https://doi.org/10.61092/iaea.4w1d-eec2

IAEA

International Atomic Energy Agency

INDC(NDS)- 0896

Distr. LP,NE,SK

INDC International Nuclear Data Committee

The Formation and Properties of Molecules in Edge Plasmas

Summary Report of the First Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

6 – 8 December 2023

Prepared by

C. Hill

December 2023

IAEA Nuclear Data Section

Vienna International Centre, P.O. Box 100, A-1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from

https://nds.iaea.org/publications

or sent as an e-mail attachment.

Requests for hardcopy or e-mail transmittal should be directed to

NDS.Contact-Point@iaea.org

or to:

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

INDC(NDS)- 0896
Distr. LP,NE,SK

The Formation and Properties of Molecules in Edge Plasmas

Summary Report of the First Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

6 – 8 December 2023

Prepared by

C. Hill

Abstract

11 experts in the field of atomic collisional physics and edge plasma modelling for magnetic confinement fusion devices, together with IAEA Staff met from 6 – 8 December 2023 for the First Research Coordination Meeting of the IAEA Coordinated Research Project (CRP) F43027: *The Formation and Properties of Molecules in Edge Plasmas*. This report summarizes the CRP participants' workplans for the duration of the project and for its first cycle (12 – 18 months). Collaborative sub-projects were initiated in the specific areas of data needed for molecular hydrogen, boron-containing species, water-derived species in glow discharge plasmas and beryllium hydrides.

December 2023

TABLE OF CONTENTS

1. Introduction

Background and Scientific Context

Molecules are known to play an important role in the physics of the edge regions of magnetically-confined plasmas. In the detached divertor region with high recycling, the isotopologues of hydrogen molecules can be present at relatively high concentrations: these molecules will undergo a variety of processes including vibrational excitation, dissociation and ionization through collisions with other energetic plasma particles.

In addition, various other hydrogen-containing molecules form, directly or indirectly as a result of interactions of plasma particles with reactor surfaces: the impact and properties of species such as BeH and BeH^+ on, for example, impurity transport remains unquantified. Furthermore, the boronization of non-beryllium wall materials in the existing and future tokamaks leads to the requirement for data on the boron hydride species formed though plasma-wall interactions under normal operation.

The goal of this CRP is to recommend fundamental data concerning the formation, spectroscopic properties and reactions of molecular species in the boundary plasmas of magnetic-confinement fusion devices; participants will be drawn from the fusion plasma modelling community and the network of computational and experimental plasma physicists working on the calculation and measurement of the collisional and spectroscopic properties of molecules under relevant conditions of temperature and density.

More details of the CRP itself are given on the website of the Atomic and Molecular Data Unit, at https://amdis.iaea.org/meetings/edge-plasmas-rcm1/.

Organizational Context

Project 1.4.1.003 of the Agency's present Programme and Budget is concerned with provision of atomic, molecular and plasma-material interaction data for fusion energy research and other plasma applications. The Subcommittee on Atomic and Molecular Data of the International Fusion Research Council ("the Subcommittee") makes recommendations to the IAEA Nuclear Data Section as to this project. At its 22nd biennial meeting, held in June 2021, the Subcommittee discussed plans and provided recommendations for two CRP proposals for the 2022—2023 biennium. The first proposed CRP to start in 2022—2023 is CRP F43026 on "Atomic Data for Injected Impurities in Fusion Plasmas." A preparatory Consultancy Meeting was held in June 2022 and the CRP had its first Research Coordination Meeting in March 2023. More details concerning this project are available at https://amdis.iaea.org/CRP/injected-impurities.

The second CRP discussed and recommended by the Subcommittee in June 2021 is the present F43027 on "The Formation and Properties of Molecules in Edge Plasmas." The Subcommittee endorsed the plans for this CRP with the objective "[to] address fundamental data needs concerning the formation, spectroscopic properties and reactions of molecular species in the boundary plasmas of magnetic-confinement fusion devices. [The CRP] will result in the establishment of a trusted repository of evaluated data concerning the molecular species, particularly metal and nitrogen hydrides, relevant to the diagnostics and safety assessment of fusion energy reactors."

Following the the preparatory Consultancy Meeting (CM), the Head of the Atomic and Molecular Data Unit, Mr Christian Hill, formally proposed the CRP at a meeting of the IAEA Committee for Coordinated Research Activities (CCRA) on 20 June 2023. The context,

scope, objectives, outcomes and possible participation of the CRP as outlined in this report were described and discussed at this meeting and the project approved as presented, with a recommendation of considering two in-person Research Coordination Meetings (RCMs) instead of three, with the possibility of the second RCM being held virtually.

Molecular Species of Interest

Molecular Hydrogen

Interactions between the plasma and hydrogen molecules play an important role in the exhaust regions of tokamak devices. These interactions are relevant to the physics of detachment (power, momentum and particle losses) and result in excited hydrogen atoms which emit strongly, with implications for the imaging and spectroscopic diagnostics used for the understanding of physics and for real-time plasma control.

In the detached divertor condition, where plasma temperatures are lower, vibrationally-excited hydrogen molecules $H_2(v)$ contribute to plasma volume recombination and hence a reduced ion particle flux through the process known as molecular assisted recombination (MAR); the relevant chains of reactions are:

1. $H_2(v) + e^- \rightarrow H^- + H$ (dissociative attachment)

   $H^- + H^+ \rightarrow H + H$ (mutual neutralization)

2. $H_2(v) + H^+ \rightarrow H_2^+ + H$ (ion conversion)

   $H_2^+ + e^- \rightarrow H + H$ and $H_2^+ + H_2 \rightarrow H_3^+ + H$ (dissociative recombination)

Additional processes, such as molecular assisted ionization (MAI):

$$H_2^+ + e^- \rightarrow H^+ + H^+ + 2e^-$$

and molecular assisted dissociation (MAD):

$$H_2^+ + e^- \rightarrow H + H^+ + e^- \text{ and } H_2^+ + e^- \rightarrow H + H$$

are also important to the overall MAR rate.

The full range of data needed for the complete modelling of these processes will be established by this CRP and these data needs met, as far as possible, in a curated database of rates that have been validated against new collisional radiative models being developed, for example as part of the UKAEA's New Exhaust Code (NEC).

Boron Hydrides

Boronization (also called boriding) is the process of treating metal or alloy surfaces to harden them through the production of metal borides which have high wear resistance. Surface boron also acts as an oxygen getter, helping to reduce the concentration of unwanted impurities in the fusion plasma that would otherwise decrease its temperature. Should ITER move away from beryllium (which is itself an excellent getter) this issue, including processes for real-time wall-conditioning and monitoring will become more important.

