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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Consultants' Meeting on "Atomic and Molecular Data Base for Hydrogen Recycling and Helium Removal from Fusion Reactors"

11-12 June 1992, Vienna, Austria

SUMMARY REPORT

Prepared by R.K. Janev

January 1993, Vienna

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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ABSTRACT

The proceedings and the main concclusions of the IAEA Consultants' Meeting on "Atomic and Molecular Data Base for Hydrogen Recycling and Helium Removal from Fusion Reactors" (June 11-12, 1992, Vienna, Austria) are described. The meeting conclusions include the results of the analysis of existing and required atomic, molecular and particle-surface interacction data bases for modeling the hydrogen recycling and helium exhaust in fusion reactors and a set of reccommended actions for improving the modelling scheme and data base situation.

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January 1993

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Appendices

1. INTRODUCTION

Following a recommendation of the IFRC Subccommittee on Atomic and Molecular (A+M) Data for Fusion, the IAEA A+M Data Unit has organized on June 11-12, 1992 at the IAEA Headquarters in Vienna a Consultants' Meeting on the "Atomic and Molecular Data Base for Hydrogen Recycling and Helium Removal from Fusion Reactors". The objectives of the meeting were to review the A+M and particles-surface interaction (PSI) data needs and to assess the status of available data bases for modelling the hydrogen recycling and helium exhaust in fusion reactor edge plasmas, as well as for diagnostics of these plasmas. The motivation for organizing this meeting was the growing awareness in the fusion research community about the critical role of the helium exhaust problem in next-step fusion devices (such as ITER), and the need to develop sufficiently accurate A+M and PSI data bases for the existing plasma edge modelling codes so that their predictive power becomes adequate for the reactor design needs. A particular goal of the meeting was to establish a "standard scheme" for the relevant A+M and PSI processes required in the H-recycling and He-exhaust modelling and in the basic edge plasma diagnosticcs, to assess the completness and quality of existing A+M and PSI data bases for such a standard scheme, and to formulate appropriate recommendations and set of actions for the IAEA A+M Data Unit and the international A+M Data Centre Network for improving the data situation. The Meeting was attended by ten participants, representing the plasma edge modelling and diagnostics segment of fusion research community, A+M Data Centre Network and the IAEA **(see Appendix 1)**. The Meeting Agenda is given in **Appendix 2**.

2. BRIEF PROCEEDINGS OF THE MEETING

The work of the meeting was organized in five sessions. The first session dealt with the A+M and PSI data needs for fusion plasma edge modelling and diagnostics in relation with the H-recycling and He-exhaust problems. **D. Reiter** (KFA, Jülich) desccribed the progress in recent edge plasma modelling with particular attention to the He-removal from ITER-type devices. He demonstrated that He-removal from the divertor is a critical issue for the reactor design, which places high demands on the predictive potential of plasma edge modelling codes and on the completness and accuraccy of associated A+M and PSI data bases. Dr. Reiter also described the A+M and PSI data bases currently included in his EIRENE neutral transport computer pacckage and discussed the further A+M and PSI data needs for improving the predictive power of the codes. He particularly emphasized the urgent need for reliable elastic ion-neutral and neutral-neutral collisions. **V. Abramov** (I.V. Kurchatov Institute, Moscow) presented results from the neutral transport codes in use in the Kurchatov Atomic Energy Institute and described the content of associated A+M and PSI data bases. He also commented on other applications of these data bases, and on their completness and accuracy. Along the same lines, **D. Stotler** (PPL, Princeton) described the A+M and PSI data bases presently included in the DEGAS neutral particle transport code, the ongoing efforts at PPPL for improvment of the content and quality of these data bases, and provided a list of A+M and PSI data to improve the predictive potential of DEGAS both for the next-step fusion devices and for analysis of recent or planned experiments on the operating large tokamaks. Particularly urgently required are the collisional data for the Be and B impurities, hydrocarbon molecules and their ions, as well as the PSI data for ion- and neutral-wall reflecction and carbon influxes into the plasma.

D. Ruzic (University of Illinois, Urbana) presented a review of the effects of the boundary conditions in neutral particle modelling. The emphasis was placed on the recent developments of the particle-surface interaction computer codes (VFTRIM), in which the surface roughness effects are included through a more realistic (fractal) surface model, and to the effects of divertor and pump duct geometry on particle recycling and exhaust. Dr. Ruzic demonstrated that ion-neutral and neutral-neutral collisions are very important processes in determining the neutral transport in the divertor region under high-recycling conditions, and have a considerable impact on the pumping speed and geometry of divertor pumping system.

