Ar ions shows that the SDTrimSP-2D code predicts the results with a good accuracy. Another extension includes the chemical sputtering and the code reproduces experimental observation such as a hydrocarbon surface bombarded with Neon and in parallel exposed to thermal hydrogen influx. (See Appendix 3 for more details)

J. Abdallah of Los Alamos National Laboratory (LANL), USA, reviewed the recent activity in his institute. The LANL contribution to the IAEA Atomic and Molecular Data Code Centre is the online version of atomic physics codes. These codes are accessed online by users to perform atomic structure calculations, including excitation and ionization cross sections, for arbitrary ions and configurations. A brief description of the online capabilities was presented. A short summary of the ATOMIC plasma modeling code was also provided. Recent improvements to the CATS code were discussed, in particular, the recently developed parallel computing capability. Several examples of the use of the LANL suite of atomic physics codes to applications of interest to magnetic fusion were discussed including recent boron power loss calculations and preliminary results for modeling low temperature tungsten plasmas.

F. Koike of Kitasato University and NIFS, Japan, reported the activities in the study of atomic structure and dynamics calculations using the GRASP (General purpose Atomic Structure Program) family codes and activities in NIFS. The projects include analysis of visible M1 lines in Tungsten ions, collisional-radiative model for W ions, a code development for single electron capture by H nucleus from metal surface, and studies of  $K\alpha$  radiation from low charge chlorine heated by an ion beam for plasma diagnostics. (See Appendix 3 for more details)

L. Vainstein of Lebedev Physical Institute, Moscow, Russia, described his work on calculations of ionization cross sections for W I and W II and codes ATOM and MZ for atomic calculations. There are good experimental data for W II single and double ionization and no direct cross section measurements for W I. Therefore he started with the ionization of W II and tests the calculations by comparison with experimental data hoping that accuracy for neutral W would be similar. The cross sections are calculated by the code ATOM in Coulomb-Born approximation (CB) with exchange and correction for the normalization by the reduced K-matrix approximation. For highly charged ions calculations, the code MZ is used using  $1/Z$  expansion method which computes energies, wave lengths, spontaneous emission rates and photo-ionization cross sections and autoionization rates.

M. Klapisch of ARTEP Inc. (USA) and Institute for Particle Physics, ETH, Switzerland, reported on the activities of HULLAC code of suite. The first version of HULLAC (Hebrew University Lawrence Livermore Atomic Code) dates back to the 1980's when he was at Hebrew University, Jerusalem, Israel, and got the support of LLNL. The concept is to generate a consistent atomic model, by using the same wave functions for computing all atomic processes relevant to plasma spectroscopy. These wave functions are obtained by solving the Dirac equation in a parametric potential. The central field model enables a convenient decoupling of the angular momentum algebra for all processes, including



electron collisions, for which the factorization-interpolation method is introduced. Recently, the whole code was re-written in a more modern way and extensively checked. It includes now a collisional radiative solver with a special scaling for improved convergence, a new fit for the cross section, the ability to use the mixed transition arrays (MUTA), and to model the effect of an external radiation field. The latter capability was used to compare with a recent experiment on the transmission of Fe at  $T_e = 156$  eV, with excellent agreement. The latest version is used by several groups, whose feedback is used to constantly improve and/or correct the code. (See Appendix 3 for more details)

I. Bray from Curtin University of Technology, Australia, reported on a considerable progress in the development of the Convergent Close-Coupling (CCC) theory. The major extension has been to institute a new parallelism paradigm. This utilizes a hybrid OPENMP/MPI combination with the main V-matrix being calculated across several nodes. Within each node the original OPENMP parallelism is used. Then, using MPI, the matrix is distributed in a block cyclic form across all the available cores suitable for solving the linear equations via the ScaLAPACK suite of routines. Consequently the CCC code is now able to be run across many nodes of memory sharing multiple cores. Both the original non-relativistic CCC and the recently developed relativistic RCCC codes have been parallelized this way. Additionally, the RCCC code has been extended to quasi two-electron targets, and highly charged ions, including Breit or Moller corrections. Recent applications of the CCC method include electron impact ionization of helium and electron-impact excitation of mercury and highly charge uranium ions. Currently the CCC method is being used to calculate electron-impact excitation and ionization of the He-like Li ion.

P. Fainstein from Centro Atómico Bariloche, Comisión Nacional de Energía Atómica (CNEA), Argentina presented their most recent calculations of different processes employing the non-relativistic Continuum Distorted Wave - Eikonal Initial State (CDW-EIS) approximation at intermediate and high energies. These include single and multiple ionization of atoms by ion impact including post collisional processes, and single ionization and electron capture in collisions between ions and molecules of biological interest. The calculations employ the independent electron model, initial and final states which verify the correct asymptotic conditions for Coulomb potentials and the straight-line version of the impact-parameter approximation which is valid at high-impact energies. Recent calculations for single and double ionization of He with a new version of the Exponential Model, modified to treat collisions with highly charged ions, were presented.

D. Reiter of Forschungszentrum Jülich GmbH, Institut für Plasmaphysik (IPP), Germany, presented the plasma code activities mainly focused on the outer layers (“edge plasma”) of magnetically confined fusion plasmas. The suit of codes ranges from dedicated local erosion-redeposition transport codes (ERO) or drift fluid turbulence codes (ATTEMPT), up to “integrated” edge codes such as B2-EIRENE (operated and maintained jointly with ITER-IO, Cadarache), EMC3-EIRENE (jointly with IPP Greifswald, mainly for stellarators, LHD, W7X), OSM-EIRENE (with ITER) and EDGE2D-EIRENE (at JET). The atomic, molecular and surface data are integrated into these models mostly via the kinetic Monte Carlo code module EIRENE. Most of the integrated edge modeling activities at FZ Jülich are under ITER contracts. (EIRENE stand alone (first wall fluxes, diagnostic mirrors), EMC3-EIRENE (3D rmp effects), B2-EIRENE (2D code benchmarks internally within SOLPS family). EIRENE resorts to a combination of external databases for which interfaces to EIRENE exist, internal (default) atomic data and collisional radiative codes integrated into the EIRENE source. The web based database and toolbox HYDKIN ([www.hydkin.de](http://www.hydkin.de)) serves to publicly expose the A&M data used by EIRENE obtained from earlier IAEA CRP’s, or as “non LTE collisional radiative” code as well as for sensitivity analysis using analytic solutions of linearized equations for sensitivity parameters. With respect to surface data EIRENE resorts to a kinetic reflection database (under [www.eirene.de](http://www.eirene.de)), based on TRIM code calculations. Distinct from other surface databases the EIRENE database format choice was driven by the need to preserve full information regarding all angular dependencies as well as energy spectra, as needed by kinetic plasma models (e.g. Monte Carlo), rather than only averaged quantities (see Appendix 3 for more details).