Work carried out recently with the Large Helical Device (LHD) describes measurements of BH and of atomic B and notes that "BH molecules will be formed less in the gas phase, but B–H bonds are formed more on the walls. B–H bonds on the surface will desorb into the gas phase via BH_n, and dissociate quickly. Therefore, BH molecular spectroscopy can be a good

diagnostic for real time monitoring of the deposition and desorption processes near the wall surface, as CH molecular spectroscopy is."

There is a need for data to support spectroscopic measurements of BH. The basic spectroscopic data (emission lines) are available, but to interpret the spectroscopy and infer source terms (and to support "S/XB" measurements) cross sections for excitation of BH (neutral) by electron impact are needed along with the lifetime of BH (neutral) in the plasma; the most important data for this is (e, e) neutral dissociation and (e, 2e) ionization and dissociative ionization.

Beryllium Hydrides

The beryllium hydrides are of much interest for JET and ITER, but this interest will be somewhat reduced if ITER decides not to use beryllium for the main wall. Data for BeH and BeH_2 are reviewed in the meeting reports of each of the RCM of CRP F43018: *Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions*, with an extensive discussion in the report of the final RCM, https://www-nds.iaea.org/publications/indc/indc-nds-0636/ (See Section 3.2 Status of Data for Light Element Molecular Processes, Beryllium hydrides: BeH and BeH_2.) The final report for this CRP contains two contributions for the BeH molecule.

Recently electron collisions with BeH and BeH_2 were comprehensively studied by the group of Jonathan Tennyson with support from JET, and electron collisions with BeH^+ at low energy were studied in the groups of Nicolina Pop and Ioan Schneider. The corresponding rate coefficients are available in the IAEA CollisionDB database. There is further recent work from the Probst group in Innsbruck, who report calculations of total (and absolute) electron-impact ionization cross sections (EICSs) for the fusion-relevant diatomic molecular species BeH, BeN, BeO, WH, WBe, WN, WO, O_2, and N_2 by means of the Deutsch-Märk and the binary-encounter-Bethe methods in the energy range from threshold to 10 keV. The Chakrabarti Group from Scottish Church College, India, provide cross sections for electronic excitation and electron impact dissociation of BeO and BeN and their positive ions. The production of BeH and BeH_2 at walls, although of lower priority for this CRP, was recently studied at the Center for Energy Research at the University of California San Diego.

The priorities for this CRP with respect to beryllium hydrides is inventorization of spectroscopic data, recommendation of data for electron collisions with BeH and BeH_2 and their ions, and the use of data on BeH and BeH_2 in fusion plasma modelling codes.

Tungsten Hydrides

There are spectroscopic investigations of WH in fusion plasma, but the knowledge base on this and related species (WH^+, WD, etc.) is incomplete. Activities concerning WH are planned by the Tennyson group during this CRP (See Section 3). Similar to the data needs for BH, in order to support spectroscopy of WH (neutral) it of interest to have data for excitation, neutral dissociation, ionization and dissociative ionization of neutral WH by electron impact. In addition, if an atomic line of W I (neutral) is used for an erosion measurement then it is necessary to know to what extent WH breaks up through neutral W and to what extent the breakup goes via WH+ to atomic ions, bypassing the neutral atom. In the preparatory consultancy meeting for this CRP data production for electron impact processes on WH and its ion was given high priority (together with data for electron impact on BH).

OH and Water-Derived Species

The spectroscopy of OH and similar species derived from water in a glow-discharge is relevant to proposed methodologies for detecting and locating leaks in magnetic confinement fusion devices such as ITER. Although many of the relevant properties, including electron impact cross sections and rates are well-known, this CRP could usefully collect these data in one place, fill data gaps where necessary, and recommend a coherent data collection methodology for this purpose. The Ghassan group (AUB) are working with ITER on the issue of leak-detection methodologies and provision of collation of the data required is one of the objectives of this CRP.

2. Proceedings

The Research Coordination Meeting was held, in person, over 2½ days from 6 – 8 December 2023 in Room C0440 of the Vienna International Centre. The list of participants and their affiliations is given in Appendix 1 of this report; the meeting agenda forms Appendix 2. The meeting was opened by Arjan Koning, Head of the Nuclear Data Section. After introductions from the participants, the first two days consisted mostly of presentations from CRP research groups on their background and proposed Workplans (Sections 3 and 4). Abstracts for these presentations are provided in Appendix 3 of this report.

The discussion session on the morning of the final day established the scope of the coordinated research to be carried out over the 5 years of the CRP and set out the collaborative subprojects described in Section 5.

3. Work Plans for the CRP

Ghassan Antar, American University of Beirut, Lebanon

Gas or water leaks always occur in tokamaks and several weeks are often needed to determine their spatial location(s). This leads to the ejection of molecules into the vacuum chamber. Leaks are going to be even more critical and time-consuming in bigger tokamaks such as ITER or DEMO. Our goal is to determine their spatial position swiftly without the need for direct intervention on the machine.

Water, as well as air leaks inside tokamaks, contain a variety of molecules that radiate when excited. They emit parts of their electromagnetic radiation spectrum in the visible range. To detect this radiation, we propose to use a visible camera equipped with an adequate optical filter that selects pre-defined wavelengths. The selected lines, determined using spectroscopy, should enable us to detect both air and water leaks. Our goal is not only to identify medium to large leaks but also to expand the capability to small and very small leaks. This means the amount of radiation that is above the background is expected to be very small. To overcome this signal-to-noise issue, we propose to use cameras that we can set integration time and that are equipped with adequate filters and image processing tools.

This investigation will occur in several steps described below:

1. Most of the tokamaks possess a glow discharge cleaning process that allows surface cleaning of the plasma-facing components. We propose to use this glow discharge cleaning to excite the impurities atoms which can then be imaged with the camera. So the first step is to ensure that the GDC setup is operational and well-equipped with the necessary diagnostics.

We need to verify the conditions of the discharges and the parameters that can be modified to increase or decrease the plasma density. The latter needs to be detected using a Langmuir probe. The neutral pressure is detected using gauges and the types of gases present in the vacuum chamber are identified using a Residual Gas Analyzer (RGA).

2. Install the air and water leak systems. Air leak is rather straightforward, it is achieved by a Leak Valve but it needs still to be calibrated as we may use a tube that is installed at the exit of the leak valve to position the leak at a given spatial location inside the vacuum vessel. A water leak requires a water reservoir that is heated up to a constant temperature so that water remains in the gaseous phase before entering the GDC chamber.

