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ATOMIC AND MOLECULAR DATA NEEDS FOR FUSION

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ABSTRACT

Atomic and molecular processes in plasmas play a crucial role in the development of net energy producing magnetic fusion devices. In light of this fact, presented here is a survey of the broad needs of fusion energy research and a review of the status of the existing database. Emphasis is placed on the relatively new needs for data as novel materials are evaluated for use in the next devices, and as components such as the divertor take on more significance for demonstration and practical reactors. Also, examples are given of recent or ongoing data evaluation efforts, the role of national and international data centers is discussed, and some summarizing comments are given.

INTRODUCTION

For nearly half a century, the goal of producing energy through controlled fusion to meet the needs of an ever expanding technological society has been envisioned and pursued vigorously. Critical to this program of research has been the availability of accurate atomic and molecular data. For example, even the earliest experiments showed that the interaction of the hot, dense plasma with the walls of the confinement vessel produces impurities whose presence even in minute quantities effects the plasma behavior with very detrimental consequences. Atomic data regarding the interaction of these impurity ions with the primary plasma constituents have, therefore, been important from the beginning of this enterprise. Thus, even though the nuclear reactions which liberate the desired energy are well understood, it is clear that the plasma and atomic physics involved in developing a net energy producing reactor presents an ongoing challenge.

In particular, atomic data have been produced and assessed to help address the need to model the interaction with the core plasma of impurity ions arising from the walls and introduced intentionally for neutral beam heating or for diagnosis. These data include large collisional and spectroscopic databases, but recently, as fusion energy development has begun to approach demonstration and engineering

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for practical reactors, needs have arisen for similar data for an expanded range of species and in new energy regimes. This has occurred as various materials are evaluated for use in the plasma facing components and for such applications as in the divertor. Concomitantly, a significant need for materials data and plasma-wall interaction properties has arisen, and planning for the construction of the International Thermonuclear Experimental Reactor (ITER) has served to focus international efforts to coordinate the evaluation of the existing data and the production of new data.

Presented here is a summary of the current broad needs of fusion research for atomic and molecular data as well as a general assessment of the ability of the existing data to fulfill these needs. Beyond the scope of this review is a survey of the needs for inertial confinement or other schemes significantly different from magnetically confined plasma approaches.

REVIEWS OF STATUS AND NEEDS

Periodically, experts working in plasma or atomic and molecular physics publish reviews concerning the status of atomic and molecular data pertaining to fusion energy research, and of the present needs for new or evaluated data. Often, this type of information can be found in the proceedings of meetings or summaries of working groups convened by the International Atomic Energy Agency (IAEA) and presented in a series of reports by the International Nuclear Data Committee. For example, committees formed by the IAEA at the request of the International Fusion Research Council recently recorded their findings on the status of the collisional, spectroscopic, and particle-material interaction databases, and on the priorities which should be established for the creation or evaluation of new data[1]. These summaries include the data requirements for both modelling and diagnosis, and emphasize such issues as power and particle control, divertor concepts and operation, neutral beam diagnostics, and physical and chemical sputtering of the vessel walls in next-step reactors, with particular attention on ITER.

Similar information can be found in more widely distributed sources such as the journals *Physica Scripta*, *Comments on Atomic and Molecular Physics*, and *Nuclear Fusion*. In fact, very detailed reviews of the database status and the needs for new data gathering efforts have recently appeared as a series of supplements to *Nuclear Fusion*[2,3,4,5]. These volumes focus on the issues involved in the edge plasma, plasma-wall interactions, impurity control, particle transport in the scrape-off layer, thermal power and helium ash exhaust, neutral beam heating, fueling, and diagnostics, and special materials such as beryllium, boron, and composites of these species especially with carbon. They present data and evaluations far beyond the scope of this brief review and are highly recommended to the interested researcher.

Forthcoming is another excellent review of the specific needs for data and data organization for present and next-step fusion reactors given by H.P. Summers[6]

Table I: Status of database for electron and heavy-particle collisions, R evaluated or recommended, A ALADDIN, S scaled or semi-empirical, I incomplete. Table adapted by permission of author[7]. (Charge Transfer is abbreviated by "CT").