I. Rabadan of Universidad Autonoma de Madrid, Spain, presented a summary of the methodologies that they have ensemble to treat ion-atom and ion-molecule collisions. Some of these methodologies

can deal with systems with more than two active electrons, which is particularly important for the intermediate range of collisional energies (around 1 keV/u). At the same time, they developed methods to treat complex systems (many electrons) using one-electron wavefunctions and/or classical mechanics. A chart of codes with a brief summary of their capabilities was presented, alongside a few examples showing recent results on isotope effects in beryllium collisions with hydrogen and collisions with molecules like CH<sub>4</sub>. The possibility of other users using the codes was also discussed.

A. Dubois of Laboratoire de Chimie Physique Universite Pierre et Marie Curie (Paris VI), France, presented the theoretical models used to evaluate cross sections of various electronic processes occurring in ion-atom and ion-molecule collisions. Lattice representation calculations are illustrated by the presentation of results for ionizing ion-molecule collisions. For atomic target, he showed double capture to autoionizing states cross sections computed by spectral methods. Finally, the presentation of his partners was done together on the implementation of the codes at the IAEA web site.

M. Capitelli of Universita di Bari, Italy, reviewed the activity in the *Plasma Chemistry* group in Bari focused on state-to-state kinetic modeling of systems of interest for technological applications ranging from fusion (negative ion sources) to aerospace. The tools for the derivation of information on the dynamics of elementary processes were described in detail. For the simulation of plasm-chemical systems, two existing codes have been coupled, the collisional-radiative model, for an atomic hydrogen plasma under shock-wave condition, and the code for calculation of synthetic hydrogen spectrum, deriving plasma optical properties. The role of non-equilibrium in internal distribution in affecting the spectrum is investigated in different position of the shock. Thermodynamics and transport of plasmas have been studied. In particular, thermodynamic properties have been calculated in the frame a novel approach that reduces complex systems of levels to an equivalent system of two-three levels by means of grouping. The quantum problem of levels for hydrogen atom confined in a spherical box has been investigated in the frame of solution of divergence of internal partition function. Modules for transport coefficients calculation have been implemented including the effects of different choices of cut-off criterion and of electronically excited states in the mixture (see Appendix 3 for more details).

Yu. Ralchenko of Atomic Spectroscopy Group, National Institute of Standards and Technology, USA presented a set of atomic structure and plasma kinetics codes that are being developed or hosted at NIST. The most advanced methods in atomic structure theory are implemented in non-relativistic Multiconfiguration Hartree-Fock (MCHF) and relativistic Multiconfiguration Dirac-Fock (MCDF) codes. Both these packages as well as some simpler codes are available for free download from the NIST web site. The NIST Atomic Spectroscopy Group also develops sophisticated collisional-radiative models for calculation of plasma population kinetics and emission characteristics. The NOMAD code is used for calculation of spectral patterns in the EBIT experiments with highly-charged ions of tungsten and other heavy elements. This detailed code is also used for simulations on neutral beam spectroscopy in fusion machines, e.g., charge exchange recombination spectroscopy and motional Stark effect. Another advanced collisional-radiative code FLYCHK developed by the LLNL researchers and available for online calculations on the NIST site is used by hundreds of researchers, including specialists in fusion plasmas for calculations of ionization distribution, radiative power losses and other important parameters (see Appendix 3 for more details)

H. Chung of International Atomic Energy Agency reviewed databases and online capabilities hosted by the IAEA Atomic and Molecular data unit. The unit hosts ALADDIN, a numerical database of collisional data of atomic and molecular processes and plasma-surface interaction data, AMBDAS, bibliographical database and GENIE, an online search engine of 9 spectroscopic databases and 6 collisional databases worldwide. The unit has simple online codes to calculate heavy particle collisional data, electron impact cross-sections and collisional-radiative calculations of charge state and radiated power in a steady state plasma. More recently, comprehensive atomic data for argon, chlorine and silicon calculated by the group at Los Alamos National Laboratory (LANL) and charge distributions calculated by FLYCHK codes are made available in addition to the access to LANL Atomic Physics Codes and FLYCHK code at NIST.

V. Lisitsa of Russian Research Centre “Kurchatov Institute”, Russia presented on fast codes for calculations of radiative-collisional processes in electron many electron ions collisions. The codes are based on quasiclassical approximation for electron motion in atomic potentials described by statistical models of the atoms (ions). Specific calculations are presented for Bremsstrahlung and radiative recombination spectra for complex ions as well as for dielectronic recombination rates for carbon Li-like ions and  $Mg^{+1}$  ion. The detailed comparison with quantum calculations was presented resulting in quite good agreements between quasiclassical and quantum numerical data. Several advantages of quasiclassical codes were discussed. Quasiclassical codes can decrease sharply the computing time as compared with quantum calculations, resulting in the possibility of their combinations with more complex plasma modeling codes, such as EIRENE or ASTRA transport codes. The codes can be used to establish quasiclassical scaling laws for probabilities of radiative-collisional processes. The precision of quasiclassical codes is quite good for most of plasma applications such as radiation background in tokamak plasmas as well as radiative and dielectronic recombination rates (see Appendix 3 for more details).

### 3. Discussions and Recommendations

The progress of recommendations of the last meeting was reviewed after presentations. As recommended, an IAEA webpage was created to list the basic information from the current code capabilities of Code Centre Network (CCN) members with a link to individual web pages at participating institutes. It was reported that the network has provided good interaction among code developers and the visibility of the network served well in attracting students to fusion related research. Feedbacks from online code users to code developers and increases in collaboration opportunities were recognized as important benefits of CCN. Providers of the plasma-surface code SDTrimSP and the suite of atomic physics codes HULLAC were invited to the network as a way of expanding the network.

A recommendation for code developers to consider an xml output utilizing XSAMS (xml schema for atomic, molecular and solids, <http://www-amdis.iaea.org/xsams>) was found too premature since XSAMS is under the development. The recommendation that code developers should attempt to estimate the accuracy of calculations in a similar manner to that of numerical databases was found difficult to meet. This led to a considerable amount of discussion on the role and future activities of the Code Centres Network.