Within the same session, **K. Behringer** (University of Stuttgart) provided an extensive review of the A+M data requirements for plasma edge diagnostics. For determination of edge plasma parameters (T_e,n_e) and particle flux densities from the line emission intensities, comprehensive collisional and radiative data bases are required for the emitting species, involving all its stages of ionization. Prof. Behringer discussed the status (including quality) of the data bases for H, He, Be, B and C atoms and ions, and provided illustrative examples of diagnostic applications of existing data bases (H- and He-collisional-radiative codes). He also reviewed the data needs and the data status for the most abundant plasma edge molecular species, such as H_2 (D_2), hydrocarbons, CO, hydrides, from the point of view of molecular radiation based diagnostics of molecular particle fluxes and chemical sputtering yields, as well as for determination of electron energy losses into vibrational and rotational excitation. The need for establishment of a collisional-radiative code for molecular hydrogen has been emphasized.

The second section of the meeting was devoted to a more detailed presentation of the status and recent developments in the collisional data bases for the major edge plasma A+M constituents. **H. Tawara** (NIFS, Nagoya) presented a critical review of the available data bases for CH_n, CO_n and H_nO molecular plasma edge impurities, including recently generated data in Japan and elsewhere. Dr. Tawara stressed the fact that the cross section information for the molecular species obtained under laboratory conditions (e.g. crossed- or merged-beams experiments), may not be always appropriate for the plasma modelling applications, since the interacting molecular species in the plasma may be in undefined vibrationally (and rotationally) excited states. The collisional cross sections for such excited species may be considerably different from those involving ground state molecular species. This aspect was further emphasized and explored in the presentation of **M. Bacal** (Ecole Polytechnique, Palaiseau), reviewing the low-energy collision processes of the ground-state and vibrationally excited hydrogen molecule and molecular ion with electrons, protons, hydrogen atoms and with surfaces. Prof. Bacal presented the available cross section information on these processes collected and evaluated by the scientific community working in the area of negative ion sources. The question of the vibrational distribution of hydrogen molecules or molecular ions, formed by surface collision processes, drew particular attention of the meeting participants. **D. Schultz** (ORNL CFADC, Oak Ridge) presented the status of the available data base for elastic and momentum transfer ion-atom collisions for species of interest to the plasma edge region. He also reported the first results of a data generation effort undertaken at ORNL CFADC for establishment a data base for the elastic and momentum transfer ion-atom collision processes. **R.K. Janev** (IAEA A+M Data Unit) presented the status of A+M and PSI data bases currently available at the IAEA, which contain information relevant for the H-recycling and He-exhaust modelling studies and plasma edge diagnostics. These data bases include: a complete recommended data base for all processes of ground-state and excited hydrogen atoms colliding with electrons, protons and fully stripped ions of He, Be, B, C, O and with A^{q+} ($q \geq 10$) ions (all the data being ALADDIN formatted), a fairly complete data base for the ground-state He atom colliding with the same species as above, and for the $He^{*}(1s2l;\ ^{2S+1}L)$ atoms colliding with electrons and multicharged ions (not all cross sections in the ALADDIN format), a fairly complete data base for the C and O plasma impurities (ALADDIN formatted), a fairly complete data base for the ground-state Be and B atoms and ions colliding with electrons and with H, He and H_2 (not ALADDIN formatted), a preliminary data base for the collisions of H_2, H_2^+, H_3 and H_3^+ with electrons and protons (the PPPL/Springer-Verlag publication; ALADDIN formatted), as well as evaluated data on light ion reflection (normal incidence) and physical sputtering of monoatomic materials upon light-ion bombardment (all of them in ALADDIN format).

In Session 3 and 4 of the meeting, the presented information during the first two session was discussed and analyzed in detail from the point of view of establishing an optimum A+M and PSI data base for H-recycling and He-removal modelling, which makes a reasonable compromise between the (predictive) modelling requirements and the realistic possibilities for providing the necessary and highly accurate, A+M and PSI data bases, and which, at the same time, could satisfy the needs of certain edge plasma diagnostics. During these discussions, several A+M and PSI data areas have been identified for which additional data information has to be compiled and evaluated, or generated. The qestion of possible effects of certain A+M processes, taking place in the edge plasmas and not included in the current modelling codes, has also been addressed. The results of the meeting work in these two session was summarized at the last meeting session and are reproduced in the next section of this Report.