Collision	Ionization	Excitation	Recombination	Dissociation
e + H, H^-	R,A	R,A	R,A	
e + He^{q+}	R,A	R,A	R,A	
e + Li^{q+}	R,A	I	I	
e + Be^{q+} ,B^{q+}	R,A	R,I	I	
e + C^{q+}, O^{q+}	R,A	R,A	R,I	
e + Si^{q+}	R,A,I	I	I	
e + Ti^{q+}	S,A,I	I	I	
e + Fe^{q+}	R,A	R,A	I	
e + Cr^{q+}, Ni^{q+}	R,A,I	I	I	
e + Mo^{q+}	S,I			
e + Ta^{q+}, W^{q+}	S,I			
e + H_2, H_2^+	R,A	R,A	R,A	R,A
e + CH_4, CH_4^+	I	I	I	I
e + C_mH_n, $C_mH_n^+$	I	I	I	I
e + O_2, O_2^+	R	I	I	I
e + CO, CO^+	R	I	I	I
e + H_2O, H_2O^+	R	I	I	I

Collision	Total CT	n, ℓ CT	Ionization	Excitation
H + H, H^-	R,A	R,A	R,A	R,A,I
H + He^{q+}	R,A	R,A	R,A	R,A,I
H + Li^{q+}	I	I	I,S	I
H + Be^{q+} ,B^{q+}	I	I	I,S	I
H + C^{q+}, O^{q+}	R,A	R,A	R,A	I
H + Si^{q+}	I		S,I	
H + Ti^{q+}	S		S	
H + Fe^{q+}	R,A,S		S	I
H + Cr^{q+}, Ni^{q+}	S		S	
H + Mo^{q+}	I		S	
H + Ta^{q+}, W^{q+}	I		S	
H + H_2, H_2^+	R,A		R,A	
H + CH_4, CH_4^+	I			
H + C_mH_n, $C_mH_n^+$	I			
H + O_2, O_2^+	I			
H + CO, CO^+	I			
H + H_2O, H_2O^+	I			

in *Advances in Atomic, Molecular and Optical Physics.* Also, a concise, critical assessment of the atomic and molecular collisional database has been given recently by R.A. Phaneuf[7]. This assessment is summarized in Table I for both electron-impact of plasma component and impurity species, and for collisions between atomic hydrogen and the plasma components and impurities, the situation being similar for molecular hydrogen and helium.

ALADDIN

In order to facilitate and standardize the exchange of atomic, molecular, and other data among international data centers, data producers, and most importantly, the community of users, the ALADDIN database system was adopted in 1989 by the IAEA Data Center Network. ALADDIN (A Labelled Atomic Data INterface) was developed by Russell Hulse[8,9] at *Princeton Plasma Physics Laboratory* using ANSI FORTRAN/77 and relying on ASCII-formatted data files. The program and all ALADDIN formatted evaluated or recommended data files are available from the IAEA† or from the present author. The program and data files can be distributed either by IBM PC-compatible floppy diskettes or through electronic mail. A manual of operations is also available for hardcopy distribution[10]. In the near future, these and other resources will be available through such facilities as anonymous *ftp* or through *telnet* over the INTERNET at both the IAEA Atomic and Molecular Data Unit and the Controlled Fusion Atomic Data Center (CFADC) at the Oak Ridge National Laboratory. ALADDIN data files which are presently available or should be in the very near future are listed in Table II.

Clearly, any data, evaluated or not, could be placed into the specified format, but the IAEA has sought to provide explicitly evaluated data. To this end, it periodically assembles working groups or enlists the involvement of experts to generate, compile, and evaluate data needed for fusion. In addition, certain international data centers or organizations submit data to the Data Unit for inclusion in the list of recommended ALADDIN data files. Several examples of these types of data files are easily identified in the table. One of the most recent additions to the list has been the recommendation of cross sections for inelastic processes involving ground and excited state hydrogen colliding with electrons, protons and multiply-charged ions[21]. This compilation was assembled to provide critically assessed and complete data for neutral hydrogen beam injection in present and next-step reactors. Neutral beam heating supplements the ohmic heating of a tokamak and also provides a means for several key diagnostics of the plasma. Along with *Elementary Processes in Hydrogen-Helium Plasmas*[18] and *Collisions of H, H_2, He, and Li Atoms and Ions with Atoms and Molecules*[19], also available in ALADDIN format, this work forms a rather complete database for inelastic collisions involving hydrogen.