There were general concerns over the accuracies of data computed with online code capabilities. Codes can provide unavailable data sets to meet comprehensive modeling needs even though accuracies of these computed data sets are unverified and generally limited. While the accuracy should be determined by the code developers, it is almost impossible to determine the accuracies of all data sets generated by the code. More often than not, code documentation is not good enough to train the code users and hence unevaluated data sets generated by inexperienced users may lead to an erroneous result when applied. In order to avoid such an adverse effect, it was suggested that either the codes should be available in collaboration with code developers to meet specific data needs of data users or only the data sets calculated by code developers with accuracy information should be available through data centres.

Participants exchanged ideas of how the CCN can contribute to the community in addition to generating new data sets. They agreed that the CCN activities should benefit the code developers as in the case of the DCN (Data Centre Network) through which data centres improve their databases by activities such as joint collaboration, technical helps and visits. Several ideas were proposed as future activities to directly help CCN members. One proposal is to organize focused meetings where code developers in the CCN can work on a formulated physics problem together. As an example, at the series of NLTE (non-local thermodynamic equilibrium) kinetics code comparison workshops, code developers compare their results together on a formulated problem, identify the sources of discrepancies among results and improve their codes. Such a workshop on a focused topic will improve the calculated data accuracy and validate the codes.

The other proposal is to develop the CCN into a structured network of data producers, data producers and experimentalists on request. Participants found the interaction with a wide range of science through the CCN useful as one finds the significant overlap among atomic, molecular and plasma-surface interaction physics. The greater visibility from the larger network with members from diverse background will be an important benefit since it will offer more collaborative opportunities and also help with recruiting young scientists.

It was the first meeting to invite researchers from the plasma modeling community who extensively use atomic, molecular and plasma-surface data in their calculations. Data users had a chance to acquire clear information on the capabilities and limits of available data, and the needs of a variety of consumer level codes and the understanding of what is needed by these codes. On the other hand, data producers had a chance to understand how their data sets are implemented in the applications. They found it necessary to establish a priority list of data needs so that they can focus more to produce unavailable data sets or improve the important data sets in fusion research. Data accuracies and validations were an important subject in this meeting and the information on the quality and availability of needed data sets are not easily obtainable. To meet the needs of both data users and producers, a decision tree of available data sets and quality information was proposed. The proposed decision tree may provide a venue to categorize available data sets and hence easy to prioritize data needs.

Every participant expressed that this meeting was extremely productive and supported that the CCN should expand the activities with a balance between computational tools and scientific interaction among participants. A DAFF (DATA For Fusion) mailing list was proposed to be used as the communication method among CCN participants. Code developers were motivated to develop further and update online codes regularly with the accuracy information in mind. More representation in the plasma surface interaction codes was recommended.

#### **4. Summary**

This was the second meeting in the code centre network, an important meeting to discuss the future direction of the network. Data users from plasma modeling community were invited to join the discussion with code developers and participants expressed that this combined meeting was very productive. It was proposed that the network should expand to more structured network of data users, data producers and possibly experimentalists. Data users expressed concerns over the quality of available data sets from online codes and proposed that the codes should be made available with expert help or only the data sets generated by experts should be available online. A decision tree was proposed as a venue to obtain information on available data with accuracy information. Data producers found the interaction with data users useful in terms of understanding the needs of plasma modeling community and suggested that there should be a priority list of important data.

## IAEA Technical Meeting on International Code Centres Network

27–28 September 2010, IAEA Headquarters, Vienna, Austria

## List of Participants

Dr Pablo Fainstein  
 Centro Atómico Bariloche  
 Comisión Nacional de Energía Atómica (CNEA)  
 Av. E. Bustillo 9500  
 8400 Bariloche  
 ARGENTINA  
 Tel.: +54-2944-445196; Fax: +54-2944-445299  
 E-mail: [pablof@cab.cnea.gov.ar](mailto:pablof@cab.cnea.gov.ar)

Prof Igor Bray  
 ARC Professorial Fellow  
 Director, Institute of Theoretical Physics  
 Deputy Director, ARC Centre for  
 Antimatter-Matter Studies  
 Curtin University of Technology  
 GPO Box U1987  
 Perth WA 6845  
 AUSTRALIA  
 Tel.: +61-8-9266-4416; Fax: +61-8-9266-1972  
 E-mail: [I.Bray@curtin.edu.au](mailto:I.Bray@curtin.edu.au)

Prof Alain Dubois  
 Laboratoire de Chimie Physique  
 Matière et Rayonnement  
 Université Pierre et Marie Curie (Paris VI)  
 UMR du CNRS 7614  
 11, rue Pierre et Marie Curie  
 F-75231 Paris Cedex 05  
 FRANCE  
 Tel.: +33-1-44276631; Fax: +33-1-44276226  
 E-mail: [ad@ccr.jussieu.fr](mailto:ad@ccr.jussieu.fr)

Dr David P. Coster  
 Max-Planck-Institut für Plasmaphysik  
 Boltzmannstraße 2  
 D-85748 Garching  
 GERMANY  
 Tel.: +49-89-32991865; Fax: +49-89-32992580  
 E-mail: [dpc@ipp-garching.mpg.de](mailto:dpc@ipp-garching.mpg.de)

Prof M. Capitelli  
 Centro di Studio per la Chimica de Plasmi  
 Dipartimento di Chimica Università di Bari  
 Via Orabona 4  
 I-70126 Bari, ITALY  
 Tel.: +39-80-544-2104; Fax: +39-80-544-2024  
 E-mail: [mario.capitelli@ba.imip.cnr.it](mailto:mario.capitelli@ba.imip.cnr.it)

Prof Fumihiko Koike  
 Physics Laboratory  
 School of Medicine  
 Kitasato University  
 Kitasato 1-15-1, Sagamihara  
 Kanagawa 228  
 JAPAN  
 Tel.: +81-427-78-8029; Fax: +81-427-78-8441  
 E-mail: [koikef@kitasato-u.ac.jp](mailto:koikef@kitasato-u.ac.jp)

Dr Valery Lisitsa  
 Russian Research Centre “Kurchatov Institute”  
 Nuclear Fusion Institute  
 Kurchatov square, 1  
 123182 Moscow  
 RUSSIAN FEDERATION  
 Tel.: +7-095-1967334; Fax: +7-095-9430073  
 E-mail: [lisitsa@nfi.kiae.ru](mailto:lisitsa@nfi.kiae.ru)

Prof L.A. Vainshtein  
 P.N. Lebedev Physical Institute  
 Leninsky pr., 53  
 119991 Moscow  
 RUSSIAN FEDERATION  
 Tel./Fax: +7-499-135-2429  
 E-mail: [vainsh@sci.lebedev.ru](mailto:vainsh@sci.lebedev.ru)