3. Purchase and install a visible spectrometer. As mentioned above, we will try to use visible imaging as tokamaks and ITER in particular will be equipped with this type of camera. The spectrometer will be used to identify and characterize the molecules that result from the leaks via their spectrum of emission. Efforts will be made to identify the various lines and to compare them with the theory. Since the GDC can last for relatively a long time, we plan on modifying the integration time of the spectrometer and investigating the minimum time needed to clearly identify a certain set of spectral signatures. The emission spectra will be determined under different plasma conditions as well as different leak rates. Moreover, we also plan on testing the effects of adding impurities to enhance the light emission, which should allow us to detect very small leaks. The results will then serve to help identify the formation of molecules at the edge of fusion plasmas during the glow discharge cleaning phase. Moreover, we will be able to identify the set of filters that we need to install in front of the visible camera for the most accurate detection.

4. A visible camera with specifications similar to the one that would be installed on ITER will be purchased and the optical filters installed. At this phase of the project, we believe that we will be able to detect the spatial position of the leak by choosing an adequate integration time that could reveal the leak's spatial location. Given that the background light is expected to be important, adequate data processing techniques will be developed to help in the detection.

5. In tokamaks like ITER, there will be lapses dedicated to the discharges as well as lapses where glow discharges will be performed for wall cleaning. Consequently, it is important to assess the formation of molecules not only during the plasma but also during the GDC. Using our setup, we will assess the formation of the molecules, by their spectroscopic signatures as a function of time. We aim to understand the role of the GDC phase in the formation of molecules.

Dmitriy Borodin, Forschungszentrum Jülich, Germany

We plan to segregate and improve the CRM employed in the established EIRENE code, make it usable standalone as well as in other transport codes. This tool "ModCR" (Fortran) should create the system of CRM data files in the JSON format (additional formats are also considerable). The output files should be in the same format as the input files, which provides a possibility to create the pipelines for multi-step formation of the final data. The final data can then be reproduced easily at any time, for instance if the basic data is updated. Those files should flexibly incorporate the data for various species with various resolution by the internal states. In addition, the user-friendly web-based data processing tool "Ploutos" should be

further developed and provide uniform and convenient access to EIRENE reaction data, including the novelly added data. We plan to produce the set of the CRM files in the interest of this CRP project (details to be liaised with other participants), test and validate those.

1) We will provide ModCR and Ploutos with documentation distributed under the "infectious open source" EPL license (www.eirene.de/EPL), thus available worldwide for scientific use.

2) We will provide the validated set of CRM files usable by EIRENE and potentially other codes employed in this CRP.

3) We will demonstrate the standalone use of the CRM together with the data files mentioned above.

4) We will provide the ready-to-use data for fusion-related species (like H_2 and isotopomers, BeH(D, T), He, etc.) very probably condensed from the basic reaction data provided by the other CRP participants on top of the older data maintained in FZJ.

5) We plan to use some *ab initio* simulations with edge plasma packages involving EIRENE (B2.5-EIRENE known as SOLPS-ITER, EMC3-EIRENE etc.) demonstrating the usefulness of the new CRMs and extended/improved data.

6) We will also do parameter studies with standalone approach investigating or demonstrating the related effects.

7) We will analyse main uncertainty sources in the frame of both 5) and 6) simulations.

8) Flexibly consider the tracking of internal states (and solving the balance equations as ODEs) instead of treating those as Monte Carlo species.

9) We study the impact of using alternative data sources (simulation methods, data resolution, additional model assumptions done to produce the final ModCR file along the pipeline) on the final result and perform reasonability checks.

10) We can try to use the meaningful simulations by SOLPS-ITER, EMC3-EIRENE or similar packages for experiments at existing devises to validate datasets and assumption-choices from 9).

We aim in finding the optimal way of condensing the very extensive A&M data (numerous states, isotopes, processes) to the essence suitable for use in the edge plasma transport codes yet capturing the main physical effects. We plan to come up with a set of the files containing up-to-date and validated data for the fusion-related tasks to be considered in the frame of this CRM.

Kalyan Kumar Chakrabarti, Scottish Church College, India

The workplan for the duration of the project will closely follow the route proposed in the original CRP proposal.

1. The calculation of detailed collision data on two or more of the molecules/molecular ions: BH, LiH, BeH_2^+, BH+, BH_2, BH_2^+. These collision data would be in the form of cross sections/rate coefficients for the following processes (i) Elastic collision (for neutral molecules); (ii) State-to-state electronic excitations; (iii) Rotational excitations (for ions only); (iv) Electron impact dissociation; (v) Estimates dissociative electron attachment to neutral molecules.

2. The analysis and evaluation of potential energy curves for the molecules studied (to be selected from the list given above), including details of resonances and their widths as a function of internuclear distance for neutral resonances and negative ion resonances (when they exist).

Dmitry Fursa, Curtin University, Australia

Molecules play an important role in the edge regions of magnetically confined plasmas. Charged particles (electrons, positrons, protons) collisions lead to molecule excitation, ionisation, and dissociation, changing, therefore, the composition and properties of plasma. Accurate modelling of fusion plasma requires detailed information on major electron impact processes involving molecules - that is given by reaction cross sections. The major objective of this project is to provide reliable cross sections for molecules of interest for this CRP. These are mostly hydride diatomic molecules: H_2, HeH^+, LiH, LiH^+, BH, BH^+. This molecules can be effectively modelled by the MCCC method. We propose to conduct detailed studies of electron collisions with these molecules and provide an accurate set of electronic and rovibrational excitation cross sections.

During the CRP timeframe, several research projects will be conducted. The objectives of the proposed research are:

1. Detailed investigation of dissociation pathways of molecular hydrogen and its isotopologues aimed to produce dissociation cross sections for dissociation products (hydrogen atoms) in particular electronic states.

2. Detailed investigation of dissociation of the HeH^+ ion and its isotopologues.

3. Investigation of electron collisions with the LiH molecule and production of a comprehensive dataset of cross sections for elastic scattering, electronic and rovibrational excitations and dissociation. Collisions with isotopologues and LiH^+ ions will be studied.

4. Investigation of electron collisions with the BH molecule and production of a comprehensive dataset of cross sections for elastic scattering, electronic and rovibrational excitations and dissociation. Collisions with isotopologues and BH^+ ions will be studied.

For all listed objectives a set of cross sections describing the collision processes will be produced. These cross sections will be made available via the MCCC database and IAEA's CollisionDB service. Several papers describing the research results will be published.

Tomoko Kawate, National Institute for Fusion Science, Japan

To achieve high-performance plasmas, wall conditioning is essential for controlling hydrogen recycling and the amount of intrinsic impurities. Boronization is one of the popular methods of wall conditioning. Spatially resolved spectroscopic measurements of boron hydride molecules and quantitative estimation of influx of these molecules are expected to be a diagnostics of boron deposition processes at plasma-facing materials, thus, the effectiveness of boronization. On the other hand, studies on the fundamental collision processes of boron hydrides and observations of these molecules in fusion devices are very limited. The objective of the project is to derive collisional cross sections for boron hydrides and to investigate the chemical kinetics of boron series in edge plasmas in LHD, which will help to discuss the validity of wall conditioning for magnetically confined fusion reactors.