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Table II: Available recommended/evaluated data sets in ALADDIN format

1. Atomic and Molecular Data for Fusion, Part I - Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions[11]
2. Recommended Data on Excitation of Carbon and Oxygen Ions by Electron Collisions[12]
3. Recommended Data on Atomic Collision Processes Involving Iron and its Ions[13]
4. Collisions of Carbon and Oxygen Ions with Electrons, H, H_2, and He, Atomic Data for Controlled Fusion Research, Vol. V[14]
5. Atomic and Molecular Data for Fusion, Part II - Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions: Fluorine to Nickel[15]
6. Recommended Data for Excitation Rate Coefficients of Helium Atoms and Helium-like Ions by Electron Impact[16]
7. Atomic and Molecular Data for Fusion, Part III - Recommended Cross Sections and Rates for Electron Ionization of Atoms and Ions: Copper to Uranium[17]
8. Elementary Processes in Hydrogen-Helium Plasmas[18]
9. Collisions of H, H_2, He, and Li Atoms and Ions with Atoms and Molecules, Atomic Data for Controlled Fusion Research, Vol. I[19]
10. Collisional Processes of Hydrocarbons in Hydrogen Plasmas[20]
11. Recommended Cross Sections for Collision Processes of Hydrogen Ground-State and Excited Atoms with Electrons, Protons, Multiply Charged Ions[21]
12. Electron-Impact Excitation and Ionization of Helium Atoms[22]
13. Recommended Cross Sections for State-Selective Electron Capture in Collisions of C^{6+} and O^{8+} Ions with Atomic Hydrogen[23]
14. Evaluated Cross Sections for Collision Processes of Li Atoms with Electrons and Protons[24]
15. Energy Dependence of Ion-Induced Sputtering Yields of Monatomic Solids in the Low Energy Region[25]
16. Energy Dependence of the Yields of Ion-Induced Sputtering of Monatomic Solids[26]
17. Particle Reflection from Surfaces: A Recommended Database[27]
18. Recommended Data for Physical Sputtering[28]
19. Thermophysical and Thermomechanical Properties of Beryllium[29]

'NEW' DATA NEEDS

The present focus on advanced development, engineering, and design of experiments and reactors requires new data not previously emphasized during phases of research which concerned primarily heating and transport in the central plasma. In particular, the data needs for modelling the properties of the edge/scrape-off plasma and the divertor performance, drive current efforts to produce and evaluate data. These regions of the reactor are characterized by higher densities, lower charge states, and lower energies than in the central plasma, and involve additional species. For example, in attempts to reduce high-Z impurities which have a deleterious effect on central plasma temperature by inducing high radiation losses, low-Z materials have become of great interest for first wall and plasma facing components. These materials must also have properties such as low physical and chemical sputtering yield, high thermal conductivity, low erosion rate, and low retention of H, D, and T. High-Z materials may still be of significant use behind the first wall for heat and radiation sinks, and for use in the divertor where extremely high heat, radiation, and particle fluxes must be handled.

The divertor for ITER is presently being designed to enable the exhaust of power and the helium ash of the fusion process. As such, it is estimated that the power density will be on the order of a gigawatt per square meter. Thus, the strategy is to operate the divertor under conditions of high density and rely on atomic processes (charge exchange, impurity radiation, hydrogen radiation, ionization, recombination, gas conduction) to spread the heat load out over the entire divertor structure. Thus, cross sections and rates for excitation, ionization, capture, recombination, and elastic scattering need to be calculated, measured, and evaluated for energies relatively low compared to the central plasma, for nearly neutral species.