Dr Ismanuel Rabadan  
 Departamento de Química, C-9-602  
 Universidad Autónoma de Madrid  
 28049 Madrid  
 SPAIN  
 Tel.: +34-91-497-4947; Fax: +34-91-497-5238  
 E-mail: [ismanuel.rabadan@uam.es](mailto:ismanuel.rabadan@uam.es)

Dr Marcel Klapisch  
 Institute for Particle Physics  
 ETH Hönggerberg HPK/G28  
 8093 Zurich  
 SWITZERLAND  
 Tel./Fax:  
 E-mail: [klapisch@phys.ethz.ch](mailto:klapisch@phys.ethz.ch)

Dr Yuri Ralchenko  
Atomic Spectroscopy Group, Stop 8422  
National Institute of Standards and Technology  
Gaithersburg MD 20899-8422  
U.S.A.  
Tel.: +1-301-975-3210; Fax: +1-301-975-4779  
E-mail: [yuri.ralchenko@nist.gov](mailto:yuri.ralchenko@nist.gov)

Dr. Hyun Kung Chung  
IAEA Atomic and Molecular Data Unit  
Wagramerstrasse 5  
P.O. Box 100  
A-1400 Vienna  
AUSTRIA  
Tel.: +43-1-2600-21729; Fax: +43-1-26007  
E-mail: [h.chung@iaea.org](mailto:h.chung@iaea.org)

Dr Joseph Abdallah, Jr.  
Los Alamos National Laboratory  
Group T-4, MS B212  
Los Alamos, NM 87545  
U.S.A.  
Tel.: +1-505-667-7388; Fax: +1-505-665-6229  
E-mail: [abd@lanl.gov](mailto:abd@lanl.gov)

Dr David Elder  
University of Toronto  
Institute for Aerospace Studies  
Fusion Research Group  
4925 Dufferin St.  
Toronto, Ontario, M3H 5T6  
CANADA  
Tel.: +1-416-667-7891; Fax: +1-416-667-7799  
E-mail: [david@starfire.utias.utoronto.ca](mailto:david@starfire.utias.utoronto.ca)

Prof Dr Detlev Reiter  
Forschungszentrum Jülich GmbH  
Institut für Plasmaphysik (IPP)  
D-52425 Jülich  
GERMANY  
Tel.: +49-2461-61-5841; Fax: +49-2461-61-2970  
E-mail: [d.reiter@fz-juelich.de](mailto:d.reiter@fz-juelich.de)

Prof Ralf. Schneider  
Institut für Physik  
Ernst Moritz Arndt Universität  
Felix-Hausdorff-Straße 6  
D-17489 Greifswald  
GERMANY  
Tel.: +49-3834-86-4735; Fax: +49-3834-86-4701  
E-mail: [ralf.schneider@physik.uni-greifswald.de](mailto:ralf.schneider@physik.uni-greifswald.de)

#### **I.A.E.A.**

Dr. Bastiaan J. Braams  
IAEA Atomic and Molecular Data Unit  
Wagramerstrasse 5  
P.O. Box 100  
A-1400 Vienna  
AUSTRIA  
Tel.: +43-1-2600-21731; Fax: +43-1-26007  
E-mail: [b.j.braams@iaea.org](mailto:b.j.braams@iaea.org)

**IAEA Technical Meeting on International Code Centres Network**

27–28 September 2010, IAEA Headquarters, Vienna, Austria

**Agenda**

**Monday, 27 September**

**Meeting Room A04-78**

09:30 – 09:40      Opening, Adoption of Agenda, R. Forrest, B. Braams

Session 1: Reports I

**Chairman:    D. Reiter**

09:40 – 10:10      D. Coster: Use of atomic, molecular, nuclear and solids data in European codes: new developments

10:10 – 10:40      D. Elder: The OEDGE code and interpretive modeling

10:40 – 11:00      *Coffee Break*

11:00 – 11:30      R. Schneider: Tools and strategies for the description of plasma-wall interaction

11:30 – 12:00      J. Abdallah: Recent developments with the Los Alamos atomic physics codes

12:00 – 12:20      F. Koike: Atomic structure and dynamics calculations using the GRASP family of codes, and an introduction of some activities in NIFS

12:20 – 12:40      L. Vainshtein: Ionization cross-sections for W I and W II and the ATOM and MZ codes

12:40 – 14:00      *Lunch*

Session 2: Reports II

**Chairman:    J. Abdallah**

14:00 – 14:30      M. Klapisch: Latest updates of HULLAC theory and applications

14:30 – 14:50      I. Bray: Recent applications of the CCC method

14:50 – 15:10      *Coffee Break*

15:10 – 15:30      P. Fainstein: Recent advances in distorted-wave calculations of ion impact single and multiple ionization of atoms and molecules

15:30 – 16:00      D. Reiter: HYDKIN: towards online hydrogen and hydride kinetics to publicly expose A+M data in particular edge modeling applications

16:00 – 16:20      I. Rabadan: Theoretical treatment of ion-atom and ion-molecule collisions

16:20 – 16:40      A. Dubois: One- and two-electron processes in multi-center collisional systems

16:40 – 17:00      M. Capitelli: State to state kinetics of molecular and atomic hydrogen plasmas

**Tuesday, 28 September**

Session 3: Reports III

**Chairman: D. Coster**

- 09:00 – 09:20 Yu. Ralchenko: NIST simulations for support of fusion research  
09:20 – 09:40 V. Lisitsa: Fast codes for modeling fusion plasma radiative properties  
09:40 – 10:00 H.-K. Chung: Code capabilities at IAEA  
10:30 – 11:00 *Coffee Break*

Session 4: Review

**Chairman: D. Coster**

- 11:00 – 12:30 All: What do we wish to get out of the CCN  
12:30 – 14:00 *Lunch*

Session 5: Plans and Recommendations

**Chairman: Y. Ralchenko**

- 14:00 – 15:30 All: Progress and plans towards goals of CCN  
15:30 – 16:00 *Coffee Break*  
16:00 – 17:00 All: Recommendations for IAEA  
17:00 – *Adjourn*



ABSTRACTS AND SUMMARIES**The OEDGE code**

J. David Elder, University of Toronto, Canada

The OEDGE code suite is used for modeling the behavior of the edge plasma of magnetic fusion devices. The OEDGE code is composed of several elements. An Onion Skin Model (OSM) can be used to create a background plasma solution for the edge plasma. This includes solving for edge plasma density, temperature, flow velocity and electric field on a 2D grid representing the poloidal magnetic structure of the fusion device. OEDGE typically assumes toroidal symmetry. OEDGE can also load a plasma solution provided by other plasma solvers in use by the fusion modeling community. After an initial plasma solution is obtained, OEDGE runs the EIRENE Monte Carlo code to obtain the distribution and magnitude of hydrogenic source terms ... ionization, recombination, power and momentum loss terms. These are then fed back to the OSM and the process is iterated until a stable plasma solution is found. OEDGE then uses the DIVIMP Monte Carlo plasma impurity code to model the impurity production, transport and deposition including such things as estimates of core impurity content, self-sputtering at surfaces and many other physics effects. The end result is a simulation of the fusion edge plasma including both hydrogenic and impurity behavior.