We plan to employ the Molpro and UKRMol+ codes to compute molecular structure and electron-impact excitation/ionization cross sections for boron hydride molecules. The calculated results will be applied to the edge plasmas in LHD for quantitative estimation for influx of boron hydrides. The calculated and experimental results will be of great importance for discussing the validity of wall conditioning by boronization in magnetically confined fusion reactors.

Anticipated outcomes are as follows:
1) Electron impact excitation/ionization cross sections and corresponding rates for boron hydrides;
2) Collisional-radiative modelling for boron hydrides;
3) Photon emissivity coefficients and S/XB values for boron hydrides;
5) Experimental results on influx of boron hydride molecules near plasma-facing materials in LHD;
6) Put theoretical data into the NIFS Atomic and Molecular Numerical Database, and make them publicly available.

In the first year, we examine and calculate essential molecular data and develop a collisional-radiative model for BH. A dataset of electron collisional excitation/ionization cross sections has been already calculated and published in Kawate et al. *PSST*, **32**, 085006 (2023). We also prepare and perform experiments in the 25th LHD experiment campaign scheduled for March to May 2024 to investigate BH_2 and BH^+ molecules during real-time boronization by the boron powder-dropping system with high-resolution visible spectroscopy.

In the second year, we examine and calculate essential molecular data and develop a collisional-radiative model for BH^+. The data will be published in a refereed paper and made available publicly. We also analyze the obtained data in the 25th LHD experiment campaign to derive the flux of BH_2 and BH^+ by using the molecular data calculated by the procedure above. If the quality of the obtained experimental data is not at a satisfactory level, we propose the same experiments in the 26th LHD experiment campaign scheduled in the middle of 2025.

In the third year, we examine essential molecular data and develop a collisional-radiative model for BH_2. The data will be published in a refereed paper and made available publicly. We also summarize the experimental data from the LHD plasmas and publish a paper on the chemical kinetics of the boron hydride system in edge plasmas and on the effect to the main plasmas during boronization.

Åsa Larson, Stockholm University, Sweden

We propose to perform *ab initio* quantum studies to supply accurate cross sections, reaction rates and final branching ratios. Electron scattering processes with molecular cations, such as dissociative recombination, ro-vibrational excitation/de-excitation and dissociative excitation can be studied. Also heavy particle collisions involving the same reaction complex, such as mutual neutralization in cation/anion collisions or inelastic scattering upon atom-atom scattering will be studied.

To obtain an accurate description of the highly excited states and non-adiabatic interactions involved in these scattering processes is challenging. It requires a balanced description of the Rydberg states, valence states, ion-pair states as well as the electronic resonant states. We have recently developed a method for this and applied it to H_2. [J. Hörnquist, A. E. Orel, and Å. Larson, *Phys. Rev. A*, **106**, 062821 (2022)] The goal is here to apply a similar method to some of the other molecular systems relevant in the edge plasmas.

Nicolina Pop, Politehnica University of Timișoara

1. Systematic calculations of DR, vibrational excitation (VE) and dissociative excitation (DE) cross sections and rate coefficients for electron impact on BeH^+ (and its isotopomers BeD^+ and BeT^+) by extending the incident electron energy above 2.7eV (the dissociative threshold of the ion). The domain of energy will be 2.7eV – 12eV. At energies higher than the dissociation threshold of the ion, we have to take into account the autoionization resulting into states from the continuum part of the vibrational spectrum, i.e., dissociative excitation (DE). When this process is included in our approach, the coupling between a given dissociation channel and an ionization one is extended to the continuum part of the vibrational spectrum. Numerically, this is achieved by discretizing the continuum using a Fourier-grid method, which gives at the same time, in one calculation, the full vibrational ladder. Every ionization channel built on the core 1is coupled to the further ionization channels built on the core 2. By the scaling laws will be obtained additionaly dissociative curves that will be included in all calculations.

2. Extensive calculations of DR and RVE (rovibrational excitation) cross sections for H_2^+ , D_2^+, HD^+ , NH^+, will be computed at high energy.The Maxwell rate coefficients of both rotational and vibrational transitions, and outline several important features, like isotopic, rotational and resonant effects will be provided displayed and highlighted.

Ioan Schneider, Université le Havre Normandie, France

- Advances in the simultaneous treatment of rotational effects, core-excited Rydberg effects, opening of Rydberg states for dissociation and vibrational continuum, using our method based on a stepwise version of the Multichannel Quantum Defect Theory (sw-MQDT). Application to H_2^+.
- Evaluation of non-adiabatic couplings in NeH^+.
- Cross section and rate-coefficient computations for H_2^+ and NeH^+ at low energy of the electron.
- Finalizing the presently ongoing calculations on C_2H^+ and N_2H^+, including isotopic effects, in order to prepare the approach of the NH_2 system by the method based on the R-matrix via the QUANTEMOL software and on the Multichannel Quantum Defect Theory (RM-QM-MQDT).
- Provided that the molecular structure data on BH^+ of A. Larson and A. Orel will be completed, sw-MQDT computation on electron/BH^+ collisions: cross section and reaction rates.
- Advances on state-to-state and branching ratios evaluations for H_2^+ and HD^+.
- Advances on state-to-state and branching ratios evaluations for D_2^+, and HT^+ at low energy.

- Computations on deuterated versions of NeH^+ and BH^+. Initiation of high energy calculations.

Jonathan Tennyson, University College London, UK

We will consider both the spectroscopy and electron collision properties of plasma edge molecules: focus will be on BH and LiH for spectroscopy and WH for electron collisions. Similar previous studies have been performed for BeH / BeD / BeT. Besides BH and WH we will also consider BH^+, OH and OH^+. Consideration will be given to performing similar treatments for NH and NH^+.

References

1. D. Darby-Lewis, J. Tennyson, S. N. Yurchenko and K. D. Lawson, Vibrational resolved electron impact electronic excitation of BeH, *J. Phys. B: At. Mol. Opt. Phys.* **53**, 135202 (2020).
2. T. Furtenbacher, S. T. Hegedus, J. Tennyson and A. G. Csaszar, Analysis of the measured high-resolution doublet rovibronic spectra of ^{12}CH and ^{16}OH, *Phys. Chem. Chem. Phys.* **24**, 19287 (2022).

Kevin Verhaegh, United Kingdom Atomic Energy Authority, UK

Background

Safe operation of fusion reactors hinges on resolving the power exhaust challenge, requiring effective divertor (power exhaust region) operation in a detached regime [1,2]. During detachment, the plasma temperature at the target drops below 5 eV, prompting plasma-neutral interactions, including molecular interactions, that concurrently remove power, momentum, and ions, leading to significant heat flux reductions [3-6].