In the divertor and also the edge plasma, since the temperatures are much lower than the central plasma, molecules can exist. In addition, since the walls may be made from such low-Z materials as boronated carbon, a wide variety of hydrocarbons may be present. Particle-surface databases are required and are being assembled to predict the species and rovibronic states that will be present. Cross sections will be needed for various fragmentation and energy redistributing reactions involving these species. It will be critical to model well the scrape-off layer since it must insulate the wall from the intense heat flux, and act to transport and control impurities. Further, important interactions involving the walls must be addressed to evaluate hydrogen retention and physical and chemical sputtering.

Neutral beams will continue to play an important role in supplementing the ohmic heating of the plasma, but they have also come to play a major role in diagnosing plasma conditions. Radiation after charge transfer with the injected beam has allowed diagnostics to be developed (e.g. charge exchange spectroscopy) for plasma temperature, ion velocity distribution, particle transport, and other important parameters. Neutral beam injection intended only for diagnosis will continue to also be important in the edge region. Edge probe species such as Li and Na have been used. Other species are puffed or otherwise introduced into the plasma for diagnosis, yielding a marker since they would not ordinarily be present in any significant quantity. One proposed species is krypton, for which present experimental and theoretical efforts are being undertaken to supply the needed database.

Given below is a broad summary of some of the more critical of the species and reactions for which data needs exist.

- Low-Z materials for first wall: Be, B, C, and composites
- Molecules: ionization, fragmentation, formation at/near wall, $C_mH_n^{q+}$, CO_n^{q+}, H_2O^{q+}
- Particle-surface interactions (realistic surfaces present in reactors)
- Total and state-selective charge transfer below 1 keV/u (C^{q+}, O^{q+}, Si^{q+}, Ti^{q+}, Fe^{q+}, Cr^{q+}, Ni^{q+}, V^{q+}, Mo^{q+}, Ta^{q+}, W^{q+}) + (H, H_2, He), especially for low charge states
- Electron collision data (excitation, ionization, dielectronic recombination, radiative recombination) for Mo, Ta, W ions
- Data for collisions involving excited/metastable reactants, e.g. H^*, He^*
- Heavy-particle, low-energy, low charge state (including neutral), elastic scattering angular distributions
- New species, e.g. injected diagnostic impurities, Kr

ROLE OF DATA CENTERS

It is the mission of a number of data centers established both in the United States and internationally to identify available data, undertake efforts to evaluate, compile, and communicate it to the fusion research community, and to periodically assess the needs for new or refined information. Such organizations exist, for example, at the National Institute for Fusion Science in Nagoya, Japan, the Oak Ridge National Laboratory, Oak Ridge, Tennessee, and the Queen's University, Belfast, North Ireland. In addition, the Atomic and Molecular Data Unit of the IAEA plays an important role to help coordinate the efforts of these data centers and other independent researchers in the international data collection, evaluation, and dissemination activity. An international data center network has been formed including fifteen participants from China, Europe, Japan, Russia, the United Kingdom, and the United States. The network assembles periodically for the coordination of efforts and exchange of data, and to assess the database status.

Another important function of the IAEA Data Unit is to enlist the aid of international teams of experts to address specific data needs. For example, recent working groups have provided important new and assessed data regarding metallic impurities, helium beam diagnostics, hydrogen recycling and helium ash removal, and boron and beryllium for plasma facing components.

Also of significance is the use of data produced for other applications, perhaps most notably, astrophysics. Data from the well known Opacity Project is rapidly entering the standard database, and has considerable relevance to fusion energy research as well as its mission to produce cross sections and rates for modelling solar (stellar) atmospheric opacity. Jean Gallagher has recently described[30] the mission, methods, resources, and contact points of several data centers through which information may be obtained.