The input to these simulations is usually the density and temperature of the plasma at the target plates as measured experimentally by Langmuir probes. The simulation results are compared to experimental measurements of hydrogenic and impurity spectral emissions, plasma condition measurements from Thomson scattering and reciprocating probes, neutral pressure measurements from in-vessel pressure gauges and many other diagnostics. Discrepancies between the simulation and experimental measurements are then investigated to determine whether physics not presently incorporated in the simulations could be the cause of the discrepancy. In this way, the OEDGE code is used to understand complex experiments with fusion edge plasmas and offers a tool giving insight into the physics underlying the experiments.

In terms of fundamental data used by the OEDGE code, there is a substantial body of data required by both EIRENE and DIVIMP in order to accomplish a simulation of this type. These codes require ionization and recombination rate data for hydrogen as well as the impurity species being modeled. The impurity species examined ranges from lithium to tungsten. This data is required for all charge states of the impurity species. Typically in DIVIMP, the code assumes a Maxwellian electron velocity distribution which then means that the code uses rate data as opposed to cross-section data. The EIRENE code also uses data for hydrogen molecules as well as atoms and ions. In addition, these codes also need line emission data for both hydrogen and specific lines for each impurity species. The specific lines are those examined experimentally so they may vary from one fusion device to another depending on the diagnostic choices made. The spectral atomic data is combined with the impurity density calculated by the code to obtain a photon emission rate for each element in the simulation. This data is then combined with diagnostic geometry data loaded into the code to generate a simulated diagnostic measurement which takes into account such things as field of view of the instrument. Finally, DIVIMP also makes use of surface sputtering data for both impurity species as well as hydrocarbon molecules. This includes both chemical and physical sputtering as well as primary (background ion) and self sputtering data. This data is used to calculate the source impurity particle distribution in the simulation. As a data consumer, OEDGE uses a broad range of atomic, molecular and surface data at a relatively processed level since the code only produces particle density estimates in the simulation and does not, at present, track the population of excited states.

As a result of these meetings at the IAEA, good information was acquired on both the capabilities and limits of data available in the atomic physics community. In addition, the needs of a variety of consumer level codes were explained so the understanding of what is needed by these codes was clarified. This may result in improvement of the data currently available for fusion edge plasma modeling.

## Tools and strategies for the description of plasma-wall interaction

Prof. Dr. Ralf Schneider, Institute of Physics, Ernst-Moritz-Arndt University Greifswald

### 1. General considerations

This has to deal with very complex and different problems, like arcs (field emission coefficients), NNBI (surface ionization, effect of Cs layers), hot spots (SEE coefficients for ions and electrons). Therefore, interaction with other fields is needed and multi-scale physics requires a combination of methods. The real structure of the material is quite important, because it determines diffusion and impurities can modify strongly surface binding energies. Molecular dynamic simulations can help to overcome some shortcomings of simpler models, but they are only as good as the quality of the interaction potentials. Also, they can deal mostly with idealized systems and have problems for realistic fusion wall materials (mixed materials with a lot of damage and impurities). For fundamental understanding model systems are needed for validation.

### 2. SDTrimSP

Sputtering of a surface exposed to a flux of energetic ions is one of the best studied effects of ion-surface interactions. The details of ion-surface interactions depend greatly on the target-projectile combination. In case the projectile being an ion of a volatile (recycling) element, sputtering is usually dominating and the surface is eroded. In this case, experiments are well described theoretically. The sputtering yield is the main parameter, which was used to validate theoretical models with experiments. Existing models like the TRIM code show good agreement with experiment for many target-projectile combinations.

If the projectile is a solid-state (non-recycling) ion, its interaction with the surface can lead to implantation, if the ion, after penetration and deceleration in the solid, remains in the surface. This leads to formation of a mixed surface of target and projectile atoms. The properties of the mixed surface may significantly deviate from the properties of original materials. Additionally, the surface composition is dynamically changed by sputtering and implantation. The study of such interactions cannot be described just by the sputtering yield behavior; it strongly depends on the elemental composition of the surface, which is, in turn, modified continuously by ion bombardment. Similar difficulties are encountered, when volatile ions interact with compounds or a surface is exposed to the mixed flux of volatile and solid-state ions. To solve this problem, a dynamic version of the TRIM code, called TRIDYN (later re-written as SDTrimSP) was developed. This is a 1D version of TRIM, where the distance from the surface into the solid is discretized on a grid and dynamical change of the surface composition along the depth due to implantation of projectiles and relocation of recoils during collisional cascades are considered. There were a number of studies comparing experiments with TRIDYN simulations showing generally good agreement.

The existing models assume that a plane and perfectly smooth surface exists and demonstrate good agreement with experiments, if well-polished specimens are used. Surface roughness is prone to increase the sputtering yield up to a factor of 5. There were a few approaches to predict sputtering yields of rough surface: Ruzic suggested considering the surface roughness having a fractal geometry; Kuestner *et.al.*, assumed that the surface can be represented as aggregates of simple surfaces at tilted angles. These approaches yield in reasonable agreement, but their intrinsic limitations had prevented further development of the models. One of them is their inability to simulate surface morphology changes by deposition and implantation.

The limitations of the approaches can be overcome by the extending the grid of the existing model into the second and third lateral dimensions. The first step in this direction has been made developing the SDTrimSP-2D code, which is capable to treat the interaction of ions with a 2D surface. An example of such a surface is a diffraction lattice. The code belongs to the TRIM family and it incorporates the same physical model, but due to existing of second lateral dimension, it requires also an advanced relaxation mechanism. It has been shown that the code predict the evolution of a Si pitch grating

exposed to 6 keV Ar ions with a good accuracy. Although this system is rather simple and governed mainly by sputtering and relaxation, the agreement between the experiment and numerical simulation demonstrates the validity of the basic physics included in the model. The code has also been used to evaluate the effect of the surface roughness of W exposed to C and C+D flux.