Plasma-molecular interactions play pivotal roles within the divertor [7-14]. Collisions between plasmas and molecules induce energy and momentum transfer, acting as sinks for momentum and power [8-10]. These collisions also induce rovibronic excitations in molecules, further engaging with the plasma in chemical reactions that yield molecular ions, e.g., D_2^+ and $D_2^- \rightarrow D^- + D$ [7,11-16]. These ions result in strong hydrogen emission [7,13-16] and promote detachment via molecular activated recombination (MAR) [7,11-13].

These plasma-molecular interactions particularly thrive in Alternative Divertor Configurations (ADC), which leverage divertor topology to enhance detachment access such as the MAST-Upgrade Super-X divertor [8,10,12,14,17]. MAST-U combines the Super-X divertor with strong baffling, amplifying plasma-neutral interactions. This has resulted in an unprecedented impact of plasma-molecular interactions on divertor physics and emission diagnostics [12,14], which has ramifications for real-time control strategies vital for reactor safety [12,18,19].

However, present plasma-molecular interaction rates used in simulations like SOLPS-ITER and Eirene lack self-consistancy, robust provenance and accuracy [7,8,13], leading to significant discrepancies between experiments and simulations [7,13]. Additionally, understanding the vibrational distribution of D_2 molecules' driving mechanisms in tokamak divertors is inadequate [7,13], necessitating modelling efforts in 0D collisional-radiative models and transport simulations like SOLPS-ITER, contributing to uncertainties in reactor extrapolations.

Addressing these challenges is one of the aims of the New Exhaust Code (NEC) in development at UKAEA, featuring Collisional-Radiative Modelling (CRM) and exhaust simulation capabilities.

Workplan

The project's first step entails curating a comprehensive list of interaction rates while considering deeply detached conditions, supported by a bibliographic review of available rate data. In this, we will provide estimates of the parameter space where inaccuracies in the currently used fundamental data are expected to cause large uncertainties in exhaust simulations or interpretations of experimental data. This provides input to other partners in the CRP on relative priorities for fundamental generation. The fundamental data can then be included in CRMs to estimate effective rates that are used in plasma-edge simulations [13]. A first attempt will be made to propagate those uncertainties in the fundamental data to uncertainty estimates for the effective rates. Additional model uncertainties arise from no transport assumptions when generating effective rates, which will be tested in a simplified 0D CRM setup [12,20].

These effective rates can then propagated into interpretive plasma edge simulations (SOLPS-ITER and NEC) [12,13]. This allows studying the impact of the improved effective rates on the plasma solution and synthetic diagnostics. Different effective rates for the interactions that are important for plasma detachment will be tested. Extensively diagnosed test-cases will be compiled from MAST-U and potentially other divertors, serving as a benchmark for code comparison studies.

Specific objectives

Objective 1: Compilation of Experimental Data for Plasma-Molecular Interactions in Tokamak Divertors

Anticipated outcome: Curate and provide extensively diagnosed experimental datasets showcasing plasma-molecular interactions within the divertor of MAST-U, and potentially other relevant tokamaks, and their impact on the divertor state. These datasets will serve as robust test cases for validating, refining and benchmarking plasma edge simulation codes.

Objective 2: Evaluation of Effective Molecular Rates Collisional-Radiative Modelling and their impact on the divertor state through Plasma-Edge Modelling

Anticipated outcomes: Propagation of the fundamental rates into effective reaction rates through collisional-radiative modelling. How these reaction rates propagate to the divertor state will be assessed through interpretive modelling and synthetic diagnostics, which will be compared against experiments (Objective 1). A first attempt on uncertainty quantification of this process will be provided. These assessments will pinpoint areas where enhanced data or knowledge is needed to improve the accuracy of plasma-edge simulations for reactor predictions.

Objective 3: Assessment of Molecular Hydrogen Data for Interpreting Tokamak Divertor Experiments and Simulations

Anticipated outcome: Compile a comprehensive list of data requirements necessary for the accurate interpretation of tokamak divertor experimental data and plasma-edge simulations,

accounting for the complex role molecules play in deeply detached plasmas. This will include a bibliographic review of existing data relevant for the CRP. Provide estimates of the parameter space where inaccuracies in fundamental data are expected to cause large uncertainties in exhaust simulations or experimental data inferences. This provides input for other CRP partners on which improvements in fundamental data are needed to understand power exhaust.

Specific workplan items

- Perform an assessment of the molecular data (rates and reactions) included in current state-of-the-art exhaust simulations such as SOLPS-ITER
- Based on this assessment, provide short and longer-term recommendations for improved data sources
- Compile extensively diagnosed test-cases from tokamak divertors, which can serve as a benchmark for code comparison studies.
- Utilise improved data sources in CRMs to compute new effective rates in collaboration with other CRP partners
- Propagate new effective rates into plasma-exhaust codes and compare the results against compiled experimental benchmark cases.
- Investigate the sensitivity of SOLPS-ITER simulations to various plasma-molecular rates
- Perform a first attempt of uncertainty propagation to plasma-molecular interaction rates

References

[1] R. Wenninger *et al., Nucl. Fusion* 2014
[2] R. Pitts *et al., J. Nucl. Mater.*, 2013
[3] K. Verhaegh *et al., Nucl. Fusion* 2019
[4] B. Lipschultz *et al., Phys Plasmas* 1999
[5] S. Krasheninnikov *et al. J. Plasma Phys.* 2017
[6] P. Stangeby, *Plasma Phys. Control. Fusion* 2018
[7] K. Verhaegh *et al., Nucl. Fusion* 2021
[8] O. Myatra *et al., Nucl. Fusion* 2023
[9] P. Stangeby and C Sang, *Nucl. Fusion*, 2017
[10] D. Moulton *et al., Plasma Phys. Control. Fusion* 2017
[11] S. Krasheninnikov *et al., Phys. Plasmas*, 1997
[12] K. Verhaegh *et al.*, submitted to *Nucl. Fusion,* arXiv: 2304.09109.
[13] K. Verhaegh *et al.*, *Nucl. Fusion* 2023, 63 076015
[14] K. Verhaegh *et al*., *Nucl. Fusion* 2023, 63 016014
[15] K. Verhaegh *et al.*, *Nucl. Mater. Energy* 2021
[16] K. Verhaegh *et al.*, *Plasma Phys. Control. Fusion* 2021
[17] E. Havlockova *et al., Plasma Phys. Control. Fusion* 2015
[18] T. Ravensbergen *et al., Nature* 2021
[19] T. Ravensbergen *et al., Nucl. Fusion* 2020
[20] S. Kobussen. MSc Internship report, 2023

4. Work Plans to RCM2

Ghassan Antar, American University of Beirut, Lebanon

For the first year, we expect to achieve items 1 to 3 from our global objectives described above. The main goal is to detect, quantify, and characterize the molecules and their behavior in a glow-discharge plasma environment. For the experiments, we aim to use the GDC that exists at the CEA-Cadarache.