3. SUMMARY OF THE MEETING WORK AND RECOMMENDATIONS

3.1 Standard scheme of A+M and PSI processes for H-recycling and He-removal modelling

The importance of particular A+M and PSI processes to be included in a neutral particle transport modelling code is judged on the basis of fractional abundance of interacting plasma edge constituents and the magnitude of the corresponding reaction rate coefficients (for A+M processes), or particle production yields (for PSI processes). A standard scheme of A+M and PSI processes that should be included in a neutral particle transport modelling code should contain the following components:

A. **A+M collisions processes**

I. **Species**

1) e, H^+, H, H^* (nl), (nl=2s, 2p; 3s,3p,3d), H^* (n>3) ,
2) He, He^* (1s, $nl^{2S+1}L$), n≤4; He^* (1s, $n^{2S+1}L$), n>5 ,
3) H_2, H_2^+, $H_2^*(v)$, $H_2^{+*}(v)$,
4) (Li), Be, B, C, O, Fe, Ni, Mo, (Ga), W, (V) ,
5) B-, C-hydrides, Be-, B-oxides, H_2O, O_2, (Li-), Be-, B-carbides.

II. **Processes**

1. Atomic H and He targets: all collision processes with electrons and protons required in a collisional-radiative model, all processes with He^+, He^{2+} and H_2^+, charge-exchange processes with major ionized impurities (particularly for excited H and He).
2. Molecular H_2, H_2^+ targets: all collision processes with electrons and protons, resonant and quasi-resonant electron- and particle exchange reactions with major atomic impurity ions (including He^+ and He^{2+}), H_2 + H_2^+ collision processes.
3. Atomic impurities (atoms and ions): all electron impact and quasi-resonant heavy-particle collision processes.
4. Molecular impurities (including their ions): all electron impact processes, including those leading to molecular dissociation and fragmentation, and quasi-resonant collision processes major edge plasma heavy constituents, including charge transfer and particle exchange.

5. Elastic ion-neutral and neutral-neutral collision processes (H, H_2, He, H^+, H_2^+, He^+, He^{2+}), including momentum transfer.
6. Radiative processes.

III. Quantities

- Cross sections and reaction rate coefficients,
- Quantum state, angular and energy distribution of reaction products,
- Preferrable: composite reaction rates from collisional-radiative codes (e.g., for H and He) with inclusion of the charge transfer on H, H_2 and He.

Comments

(1) The A+M data base outlined above should also be sufficient for diagnostic purposes, with electron capture treated as a state-selective process.

(2) In a crude modelling scheme for neutral particle transport, the processes involving excited states (except perhaps the first few) may be omitted.

(3) The effects of collision processes involving vibrationally excited H_2, H_2^+ (and molecular impurities) on the modelling code results has not as yet been investigated, although from a physical point of view (significant changes in the reaction thresholds, reaction rate coefficients, energy distributions of reaction products) these effects may be expected to be important. If proven so (to be checked by edge plasma modellers), practical methods have to be developed to effecctively include these processes in the computational scheme (e.g. dividing the vibrational spectrum into several groups, or introducing effective rates for molecular processes based on certain type of averaging or on an auxilliary

vibrational radiative-collisional model).

(4) Except for the H-target, the collisional data bases for other targets are still not complete, or contain data for certain processes of insufficient accuracy. It is of critical importance to continue and accelerate the work on completing and improving the data bases for He, H_2, Be, B, hydrocarbons, and their ions.

(5) Establishment of a complete and evaluated data base for elastic ion-neutral and neutral-neutral collisions for the edge plasma relevant species is of highest priority. The initial efforts along this line of the ORNL group are described in **Appendix 3**.

B. PSI Processes

I. Collision species

Projectiles: light-element atoms and ions (H- and He-isotopes, Be, B, C, O), self-ions;

Targets: mono-atomic and composite plasma facing candidate materials.

II. Processes

1. Particle reflection,
2. Physical sputtering, chemical erosion and RES,
3. Thermal and particle-impact induced desorption,
4. Low-energy collisions of hydrogen atoms and molecules (and their ions) with surfaces,
5. Surface molecule formation and release,
6. Processes related to local, hot spot phenomena, e.g. evaporation, disruption erosion, etc.

III. Quantities

- number, angle and energy distributions of reflected, sputtered and desorbed particles as function of incident angle, energy, and species,

- rates of thermally induced or other particle release processes as function of surface temperature, material and other parameters characteristic for the release mechanism,
- quantum and charge state of reflected, sputtered and desorbed particles,
- charge and chemical composition of released particles.

Comments

(1) Characterization of particle influxes from the walls is also important for the edge plasma diagnostic schemes.