Another extension of the code is the inclusion of chemical sputtering by combining the local chemistry model of Mech et al. (based on work by Küppers et al.) with the experimental flux scaling from Roth et al. and the concept of escape probabilities for hydrocarbons depending on the distance to the surface (see Jacob et al.). This code reproduces a large number of experiments including the observation that a hydrocarbon surface bombarded with Neon (producing damage) and in parallel exposed to thermal hydrogen influx shows strong chemical sputtering.

### **Recent developments with the Los Alamos atomic physics codes**

J. Abdallah, Jr., M.S. Sherrill, C.J. Fontes, H.L. Zhang, J. Oelgoetz and D.P. Kilcrease, Los Alamos National Laboratory, USA

The LANL contribution to the IAEA Atomic and Molecular Data Code Centre is the online version of atomic physics codes. These codes are accessed online by users to perform atomic structure calculations, including excitation and ionization cross sections, for arbitrary ions and configurations. A brief description of the online capabilities was presented. A short summary of the ATOMIC plasma modeling code was also provided. Recent improvements to the CATS code were discussed, in particular, the recently developed parallel computing capability. Several examples of the use of the LANL suite of atomic physics codes to applications of interest to magnetic fusion were discussed including recent boron power loss calculations and preliminary results for modeling low temperature tungsten plasmas.

### **Atomic structure and dynamics calculations using the GRASP family of codes, and an introduction of some activities in NIFS**

Fumihiro Koike, Kitasato University and NIFS (National Institute of Fusion Science), Izumi Murakami, Daiji Kato, Xiaobin Ding, NIFS, Tohru Kawamura, TITECH

We have briefly reported the activities in the study of atomic structure and dynamics calculations using the GRASP (General purpose Atomic Structure Program) family codes and also of some activities in NIFS. We have introduced the following items: 1. Analysis of Visible M1 Lines in Tungsten Ions, 2. Collisional-radiative model for W ions, 3. Code development for single electron capture by H nucleus from metal surface, 3.  $K\alpha$  radiation from low charge chlorine heated by an ion beam for plasma diagnostics, 4. Code Availability. And we have summarized the talk.

The visible lights emitted from highly charged tungsten ions are of special interest; they are mainly realized by magnetic dipole transitions between the fine structure levels of ions and therefore they suffer less self-absorption by surrounding plasmas providing us with a great advantage for the diagnostics of core plasmas. We have studied the source of these visible line emissions in terms of accurate non-empirical atomic structure calculations and of population kinematics analyses. The GRASP package [1] for multi-configuration Dirac-Fock atomic structure calculation have provided us with the transition energies that are accurate enough to discriminate the states and the charges of tungsten ions. We tried, further, to reproduce the emission spectra by modifying a population kinetics code that has been used for the analysis of boron like ion plasmas [2]. We have assigned new visible emission lines. We have shown that the use of the GRASP family of codes is quite effective for the spectroscopy of the visible line emissions of tungsten ions and for the diagnostics of the MCF plasmas.

We have extended a CR model calculation code[2] to include the case of tungsten ions plasmas; the atomic data have been calculated using HULLAC code. We have applied the code to the analysis of  $W^{35+}$  to  $W^{37+}$  plasmas. The code is now still under development. We have now under the development

of a code for single electron capture by H nucleus from metal surface. The features of theoretical method implemented with the code are: 1. semi-classical treatment of H nucleus-metal surface collision, 2. static linear density response of target electron gas induced by external nuclear charge, 3. direct numerical solution of time-dependent Schrödinger equation of electron wave-function, 4. adiabatic expansion of wave-function, and B-spline method and discrete-variable-representation of adiabatic state function. We have obtained the level populations created by electron capture from molybdenum surfaces. It is found that the code can be improved substantially (e.g. more realistic target description, beyond jellium model), and that validation of theoretical methods implemented in the code requires more comparison with experimental results. This code is, at present, not ready to open for public.

We have investigated the  $K\alpha$  radiation from low charge chlorine heated by an ion beam for ICF plasma diagnostics. In those plasmas, many  $K\alpha$  lines are distributed over photon energy according to the ionization state, and, therefore,  $K\alpha$  photon energies show the characteristic charge state of plasmas. The  $K\alpha$  with M-shell electrons may be useful for the diagnostics of lower temperature plasmas. In the ions with K-shell vacancies, many Auger channels compete with radiative processes, and are indispensable to estimate  $K\alpha$  yield.

We have discussed the availability of computer codes for open computing. We have listed out the following codes that are to be considered. 1. GRASP and GRASP2, 2. GRASP92 + RATIP, 3. GRASP2K, 4. CR-Model Code based on HULLAC, Code for single electron capture by H nucleus from metal surface.

#### References

- [1] P. Jönsson et al., *Comp. Phys. Communications*, 177, 597-622 (2007).
- [2] I. Murakami et al., *Annual Report of NIFS*, April 2005 to March 2006, 425 (2006).

#### **Ionization cross-sections for W I and W II and the ATOM and MZ codes**

L.A. Vainshtein, P.N. Lebedev Physical Institute, Moscow, Russian Federation

The problems of ionization of the atom W and ion  $W^+$  are of similar complexity. There are good experimental data for  $W^+$  single and double ionization and no direct cross section measurements for W. By this reason we start with the ionization of  $W^+$  and test the calculations by comparison with experimental data hoping that accuracy for neutral W would be similar. Most of the calculation details are the same (or at least similar) for the atom W and ion  $W^+$ . Ionization of  $W^+$  can be produced either by direct ionization (DI) or through excitation of inner shells followed by autoionization (EA). Ionization from the inner shells (IA) is followed by autoionization and therefore results in the double ionization. The cross sections are calculated by the code ATOM in Coulomb-Born approximation (CB) with exchange and correction for the normalization effect (account for the electron flux conservation) by the reduced K-matrix approximation. This considerably improves the results due to account for strong virtual excitations. The contribution of EA through  $4f^{13}5d^5$  and  $5p^55d^5$  and the double ionization due to ionization from those shells followed by autoionization (IA) are calculated. The double ionization cross section can be directly measured in beam experiments. On the other hand, in calculations of the ionization equilibrium and other plasma kinetic problems the double ionization should be included in the total ionization rate. In addition to the cross sections we calculated the rate coefficients  $\langle v\sigma_{iz} \rangle$  for Maxwell electron energy distribution with the temperature T as well as 3 adjusted parameters for fitting formula.

The calculated  $\sigma_{iz}^{(1)}$  overestimate the cross section by 20% at the cross section maximum. For such complicated ion as  $W^+$  this accuracy is rather good. Without the correction for normalization the error is twice as much. Ionization of atoms W I was considered in the way similar to W II.