Our first task will be to have a complete design of the experiment. It is followed by identifying the hardware needed and procuring the various components.

In parallel, we will commission the GDC device and perform the necessary tests in order to ensure that it is functioning as designed. Glow discharges will be conducted with different biasing schemes and at different neutral pressures and the plasma properties will be measured as a function of the various parameters of the GDC.

After receiving the equipment dedicated to introducing air and water we need to install them and calibrate the two setups. In parallel, we will be installing the spectrometer and performing the necessary calibration.

The first set of experiments will be done using Helium plasma and argon leak to make sure that the whole system is operational. Spectroscopic measurements will be taken with and without the gas puffing in order to assess the background radiation and its dependence not only on the discharge parameters but also on time.

The second set of experiments will be done with helium plasma but with a controlled air leak. We will change the following parameters:

With all plasma and leak properties constant we will increase the spectrometer integration time in order to define the optimal time corresponding to the best signal-to-noise ratio.

For a constant leak determine the spectroscopic properties of the light emission as a function of the bias voltage and the glow discharge properties. The goal is to identify the best scenario with the highest signals.

Since the molecular population could change over time, we will conduct spectroscopic measurements as a function of time. This will reveal whether time plays a role in the type of molecules that are formed during the GDC.

At this stage, all the parameters related to the discharge are known, mainly their spectroscopic signatures. We will thus proceed with introducing the air molecules into the vacuum chamber to study their emission with respect to the background. For a constant small leak, we will investigate the minimum integration time needed to have an accurate spectrum that is above the background noise.

We will change the leak rate and determine the minimum integration needed to have a signal that is well above the noise levels. A curve should be established, which summarizes the results, for the different rays where the minimum integration time is plotted as a function of the leak rate.

A study will be made about the addition of a gas, probably argon, that could enhance the radiation coming from the air molecules. After completing the spectroscopic studies of air, we

turn to the case of a water leak where the same procedure is followed leading to a full characterization of the radiation in the visible domain in a glow-discharge plasma.

Dmitriy Borodin, Forschungszentrum Jülich, Germany

Liaise with the other CRP participants the scope of physical tasks and relevant data (species, processes) including the prioritization. Establish cooperation on this with basic data delivers (e.g. MCCC, ADAS) as well as partners in modelling (e.g. SOLPS-ITER) and validation. Identify necessary simulation cases with parameter ranges to be studied in a view of applications to both the existing experiments and upcoming ones like ITER and DEMO (for UQ).

Finalize the ModCR input (equal to output) format, demonstrate the work on part of the selected above simulations cases (starting with H_2).

Further steps: Communicate with the other CRP members on validation results as well as usage experience of the new CRMs incl. the particular datasets. Iterate the assumptions for getting the best match to experiments and general reasonability of the results.

Kalyan Kumar Chakrabarti, Scottish Church College, India

The workplan for the coming 18 months will be the following.

1. Electron collision calculations on the BH molecule will be performed and cross sections for collision processes, namely elastic scattering, state-to-state excitation and electron impact dissociation will be evaluated. Molecular states of BH and anionic resonance curves of BH^- and widths as a function of geometry would be obtained. We will also try to provide an estimate of the cross section for dissociative electron attachment to BH.

2. Calculations of electron collision with the BeH_2^+ molecular ion will be undertaken using the R-matrix method. We expect to provide cross sections for state-to-state excitations and electron impact dissociation.

Dmitry Fursa, Curtin University, Australia

The set of vibrationally resolved cross sections for molecular hydrogen (and its isotopologues) will be used to produce detailed dissociation cross sections for dissociation products in particular electronic states. This study requires a careful analysis of radiative cascades in the molecular spectrum. Most of the collision and radiative transition data are already available. A computer program modelling electronic and vibrational excitation and the radiative cascades will be produced and required cross sections for producing the dissociation products in particular electronic states will be established.

A similar research program is planned to study the dissociation of the HeH^+ ion and its isotopologues.

Target structure models for LiH, LiH^+, BH, BH^+ molecules and their isotopologues will be produced.

Electron collisions with LiH molecule will be studied and a comprehensive set of electronic and rovibrational excitation cross sections will be produced together with cross sections for elastic scattering and ionisation.

Tomoko Kawate, National Institute for Fusion Science, Japan

We examine and calculate essential molecular data and develop a collisional-radiative model for BH. A dataset of electron collisional excitation/ionization cross sections has been already calculated and published in Kawate et al. *PSST* **32**, 085006 (2023). We also prepare and perform experiments in the 25th LHD experiment campaign scheduled for March to June 2024 to investigate BH_2 and BH^+ molecules during real-time boronization by the boron powder-dropping system with high-resolution visible spectroscopy.

Åsa Larson, Stockholm University, Sweden

Workplan for the first year

- Dissociative recombination and ion-pair formation in electron collisions with H_2^+ (and its isotopologues) will be studied using the newly developed model of the H_2 reaction complex.

- Quantum chemistry structure calculations will be performed on BH using the multi-reference configuration interaction method. Fixed nuclei electron scattering calculations on BH^+ will be carried out using the Complex Kohn variational method. We will then work on extracting the "diabatic model" of the involved states.

Workplan for the second year

- Studies on Dissociative recombination of BH^+ will be carried out in collaboration with the group of Prof. I. F. Schneider and Z. Mezei using the Multi-Channel Quantum Defect theory. The process can also be studied using a coupled-channel approach.

- Heavy particle collisions such as H + B and H^- + B^+ will be studied using a log-derivative method to solve the coupled Schrödinger equation.

- Structure and electron scattering calculations will be initiated on the OH reaction complex.

Nicolina Pop, Politehnica University of Timișoara

Our previous studies of dissociative recombination, vibrational excitation and vibrational de-excitation of the BeH^+ ion, based on the MQDT method, will be extended to collision energies above the dissociation threshold, taking into account the vibrational continua of the BeH^+ ion and, consequently, its dissociative excitation. We will also significantly increased the number of dissociative states of $^2\Pi$, $^2\Sigma^+$ and $^2\Delta$ symmetry included in our cross section calculations, generating the most excited-ones by using appropriate scaling laws. Our results in terms of DR, VE, VdE and DE cross sections and rate coefficients for BeH^+ will be suitable for modeling the kinetics of BeH^+ in edge fusion plasmas for collision energies up to 12 eV.