(2) Characterization of the surface state, in both morfological and physico-chemical sense, is important in the description of above processes.

(3) Most complete information on particle reflection and physical sputtering can presently be obtained by the VFTRIM code (D. Ruzic), which has already been coupled to the 3D neutral transport modelling codes. Analytic models for the plasma-entering particle distributions (in angle and energy) would be very valuable for reducing the computational time.

(4) Desorption processes need a better description in the present versions of modelling codes. The low-energy atom/molecule-surface collision processes (different than those included in particle reflection codes) are presently not included in the modelling codes, and the surface molecule formation and release processes are treated in a crude phenomenological manner (e.g. by adopting an ad hoc number for the H/H_2 ratio of reflected and/or surface released hydrogen). Improvement of this situation, both on the data and the code side, is an important task. Similar is the

situation with the chemical and other erosion processes.

3.2 **Priorities in data compilation and new data generation for neutral particle modelling and edge plasma diagnostics**

The basic data collections currently used in neutral particle transport modelling and edge plasma diagnostics are the Springer-Verlag book of Janev et al, PPPL compilation on hydrocarbons by Erhardt and Langer, the JET A+M data base, the Johnson/Hinnov and Fujimoto collisional-radiative models for H and He, respectively, and the TRIM code (or its VFTRIM, and other versions) for describing particle reflection and sputtering processes. All these data compendia need serious updating and should be complemented by new sets of data on processes not covered there.

The priorities in the data compilation and generated work for completion or improving the A+M and PSI data bases required in plasma edge neutral gas modelling and diagnostics are:

1. Updating and completion of the data file for processes involving H_2 and H_2^+, particularly those leading to dissociation and formation of excited products. A more detailed information on the angular and energy distribution of dissociative reaction products (as well as the secondary electrons from ionization) is urgently required. Inclusion in the data base of processes involving vibrationally excited states (at least in an effective way) would be highly desirable, but the required effort seems to be too large and incombatible with the present resources.
2. Updating and completion of the data file for the processes involving He, He^+ and He^{2+} with edge plasma constituents is also urgently required for adequate

description of the He transport in and its removal from a high-recycling divertor region.

3. Establishment of an evaluated data file for ion-neutral and neutral-neutral elastic and momentum transfer collisions (H^+, He^+, He^{2+}, H_2^+, low-q impurities - H, He, H_2).
4. Completion of the collisional data bases for Be, B, and other low-Z impurities.
5. Updating and extension of the collisional data bases for hydrocarbons and other plasma edge impurity molecules.
6. Establishment of data bases for PSI processes other than those described by the TRIM-based codes (see comment (4) in 3.1.B above).

3.3 Recommended Actions

In order to accelerate the establishment of a complete data base for modelling of H-recycling and He-removal from fusion reactors, the following actions are recommended:

1. The A+M Data Centre Network (DCN) should give a high priority to the compilation and evaluation of A+M and PSI data involved in the "standard scheme" described in Section 3.1, and the IAEA A+M Data Unit should promote more vigorously the data generation for relevant A+M processes in the atomic collision physics community.
2. It is suggested that IAEA initiate in 1993 a Co-ordinated Research Programme (CRP) devoted to the improvement of A+M and PSI data bases and the A+M and PSI physics of neutral transport modelling codes. The conclusions of the present Consultants' Meeting may serve as guidelines for the scope and objectives of the suggested CRP. The composition of this CRP should include representatives from the most active neutral transport modelling groups, the A+M Data Centre Network and atomic collision physics laboratories.

Appendix 1

IAEA Consultants' Meeting on "Atomic and Molecular Data Bases for Hydrogen Recycling and Helium Removal from Fusion Reactors"

11 - 12 June 1992, IAEA Headquarters, Vienna, Austria

LIST OF PARTICIPANTS

Dr. M. Bacal	Laboratoire de Physique des Milieux Ionises, Eccole Polytechnique, F-91128 Palaiseau Cedex, **FRANCE**
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Dr. V.A. Abramov	Institut Atomnoi Energii I.V. Kurchatova, Ploshchad I.V. Kurchatova, Moscow D-182, 123182, **RUSSIAN FEDERATION**
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Appendix 2

IAEA Consultants' Meeting on "Atomic and Molecular Data Bases for Hydrogen Recycling and Helium Removal from Fusion Reactors"