## Latest updates of HULLAC theory and applications

M. Klapisch, ARTEP Inc. USA, Institute for Particle Physics, ETH, Switzerland

The first version of HULLAC (*Hebrew University Lawrence Livermore Atomic Code*) dates back to the 1980's when M. K. was professor at Hebrew University, Jerusalem, Israel, and got the support of LLNL. The concept is to generate a consistent atomic model, by using the same wave functions for computing all atomic processes relevant to plasma spectroscopy. These wave functions are obtained by solving the Dirac equation in a parametric potential [1]. The central field model enables a convenient decoupling of the angular momentum algebra [2] for all processes, including electron collisions, for which we introduced the factorization-interpolation method [3]. Recently, the whole code was re-written in a more modern way [4] and extensively checked. It includes now a collisional radiative solver with a special scaling for improved convergence, a new fit for the cross sections [5], the ability to use the mixed transition arrays (MUTA) [6], and to model the effect of an external radiation field. The latter capability was used to compare with a recent experiment on the transmission of Fe at  $T_e=156\text{eV}$  [7], with excellent agreement [8]. The latest version is used by several groups, whose feedback is used to constantly improve and/or correct the code.

### References

- [1] M. Klapisch, *Comput. Phys. Comm.*2, (1971) 239 -60.
- [2] A. Bar-Shalom and M. Klapisch, *Comput. Phys. Comm.*50, (1988) 375 - 93.
- [3] A. Bar-Shalom, M. Klapisch, and J. Oreg, *Phys. Rev. A*.38, (1988) 1773- 84.
- [4] M. Klapisch, M. Busquet, and A. Bar-Shalom, *AIP Conference Proceedings*926, (2007) 206-15;  
M. Busquet, M. Klapisch, and A. Bar-Shalom, *Bull. Am. Phys. Soc.*49, (2004) 114.
- [5] M. Busquet, *High Ener. Dens. Phys.*3, (2007) 48 - 51.
- [6] S. Mazevet and J.J. Abdallah, *J. Phys. B.: At. Mol. Opt* 39, (2006) 3419-29.
- [7] J.E. Bailey, G.A. Rochau, C.A. Iglesias, J.J. Abdallah, J, et al. *Phys. Rev. Lett.*99, (2007) 265002-4.
- [8] M. Klapisch and M. Busquet, *High Ener. Dens. Phys.*5, (2009) 105-9.

## Recent applications of the CCC method

I. Bray, Curtin University, Australia

There has been considerable progress in the development of the Convergent Close-Coupling (CCC) theory. The major extension has been to institute a new parallelism paradigm. This utilizes a hybrid OPENMP/MPI combination with the main V-matrix being calculated across several nodes. Within each node the original OPENMP parallelism is used. Then, using MPI, the matrix is distributed in a block cyclic form across all the available cores suitable for solving the linear equations via the ScaLAPACK suite of routines.

Consequently the CCC code is now able to be run across many nodes of memory sharing multiple cores. Both the original non-relativistic CCC and the recently developed relativistic RCCC codes have been parallelized this way. Additionally, the RCCC code has been extended to quasi two-electron targets, and highly charged ions, including Breit or Moller corrections.

Recent applications of the CCC method include electron impact ionization of helium and electron-impact excitation of mercury and highly charge uranium ions. Currently the CCC method is being used to calculate electron-impact excitation and ionization of the He-like Li ion.

## Recent advances in distorted-wave calculations of ion impact single and multiple ionization of atoms and molecules

P. Fainstein, Centro Atomico Bariloche, Commission Nacional de Energia Atomica , Argentina

In this talk I will present our most recent calculations of different processes employing the non-relativistic CDW-EIS approximation at intermediate and high energies. These include single and

multiple ionization of atoms by ion impact including post collisional processes, and single ionization and electron capture in collisions between ions and molecules of biological interest. We employ the independent electron model, initial and final states which verify the correct asymptotic conditions for Coulomb potentials and the straight-line version of the impact-parameter approximation which is valid at high-impact energies.

Recent calculations for single and double ionization of He with a new version of the Exponential Model, modified to treat collisions with highly charged ions, will be also presented.

### **HYDKIN: towards online hydrogen and hydride kinetics to publicly expose A+M data in particular edge modeling applications**

D. Reiter, Forschungszentrum Jülich GmbH, Institut für Plasmaphysik (IPP), Germany

The FZ Juelich plasma codes activities are mainly focused on the outer layers (“edge plasma”) of magnetically confined fusion plasmas. The suit of codes ranges from dedicated local erosion-redeposition transport codes (ERO) or drift fluid turbulence codes (ATTEMPT), up to “integrated” edge codes such as B2-EIRENE (operated and maintained jointly with ITER-IO, Cadarache), EMC3-EIRENE (jointly with IPP Greifswald, mainly for stellarators, LHD, W7X), OSM-EIRENE (with ITER) and EDGE2D-EIRENE (at JET).

The atomic, molecular and surface data are integrated into these models mostly via the kinetic Monte Carlo code module EIRENE. Most of the integrated edge modeling activities at FZ Juelich are under ITER contracts. (EIRENE stand alone (first wall fluxes, diagnostic mirrors), EMC3-EIRENE (3D rmp effects), B2-EIRENE (2D code benchmarks internally within SOLPS family). With respect to numerical data EIRENE resorts to a combination of

1. external databases for which interfaces to EIRENE exist. Some of these are homemade and web-based (HYDKIN, AMJUEL), others are obtained from database centers (ALADDIN, ADAS)
2. internal (default) atomic data,
3. collisional radiative codes integrated into the EIRENE source.

The web based database and toolbox HYDKIN ([www.hydkin.de](http://www.hydkin.de)) serves to publicly expose the A&M data used by EIRENE obtained from earlier IAEA CRP's, as “non LTE collisional radiative” code as well as for sensitivity analysis using analytic solutions of linearized equations for sensitivity parameters.

With respect to surface data EIRENE resorts to a kinetic reflection database (under [www.eirene.de](http://www.eirene.de)), based on TRIM code calculations. Distinct from other surface databases the EIRENE database format choice was driven by the need to preserve full information regarding all angular dependencies as well as energy spectra, as needed by kinetic plasma models (e.g. Monte Carlo), rather than only averaged quantities. This is achieved by storing the multidimensional data in form of conditional quantiles (loc. cit.).