Whereas in our previous works the energy of the incident electron was less than 2.7 eV, in this work the energy range of the incident electron is extended up to 12 eV. This means the inclusion of more than 180 ionization channels in addition to the 18 vibrational levels of the ground electronic states of the cation. We will perform a convergence study by continuously increasing the number of generated dissociative states, by imposing an overall change in the DR cross section.

Ioan Schneider, Université le Havre Normandie, France

- Finalizing and publishing the presently ongoing calculations on C_2H^+ and N_2H^+, including isotopic effects.
- Evaluation of non-adiabatic couplings in the NeH^+ system and cross section and rate-coefficient computations for electron collisions with NeH^+ at low impact energy.
- Advances in the simultaneous treatment of rotational effects, core-excited Rydberg effects, opening of Rydberg states for dissociation and vibrational continuum. Application H_2^+: cross section and rate-coefficient computations.
- Start the approach of the NH_2^+ system by the RM-QM-MQDT method.
- Provided that the molecular structure data on BH of A. Larson and A. Orel will be completed, sw-MQDT computations on BH: cross section and reaction rates.

Jonathan Tennyson, University College London, UK

1. Generate a spectroscopic model for BH suitable for modelling observed BH/BD emissions in fusion plasmas. Similar models will be generated for OH and OH^+.
2. Facilitate the the upgrade of UKRmol+/QEC to use effective core potentials (ECP) with the aim of using them in future studies.

Kevin Verhaegh, United Kingdom Atomic Energy Authority, UK

- Perform an assessment of the molecular data (rates and reactions) included in current state-of-the-art exhaust simulations such as SOLPS-ITER
- Based on this assessment, provide short and longer-term recommendations for improved data sources
- Provide post-processing tools for investigating the sensitivity of different reaction rates to simulations non self-consistently
- Start compilation of experimental benchmark cases.
- Start providing new rate calculations, based on CRM calculations, in collaboration with CRP partners.
- Start SOLPS-ITER simulations on these new rates, applied to the experimental benchmark cases.

5. Collaborative Subprojects

5.1 Data for Molecular Hydrogen

Power exhaust, whilst maintaining an acceptably high level of core performance, is a major challenge for the realization of fusion energy. Alternative Divertor Configurations (ADCs), often featuring strongly baffled divertor chambers and long divertor legs, paired with divertor detachment is a solution to the power exhaust challenge that is being investigated, and that is actively planned for SPARC, ARC and STEP. Plasma-molecular interactions can have profound impacts on detachment physics, interpretation of optical emission diagnostics and detachment control, particularly in strongly baffled ADCs. Recent work showed the importance of such processes experimentally and has shown strong contrasts between experiments and simulation results, due to inaccuracies in the hydrogen molecular data used

in exhaust simulations. Post-processing reactor-class STEP simulations with updated rate data showed that such interactions can extend to reactor designs and can impact detachment physics, detachment control and the development of diagnostics for reactors.

To address these challenges, the used rate data in plasma-edge simulations requires revision. First, an overview and assessment of currently used rate data is performed (UKAEA). Through interaction with CRP partners, recommendations are received on how this rate data can be revised (UCL, Forschungszentrum Jülich, Curtin University, Université Le Havre, Stockholm University…). This will result in a new list of fundamental data requirements for molecular hydrogen, preferably with uncertainties. This new data will be integrated with collisional-radiative modeling (Forschungzentrum Jülich, UKAEA, …) to generate new, effective, rates that can be used in exhaust simulations. Post-processing tools will be developed (UKAEA) to investigate the potential impact of such rate modifications to detachment physics and synthetic diagnostic predictions, in a range of different interpretive (for comparisons against experiments) and non-interpretive (for assessing the impact on reactor-class devices) simulations (Forschungszentrum Jülich, UKAEA, EuroFusion, …). New interpretive simulations will be performed in conditions where post-processing illustrates strong modifications, to investigate the impact of the revised rates on interpretive simulations that can be compared against experiments (UKAEA).

The outcome of this collaborative project will be an updated set of fundamental (and, self-consistent, effective rate) data for plasma-molecular interactions in divertor, together with an assessment of how these rate updates can impact detachment physics, diagnostic design and real-time control in both current day devices as well as reactors.

5.2 Data for Boron-containing species

This planned collaboration between Forschungszentrum Jülich, Germany and the National Institute for Fusion Science, Japan will aim to validate the modelling of boron-containing molecules, ions and radicals, including BH and BH^+ using data from the Large Helical Device (LHD) which has undergone boronization for wall-conditioning in several experimental campaigns. Simulations using the Edge Monte Carlo 3D code EMC3-EIRENE will be compared to experiment, with details of the activity to be established at the next RCM of this CRP, probably in late 2025. in the meantime, the groups of Stockholm and Le Havre Universities will collaborate on the theoretical evaluation of the rate coefficients for electron/ BH^+ collisions.

5.3 Data for Water-derived species in glow discharges for leak detection

The main idea that is being pursued is to spatially localize the position of air or water leaks in tokamaks based on several processes. We will be using a glow discharge plasma, thus with electron energies around 1 eV to excite the molecules and then record their radiative de-excitation. It is thus a two-step process: excitation and radiation de-excitation. Several of the reactions were already investigated in the past and some need to be simulated in the framework of this CRP.

Electrons interacting with the water molecules can lead to different processes.

1. Excitation, where the electrons and ions of the plasma glow discharge interact with the leaked gas and excite its molecules. In this case, we have interactions leading to:

(a) Higher electronic energy levels are achieved by momentum transfer:

$$e^- + H_2O \rightarrow H_2O^* + e^-,$$

followed by a de-excitation leading to a release of a photon:

$$H_2O^* \rightarrow H_2O + photon.$$

(b) Higher vibrational energy levels refer to the energy associated with the vibrational motion of the atoms within the molecule. Water has three vibrational modes: symmetric stretch, asymmetric stretch, and bend.

$$e^- + H_2O(000) \rightarrow H_2O^*(010) + e^-$$

$$e^- + H_2O(000) \rightarrow H_2O^*(100) + e^-$$

This is followed by a modification of the emission spectra.

(c) Higher rotational energy levels refer to the energy associated with the molecule's total rotational angular momentum.

$$e^- + H_2O\ (J'') \rightarrow H_2O^*\ (J' > J'') + e^-$$

They are followed by a modification of the emission spectrum.