In particular, the Oak Ridge National Laboratory Controlled Fusion Atomic Data Center identifies, compiles, evaluates, and recommends atomic and molecular data relating primarily to collisions. To facilitate these activities, a database of categorized references is maintained and additions are made to it by a group of expert consultants. This database currently contains references to over 25,000 journal articles dating from 1978 to the present, and in collaboration with a group from the National Institute for Standards and Technology, conversion of archival tapes to modern format is currently making accessible over 40,000 additional entries dating from around 1950 to 1978. All of these entries and those which will continue to be added to the database, will be available to be searched over the INTERNET computer network in the near future, along with other services, such as access to ALADDIN. Currently, the CFADC answers individual requests to search the bibliographic database or to help provide access to other numerical atomic and molecular data at the rate of once or twice weekly. The CFADC bibliography forms a major part of the IAEA publications *International Bulletin on Atomic and Molecular Data for Fusion*, which is published periodically, and two publications which summarized the bibliographic information as of 1980 (*CIAMDA 80*)[31] and 1987 (*CIAMDA 87*)[32].

A condensed summary of the reaction categories for which bibliographic references are compiled regarding species relevant to fusion research is given below.

1. Heavy Particle - Heavy Particle Collisions:
   Elastic, Excitation, Dissociation, Electron Capture, Ionization, Recombination, Stripping, Recombination, Mutual Neutralization, Energy Transfer, Interaction Potentials, Line Broadening, Electron Detachment, De-excitation

2. Interaction with Fields:
   Atoms or Molecules in External Fields, Collisions in Fields

3. Particle Penetration in Matter:
   Energy Loss and Stopping Power, Particle Range, Multiple Scattering, Charge State Population, Excited State Population

4. Particle Interactions with Surfaces:
   Sputtering, Secondary Electrons, Photoelectrons, Reflection, De-excitation, Neutralization, Ionization, Dissociation, Sticking, Adsorption, Desorption, Chemical Changes, Trapping and Re-emission of H and He

5. Electron - Particle Collisions:
   Elastic, Excitation, Dissociation, Ionization, Recombination, De-excitation, Line Broadening, Negative Ion Formation, Bremsstrahlung, Electron Detachment, Fluorescence, Angular Scattering, Momentum Transfer

6. Photon Interactions with Heavy Particles and Electrons:
   Absorption, Elastic, Excitation, Dissociation, Ionization, Photodetachment, Fluorescence, Inverse Bremsstrahlung

7. Data Compilations, Reviews and Books, Bibliographies:
   Electrons, Heavy Particles, Photons, Particles on Solids, Transport, Structure

The CFADC also periodically publishes compilations and recommendations through the series *Atomic Data for Fusion*[14,19,33,34,35], commonly referred to as the "Redbooks", and through other topical reports and articles. The activities of the CFADC are coordinated closely with those of the International Atomic and Molecular Data Center Network, through which data needs are identified and the status of the available database is assessed.

SUMMARY AND COMMENTS

In summary, the need in fusion plasma research for compilation and evaluation of atomic and molecular data persists, and efforts by the community of atomic, molecular, and plasma physicists continue to help to ameliorate this situation. The needs for data also continue to change as new materials or new concepts are evaluated for next-step devices. National and international data centers play an important role by coordinating the efforts to produce, compile, and evaluate the required data, and by providing centralized repositories at which the databases may be assembled and maintained. The International Atomic Energy Agency helps to insure the efficient cooperation of these data centers, and coordinates groups of researchers brought together to address specific needs. A significant advancement in the standardization and communication of data has been made by the adoption and expanding use of ALADDIN.

Many of the bibliographic and numerical databases which are presently either searched on local systems or distributed on a rather limited basis, will soon become available through access to workstations over the INTERNET computer network. It is hoped that this will allow a significantly easier method of obtaining data for the intended end users in the fusion energy and atomic and molecular research communities. In addition, informal surveys of the user community indicates that not only bibliographic and raw cross section data are desired, but also various forms of "derived" data. Perhaps the simplest such form would be rate coefficients, obtained from some adjunct code interfaced to the cross section database, but needs also extend to such data as could be derived from a collisional-radiative model. The advent of workstations through which bibliographic and numerical cross section data could be retrieved also holds the promise that these derived data needs may be addressed since sufficient computational power would then exist for the easy interface of auxiliary programs.

It is hoped that the communication between the atomic and molecular and the plasma communities, as well as between data producers and evaluators, can continue to be encouraged, as the next phase of work begins towards the goal of net energy producing fusion energy reactors.

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