11 - 12 June 1992, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

THURSDAY, June 11 **(Meeting Room: A-07-42)**

09:30 - 09:45 - Opening Remarks (**R.K. Janev**)
- Adoption of Meeting Agenda

Session 1: A+M Data Needs for Fusion Plasma Edge Modelling and Diagnostics

Chairman: V.A. Abramov

09:45 - 10:15	**D. Reiter**:	Progress in fusion plasma edge modelling and status of A+M data in present computer codes.
10:15 - 10:45	**V.A. Abramov**:	A+M data base of Kurchatov Institute plasma edge modelling codes.
10:45 - 11:00	**Coffee break**	
11:00 - 11:30	**K. Behringer**:	Plasma edge spectroscopy of some atoms and molecules.
11:30 - 12:00	**D. Ruzic**:	Effects of boundary conditions in neutral particle modelling.
12:00 - 12:30	**D. Stotler**:	A+M data needs for the PPPL plasma edge modelling codes.
12:30 - 14:00	**Lunch**	

Session 2: Status of A+M Data Base for Fusion Plasma Edge Modelling and Diagnostics

Chairman: D. Reiter

14:00 - 14:30	**H. Tawara**:	Data for some A+M processes in the plasma edge: need for redetermination.
14:30 - 15:00	**M. Bacal**:	Data for processes involving vibrationally excited states.
15:00 - 15:15	**Coffee break**	
15:15 - 15:45	**D. Schultz**:	Towards an elastic and momentum transfer cross section data base for 1 to 1000 eV collisions involving A^{q+} + H, He and H_2.

15:45 - 16:15 **R.K. Janev:** IAEA data bases for the ccollision processes in plasma edge region.

16:15 - 16:30 **Coffee break**

Session 3: **Assessment of the A+M Data Status and Needs for H-Recycling, He-Removal and Edge Plasma Diagnostics**

Chairman: R.K. Janev

16:30 - 17:30

a) Establishment of "standard schemes" of A+M and PSI processes required in the H-recycling and He-exhaust modelling and in the basic edge plasma diagnostics;

b) Assessment of the completness and quality of existing A+M and PSI data bases for such "standard schemes";

c) Formation of Working Groups on:

   A) Formulation of A+M + PSI data requirements for H-reccycling and He-exhaust modelling and specific edge plasma diagnostics

   B) Critical analysis of available A+M and PSI data.

FRIDAY, June 12

Session 4: **Detailed Analysis and Formulation of Data Requirements and of Recommended Data Sets**

09:00 - 12:30 Parallel Working Group Sessions:

WG-A: Meeting Room: A-07-42
Participants: Abramov, Behringer, Reiter, Ruzic, Stotler

TASK: Specification of all relevant A+M and PSI processes and related reacction characteristics required in H-reccycling and He-exhaust modelling and in the common plasma edge diagnostics; pecification of required data acccuracies for particular processes and reactions; specification of desirable data presentation formats.

WG-B: Meeting Room: A-07-43
Participants: Bacal, Botero, Janev, Schultz, Tawara

TASK: Critical analysis of the available data information; selection of best data sets; identification of important data gaps or sets of inadequate data, and suggestion of research groups for generation of required data.

12:30 - 14:00 **Lunch**

Session 4: **Review and evaluation of existing data base and selection of best available data sets**

14:00 - 15:30 **Session 4 (contd.):**

- Continuation of Working Group analyses
- Preparation of Working Group reports

15:30 - 16:00 **Coffee break**

Session 5: **Summary of the Meeting Work (Joint Session)**
Room: A-07-42

16:00 - 17:30
- Discussion of Working Group reports
- Formulation of Meeting conclusions and Reccommendations

17:30 - **Adjourn of the Meeting**

Appendix 3

Towards an elastic and momentum transfer cross section data base for 1 to 1000 eV collisions involving A^{q+} + H, H_2 and He

Summary of presentation by D.R. Schultz at IAEA Consultants' Meeting on Atomic and Molecular Data Base for Hydrogen Recycling and Helium Removal from Fusion Reactors

As the design and engineering phases of the development of ITER are entered, a greater emphasis is being placed on the physics of the edge plasma (scrape-off layer). The atomic and molecular physics concerning this regime is characterized by radically lower temperatures than those in the core plasma region, or those generally encountered in such aspects of fusion technology as neutral beam injection. Consequently, the new focus on the edge plasma demands a reappraisal of the atomic and molecular data available for plasma modelling and diagnostics.

