Recent Developments at the Atomic and Molecular Data Unit of the International Atomic Energy Agency

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INTRODUCTION

The main purpose of the Atomic and Molecular (A+M) Data Unit of the IAEA is to establish and maintain databases in support of nuclear fusion energy research. This encompasses a very large number of processes in atomic, molecular, and plasma-material interaction physics. Data for these processes are supplied by research centres around the world participating in several different activities, such as Co-ordinated Research Projects (CRP), a Data Centre Network, and individual consultant agreements. The resulting data are incorporated into the databases maintained at the A+M Data Unit at the IAEA Headquarters in Vienna. These databases are now available through the world-wide-web.

This talk will focus on recent improvements and additions to these databases. Notable points include a new search engine developed by Yuri Ralchenko and Denis Humbert, energy and angle dependent data for physical sputtering and radiation enhanced sublimation, effective rate coefficients for several elements relevant to fusion machines, as well as some new interfaces in the web site. In the near future more data from recently concluded CRPs will be added. In addition, two new CRPs have recently started and a third is scheduled to begin in 2002. These CRPs will generate needed data on molecular processes affecting the edge plasma, data needed for diagnostics in fusion machines, and data for assessing the total tritium inventory in plasma machines.

SEARCH ENGINE

As the number of electronic databases available on the Internet increases, it has become increasingly difficult for any one user to become proficient in using them. Each site has its own format and the user must learn this format for each web site. Discussions have been held on the possibility of constructing one interface that could take a user request and formulate the request for each of several different databases. The requests would then be sent to each database in turn and the results returned to the user.

There is now a prototype of such an interface. Yuri Ralchenko of the Weizmann Institute in Israel and Denis Humbert of GAPHYOR in France have developed the search engine called GENIE. This search engine currently searches five different sites for radiative data and two sites for electron impact excitation and ionisation data. The format is simple and easy to understand. The underlying code is easy to expand for more databases and other types of data. The prototype version is available at the web sites at the IAEA, the Weizmann Institute, and GAPHYOR.

PHYSICAL SPUTTERING AND RADIATION ENHANCED SUBLIMATION

The CRP on "Plasma-Interaction Induced Erosion of Fusion Reactor Materials" produced a large volume of data on erosion of materials. This large volume of data was carefully evaluated by several members of the CRP. The best quality data were then fitted to physically realistic forms for angle dependence and for energy dependence. The resulting fits were

checked for accuracy in reproducing the original data and to insure smooth behaviour over the entire range of validity. The results of this work were published in Volume 7B of the journal series *Atomic and Plasma-Material Interaction Data for Fusion.* The fit coefficients have been added to the online electronic database along with the evaluation functions so that users can obtain the data for arbitrary energy or angle.

EFFECTIVE RATE COEFFICIENTS

The computer modelling of non-LTE plasmas can be very time consuming. It is often the case that the densities are such that a simple coronal model is not sufficient. In such a case, each individual energy level of each ion must be included in the solution of the rate equations. This can result in massive amounts of data and solutions of very large sets of equations. In a CRP on radiative power losses in plasmas, many such lengthy modelling calculations were carried out. In addition to providing the calculated radiated power, effective ionisation and recombination rate coefficients were derived. These data were stored along with the populations of the ion stages as well as the total radiation from each ion stage. It is possible to use these data to interpolate in temperature and electron density to obtain the radiated power at an arbitrary temperature and density. In the steady state case this does not require the use of the effective rate coefficients. The effective rate coefficients are needed in the case of a plasma that is evolving with time. In that case it is possible to use interpolated effective rate coefficients to solve the time dependent problem and obtain the populations of each ion stage as well as the total radiated power. Since the effective rates coefficients do not require any explicit energy levels, this calculation is very quick computationally. These effective rate coefficients will soon be available on the A+M Data Unit web site.

NEW INTERFACES

Recent work by Jeff Stephens and Yuri Ralchenko has resulted in a preliminary version of a new interface to the bibliographic database at the A+M Data Unit. In the past, access to the bibliographic data was possible only through a Telnet session. That method is no longer adequate and a new interface was needed. While at the A+M Data Unit, Stephens did a large amount of work on the bibliographic database to bring it into a form suitable for more modern database management. During a recent period as a consultant, Ralchenko continued this work and put a preliminary version of an interface on the Unit web page. This interface allows the user to search the extensive bibliographic database by author and/or keyword. The resulting references are displayed along with a link to the home page of the journal where possible.

In may cases it is necessary to model a particular element for which data such as electron impact excitation cross sections, are not available. Such data may take a considerable time to generate. Often it would be of great value to have at least a good estimate of these data. This is now possible for electron impact excitation of atomic ions. During a consultancy visit to the Unit, James Peek installed a code for calculation of these cross sections using the so-called "average approximation". Along with the cross section code, a version of the Hartree-Fock atomic structure code of R. Cowan was also installed. It is now possible to run these codes through an interface at the Unit web page. This allows the calculation of cross section versus impact electron energy for an arbitrary ion in a relatively short time, typically a second for each energy point. The calculations are all in configuration average mode only, no angular coupling to form LS terms is carried out. However, the results should be useful in cases where no other data exist. In most cases the average approximation is fairly accurate compared to a distorted wave calculation. The worst case is for singly ionised at very close to threshold energy, where the average approximation could be in error by as much as a factor of

two. For higher ion stages and for higher energies, the average approximation is within approximately 10% of the distorted wave.

NEW CO-ORDINATED RESEARCH PROJECTS

In the past year two new CRPs have been started, one on the subject of "Data for molecular processes in edge plasmas", the other on the subject "Atomic and molecular data for fusion plasma diagnostics". Each CRP had a research co-ordination meeting last fall and each group formulated a plan for research in these areas. In addition a new CRP to assess the overall inventory of tritium in fusion reactors will start this year. This CRP will include processes that retain tritium as well as methods to release the tritium back to the plasma.

THE URL FOR THE ATOMIC AND MOLECULAR DATA UNIT IS:

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