### **Theoretical treatment of ion-atom and ion-molecule collisions**

Ismanuel Rabadan, Universidad Autonoma de Madrid, 28049-Madrid, Spain

I presented a summary of the methodologies that we have ensemble to treat ion-atom and ion-molecule collisions. Some of these methodologies can deal with systems with more than two active electrons, which is particularly important for the intermediate range of collisional energies (around 1 keV/u). At the same time, we have developed methods to treat complex systems (many electrons) using one-electron wave functions and/or classical mechanics.

A chart of codes with a brief summary of their capabilities was presented, alongside a few examples showing recent results on isotope effects in beryllium collisions with hydrogen and collisions with molecules like CH<sub>4</sub>. The possibility of other users using the codes was also discussed.

### **One- and two-electron processes in multi-center collisional systems**

Alain Dubois, Laboratoire de Chimie Physique-Matière et Rayonnement, Université Pierre et Marie Curie - CNRS, Paris, France

In the presentation, we present briefly the theoretical models used to evaluate cross sections of various electronic processes occurring in ion-atom and ion-molecule collisions. Lattice representation calculations are illustrated by the presentation of results for ionizing ion-molecule collisions. For atomic target, we show double capture to autoionizing states cross sections computed by spectral methods. Finally, before some conclusive remarks, the presentation of our partners is done together with the implementation of the codes at the IAEA web site.

### **State-to-State Kinetics of Molecular and Atomic Hydrogen Plasmas**

Mario Capitelli, University of Bari, CNR Institute of Inorganic Methodologies and Plasmas Bari, Italy

The activity in the *Plasma Chemistry* group in Bari is focused on state-to-state kinetic modeling of systems of interest for technological applications ranging from fusion (negative ion sources) to aerospace. Concerning the tools for the derivation of information on the dynamics of elementary processes, recent results include:

- the implementation of a simplified theoretical approach, the *similarity function*, for the calculation of cross sections for electron-impact induced vibronic excitation in diatomic molecules with resolution on internal degrees of freedom, giving results that compares well both to theory and experiments in the case of e-H<sub>2</sub> excitation and avoiding the high computational load of more accurate methods
- new implementation of the code for resonant processes in electron-molecule collisions (resonant vibrational excitation and dissociative attachment) for the investigation of isotopic effects, considering the different role for the three relevant resonances in e-H<sub>2</sub> scattering
- the inclusion of non-adiabatic effects, due to coupling among different potential energy surface, in the QCT (quasi-classical trajectory) code for the treatment of H<sup>+</sup>+H<sub>2</sub> system, representing a new frontier including quantum effects in the dynamics
- the implementation of a numerical tool based on the Downhill Simplex Method for the deconvolution of rate coefficients to cross sections, validated in the case of well-known systems as H+H<sub>2</sub>
- the code for the semi-classical treatment of heterogeneous processes of atom recombination at the surface, has been used for the investigation of isotopic effect in the Eley-Ridael mechanism of deuterium on graphite

For the simulation of plasm-chemical systems, two existing codes have been coupled, the collisional-radiative model, for an atomic hydrogen plasma under shock-wave condition, and the code for calculation of synthetic hydrogen spectrum, deriving plasma optical properties, i.e. emissivity and absorption coefficient. The role of non-equilibrium in internal distribution in affecting the spectrum is investigated in different position of the shock.

Finally thermodynamics and transport of plasmas have been studied. In particular, thermodynamic properties have been calculated in the frame a novel approach that reduces complex systems of levels to an equivalent system of two-three levels by means of grouping. Moreover the quantum problem of levels for hydrogen atom confined in a spherical box has been investigated in the frame of solution of divergence of internal partition function.

Modules for transport coefficients calculation have been implemented including the effects of different choices of cut-off criterion and of electronically excited states (EES) in the mixture.

### **Atomic and plasma codes at NIST**

Yuri Ralchenko, National Institute of Standards and Technology (NIST), Gaithersburg, USA

We present a set of atomic structure and plasma kinetics codes that are being developed or hosted at NIST. The most advanced methods in atomic structure theory are implemented in non-relativistic Multiconfiguration Hartree-Fock (MCHF) and relativistic Multiconfiguration Dirac-Fock (MCDF) codes. An example of an MCDF code is provided by the GRASP2K package which is being maintained and improved by C. Froese Fischer in collaboration with several researchers from other countries. C. Froese Fischer also develops the MCHF code. Both these packages as well as some simpler codes are available for free download from the NIST web site. Yu. Ralchenko presented some examples of recent highly accurate results obtained with MCHF and GRASP2K codes for atoms and ions of relevance to fusion research.

The NIST Atomic Spectroscopy Group also develops sophisticated collisional-radiative models for calculation of plasma population kinetics and emission characteristics. The NOMAD code is used for calculation of spectral patterns in the EBIT experiments with highly-charged ions of tungsten and other heavy elements. This detailed code is also used for simulations on neutral beam spectroscopy in fusion machines, e.g., charge exchange recombination spectroscopy and motional Stark effect. Another advanced collisional-radiative code FLYCHK developed by the LLNL researchers and available for online calculations on the NIST site is used by hundreds of researchers, including specialists in fusion plasmas for calculations of ionization distribution, radiative power losses and other important parameters.

### **Fast quasiclassical codes for radiative-collisional processes**

V.S. Lisitsa , RRC Kurchatov Institute, Moscow, Russian Federation

Fast codes for calculations of radiative-collisional processes in electron many electron ions collisions are presented. The codes are based on quasiclassical approximation for electron motion in atomic potentials described by statistical models of the atoms (ions). Specific calculations are presented for Bremsstrahlung and radiative recombination spectra for complex ions as well as for dielectronic recombination rates for carbon Li-like ions and  $Mg^{+1}$  ion. The detail comparison with quantum calculations is presented resulting in quit good agreements between quasiclassical and quantum numerical data.

The advantages of quasiclassical codes are as following:

1. Quasiclassical codes can decrease sharply the computing time as compared with quantum calculations, resulting in the possibility of their combinations with more complex plasma modeling codes, such as EIRENE or ASTRA transport codes;
2. The codes discover quasiclassical scaling laws for probabilities of radiative-collisional processes pointed above which are followed by quantum numerical data as well; it makes possible to propose universal scaling laws for the processes applicable for every kind of multi-electron ions;

The precision of quasiclassical codes is quite good for most of plasma applications such as radiation background in tokamak plasmas as well as radiative and dielectronic recombination rates.



---

Nuclear Data Section  
International Atomic Energy Agency  
P.O. Box 100  
A-1400 Vienna  
Austria

e-mail: [services@iaeand.iaea.org](mailto:services@iaeand.iaea.org)  
fax: (43-1) 26007  
telephone: (43-1) 2600-21710  
Web: <http://www-nds.iaea.org>

---