In fact, requests to the Atomic and Molecular Data Unit of the IAEA, and the comments of modellers at the present meeting have highlighted the need for elastic and momentum transfer (diffusion) cross sections relevant to the edge plasma. Specifically, the energy regime of interest is one characteristic of the low scrape off layer temperatures, namely 1 to 1000 eV, with the greatest emphasis on the range 1 to 200 eV, and the collision systems of interest fall into two categories. Of primary interest are ion-neutral and neutral-neutral collisions between H, H_2 and He, i.e.

$$H^+ + H, H_2, He \tag{1}$$

$$He^{+,2+} + H, H_2, He \tag{2}$$

$$H, He + H_2 \tag{3}$$

and where the isotopes D and T may replace any of the atomic hydrogen components. Of secondary interest are collisions involving the major impurity ions which enter the plasma through sputtering from the wall or by injection (e.g. Li, Be, B, C, O and Fe),

$$A^{q+} + H, H_2, He \tag{4}$$

where the charge state, q, of these ions is primarily low owing to the low temperature of this region, and again the isotopes of hydrogen may be substituted. The greater immediate importance attributed to the collisions between helium and hydrogen and amongst the isotopes of atomic and molecular hydrogen reflects the fact that these are the particles which the next step fusion reactors will seek to remove from the plasma for recycling or as waste. It is therefore extremely important to model their interactions near the divertor plates and throughout the pump duct system. Data concerning the other heavier impurities present in these regions should become more important at subsequent stages of the development.

The primary quantities of interest are the total elastic cross section, Q, and the momentum transfer (diffusion) cross section, Q_D. However, since the momentum transfer cross section is given by

$$Q_D = 2\pi \int (1 - cos\theta) \frac{d\sigma^{elastic}}{d\Omega} d\Omega \tag{5}$$

where θ is the scattering angle in the center of mass, the most useful quantity would be the differential elastic scattering cross section which could be integrated to obtain both Q and Q_D. The momentum transfer cross section is a measure of the average forward momentum lost by the projectile in an elastic scattering encounter.

The goal for data compilation concerning these cross sections should be to survey the existing atomic and molecular research which is pertinent, encourage calculations to be made to fill in the gaps and finally to produce a recommended set of values. The results of a preliminary survey of the existing works has been performed at the ORNL Controlled Fusion Atomic Data Center and is summarized in the table below. Most of the data which exists concerns total elastic cross sections for collisions of H^+, He^+ and He^{2+} with H and He. Elastic differential cross sections and momentum transfer cross sections also exist for these systems but do not adequately cover the impact energy range of interest. Very few works, covering only very limited energy ranges, exist for the neutral-neutral systems, H + H_2, He + H_2. The primary conclusion of the search is therefore that the vast majority of the data required with have to be generated theoretically.

Due to the complex nature of the quantum mechanical calculations required to fully treat elastic scattering of these species at low impact energy (i.e. many molecular states and many reaction channels), some simplified models will have to be used to produce the needed cross sections. In particular, the influence of the charge transfer channel in both depleting the elastic channel and modifying the shape of the elastic differential cross section, and therefore the magnitude of the momentum transfer cross section, is a leading complication that should be treated. Figure 1 shows this influence on the momentum transfer cross section by comparing two-channel S-matrix calculations [1] including and and neglecting the charge transfer channel in C^{6+} + H collisions, as a function of impact energy. Also shown is a simple scaling (Langevin formula) based only on the polarizability of the H target. Figure 2 illustrates the relative magnitudes of the elastic, charge transfer and momentum transfer cross sections for this same system.

Thus, the conclusions of the present meeting concerning the data base relevant to hydrogen recycling and helium exhaust indicate that of primary importance is the compilation of elastic differential cross sections, and derived elastic total and momentum transfer cross sections, for 1 to 200 eV (1000 eV) collisions of H, H^+, H_2, He, He^+ and He^{2+} with H, H_2 and He (and all D and T substituted reactions as well). Secondarily, cross sections for the same processes involving impurity ion collisions with H, H_2 and He may also be important as development of the edge plasma models continues. The preliminary findings of a search of the existing literature indicate that the majority of the data of interest must be calculated and that due to the sophistication of robust models of these low energy, molecular collisions, simplified models should be useful alternatives to allow urgently needed data to be supplied in a timely fashion.

References

[1] D.R. Schultz and R.E. Olson, unpublished contribution to this meeting.

Figure Captions

Figure 1. The momentum transfer (diffusion) cross section for C^{6+} + H as a function of impact energy in the center of mass calculated using a two-channel S-matrix approximation including charge transfer, a one-channel S-matrix approximation neglecting charge transfer and the simple Langevin formula dependent only on the polaribility of H, showing the importance of treating the charge transfer channel.

Figure 2. The elastic, charge transfer and momentum transfer (diffusion) cross section as a function of impact energy in the center of mass for C^{6+} + H using a two-channel S-matrix approximation, indicating their relative magnitudes.

Preliminary evaluated status of existing data

Elastic Collisions of 1 to 1000 eV A^{q+} + H, He

Ion Species	Elastic Total Cross Section	Elastic Diff. Cross Section	Diffusion Cross Section
Hydrogen	B	F	F
Helium	B	F	F
Lithium	N	N	N
Beryllium	N	N	N
Boron	F	N	N
Carbon	F	F	N
Oxygen	F	F	N
Iron	N	N	N

A to F: decreasing amount of data available

N: no data available

TABLE 1

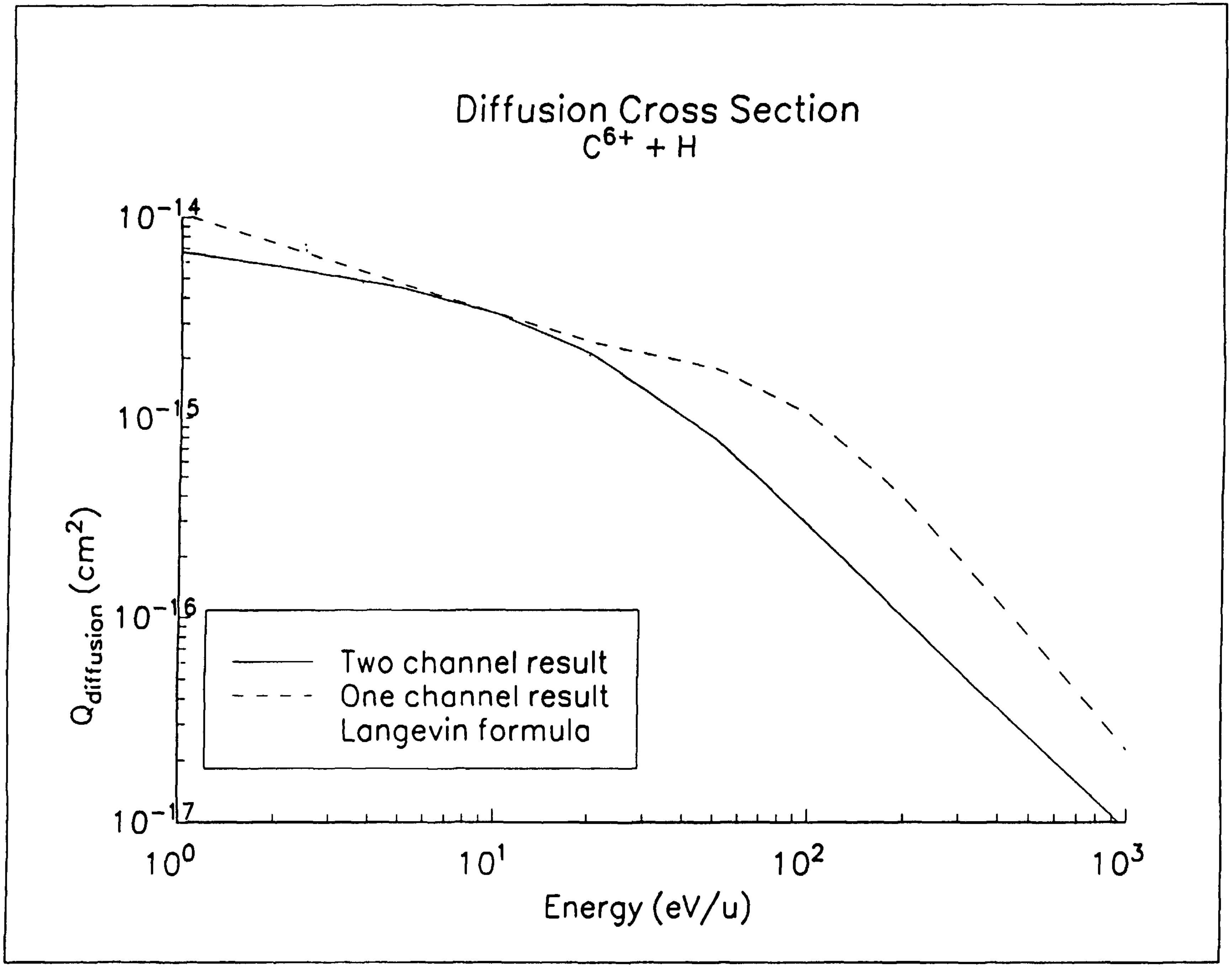
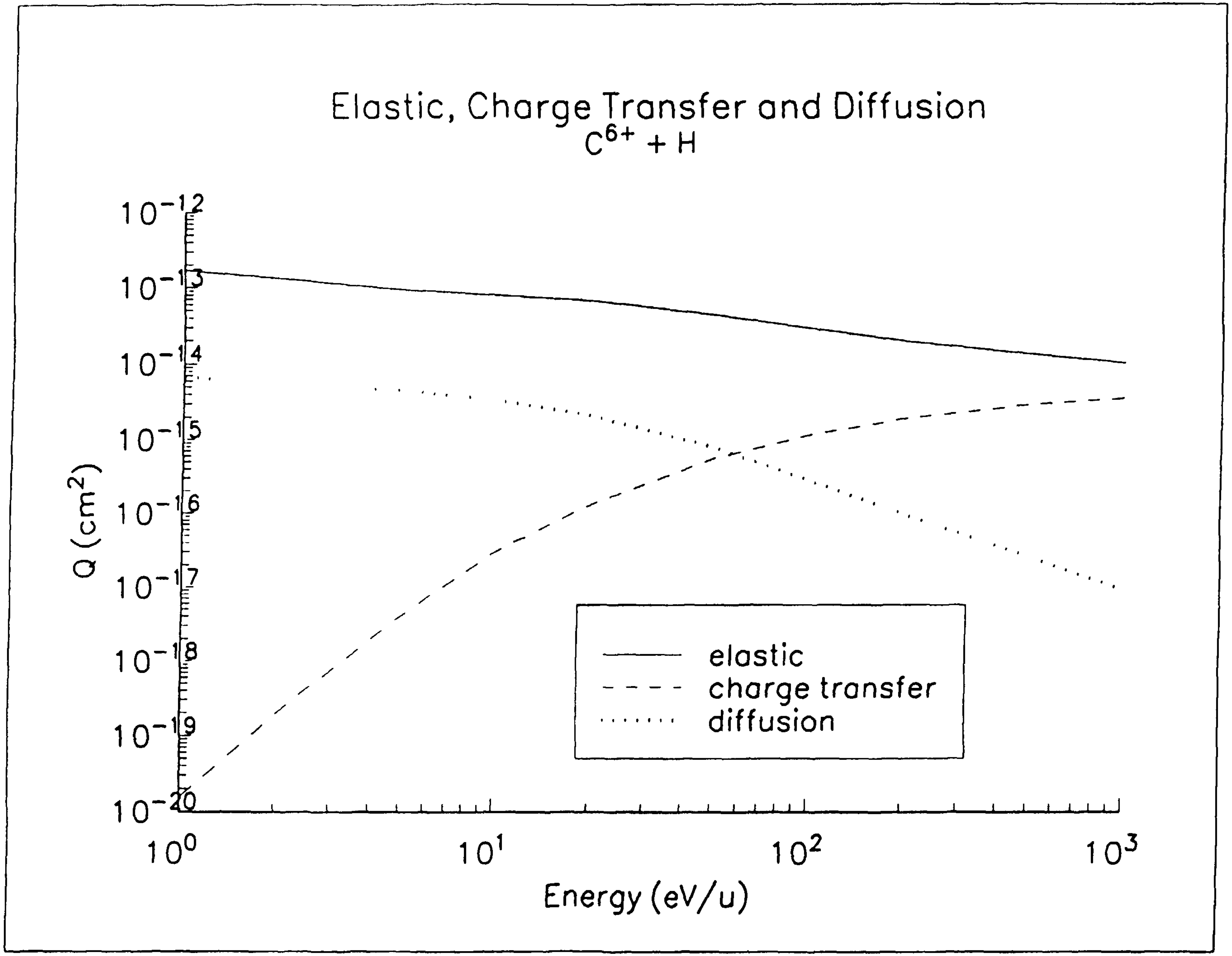

Diffusion Cross Section
C6+ + H
10−14
10−15
10−16
10−17
Qdiffusion (cm2)
10^0
10^1
10^2
10^3
Energy (eV/u)
Two channel result
One channel result
Langevin formula

FIGURE 1



Elastic, Charge Transfer and Diffusion
C^{6+} + H
10^{-12}
10^{-13}
10^{-14}
10^{-15}
10^{-16}
10^{-17}
10^{-18}
10^{-19}
10^{-20}
Q (cm^2)
10^0
10^1
10^2
10^3
Energy (eV/u)
elastic
charge transfer
diffusion

FIGURE 2