2. Dissociation, where the water molecule is split according to

$$e^- + H_2O \rightarrow OH^* + H^* + e^-$$

which could be followed by deexcitation and the emission of a photon:

$$H^* \rightarrow H + photon$$

$$OH^* \rightarrow OH + photon$$

3. The ionization by electron impact with a threshold of about 7.4 eV:

$$e^- + H_2O \rightarrow H^+ + OH^- + e^-$$

is followed by the radiative recombination.

$$e^- + H^+ \rightarrow H^* \rightarrow H + photon$$

$$OH^- + H^+ \rightarrow H_2O^* \rightarrow H_2O + photon$$

Since we will be detecting the light emitted from the plasma-water interaction, we would want to understand the optical emission spectra in the visible range. The interaction between the experiment and the theory should help identify the processes that are taking place during a glow discharge plasma.

5.4 Data for BeX, BeX^+ (X=H, N, O) and BeH_2^+

The interests and priorities for BeH, BeH^+, BeH_2 data were laid down in the Summary Report of the Consultancy Meeting in preparation of a Coordinated Research Project on *The Formation and Properties of Molecules in Edge Plasmas*, held in IAEA Headquarters Vienna during 20 – 21 April 2023. To this we added BeH_2^+.

At the time of writing (February 2024), JET is known to be decommissioned and there are informal reports on future plans of ITER to use tungsten walls although no announcements has been made on the ITER website. This may seem to decrease the priority of the need for beryllium data. However, beryllium data is still not totally irrelevant as JET used beryllium walls and the JET data on beryllium still awaits to be analysed and is expected to be useful for future tokamaks that may use beryllium walls. Be is a neutron multiplier, so it is likely to be used in the blanket modules though of course largely protected from the erosion by plasma. Be will likely remain as a fall back solution for the case of critical issues revealed for the W wall.

Electron collision studies on BeH and BeH_2 have been undertaken by the UCL group lead by Jonathan Tennyson [1 – 3]. Electron impact ionization of a series of beryllium compounds (among others), namely BeH, BeN, BeO, were undertaken by the Innsbruck group of Probst *et al* [4]. More recently, a series of electron collision studies on BeO, BeN and BeO^+ were reported by Chakrabarti *et al* [5 – 7] giving collision cross sections for elastic scattering (for neutrals), electronic excitations, dissociation and rotational excitation (for ions). There has also been significant contribution towards dissociative recombination, vibrational excitation and de-excitation of BeH^+ and its isotopologues from the Le Havre University group of Ioan Schneider [8 – 11].

The JET and PISCES-B studies show that much of Be is released due to chemically assisted physical sputtering (CAPS). It needs certain ion energy and depends on it as well as on the surface temperature. It was shown that the surface T of about 500C leads to the full suppression of Be CAPS in JET (I. Borodkina et al., submitted to *Nuclear Fusion* in January 2024). The molecular dynamics (MD) studies indicate that also the stoichiometry (n) of released BeX_n may depend on the plasma and surface conditions [12]. Very recently those (MD) studies are continued by the A. Lasa group (Helsinki, Finland).

As stated in the Summary Report of the Consultancy Meeting, the data arising from these studies need to be inventorized, and collision cross sections need to be selected and recommended for use in fusion plasma modelling codes.

References

[1] Darby-Lewis, Daniel, Zdeněk Mašín, and Jonathan Tennyson. "R-matrix calculations of electron impact electronic excitation of BeH." Journal of Physics B: Atomic, Molecular and Optical Physics **50**, no. 17 (2017): 175201 (https://doi.org/10.1088/1361-6455/aa8161)

[2] Gupta, Dhanoj, Mi-Young Song, Heechol Choi, Deuk-Chul Kwon, K. L. Baluja, and Jonathan Tennyson. "R-matrix study for electron scattering of beryllium dihydride for fusion plasma." Journal of Physics B: Atomic, Molecular and Optical Physics **52**, no. 6 (2019): 065204 (https://doi.org/10.1088/1361-6455/aafdc4).

[3] Darby-Lewis, D., J. Tennyson, S. N. Yurchenko, and K. D. Lawson. "Vibrationally resolved electron impact electronic excitation of BeH." Journal of Physics B: Atomic, Molecular and Optical Physics **53**, no. 13 (2020): 135202 (https://doi.org/10.1088/1361-6455/ab87e9).

[4] Huber, Stefan E., Andreas Mauracher, Daniel Süß, Ivan Sukuba, Jan Urban, Dmitry Borodin, and Michael Probst. "Total and partial electron impact ionization cross sections of fusion-relevant diatomic molecules." The Journal of Chemical Physics **150**, no. 2 (2019): 024306 (https://doi.org/10.1063/1.5063767).

[5]. N. Mukherjee, K. Chakrabarti. "Theoretical study of low energy electron collisions with the BeO molecule." Journal of Physics B: Atomic, Molecular and Optical Physics **56** (2023) 015202 (https://doi.org/10.1088/1361-6455/acac56)

[6] Chakrabarti, Kalyan and Dinda Sayantan. "Calculated cross sections for electron collisions with the BeN molecule." Plasma Physics and Controlled Fusion **65** (2023) 085017 (https://doi.org/10.1088/1361-6587/ace3f3)

[7] Mukherjee Nilanjan, Bhattacharyya, Abhijit and Chakrabarti, Kalyan. "R-matrix Calculation of Electron Collision with the BeO^+ Molecular Ion.", Atoms **2024**, 12, 2. (https://doi.org/10.3390/atoms12010002)

[8] Mezei, J. Zs, S. Niyonzima, D. Backodissa, N. Pop, F. O. Waffeu Tamo, K. Chakrabarti, O. Motapon et al. "Electronic and photonic reactive collisions in edge fusion plasma and interstellar space: Application to H_2 and BeH systems." In Journal of Physics: Conference Series 576, no. 1 (2015): 012005. (https://doi.org/10.1088/1742-6596/576/1/012005).

[9] Laporta, V., K. Chakrabarti, R. Celiberto, R. K. Janev, J. Zs Mezei, S. Niyonzima, J. Tennyson, and I. F. Schneider. "Theoretical resonant electron-impact vibrational excitation, dissociative recombination and dissociative excitation cross sections of rovibrationally excited BeH + ion." Plasma Physics and Controlled Fusion 59, no. 4 (2017): 045008 (https://doi.org/10.1088/1361-6587/aa5c56).

[10] Niyonzima, S., N. Pop, F. Iacob, Å. Larson, A. E. Orel, J. Zs Mezei, K. Chakrabarti et al. "Low-energy collisions between electrons and BeD + ." Plasma Sources Science and Technology 27, no.2 (2018): 025015 (https://doi.org/10.1088/1361-6595/aaabef).

[11] Pop, N., F. Jacob, S. Niyonzima, A. Abdoulanziz, V. Laporta, D. Reiter, I. F. Schneider, J. Zs. Mezei. "Reactive collisions between electrons and BeT: Complete set of thermal rate coefficients up to 5000 K," Atomic Data. Nucl. Data Tables, **139** (2021): 101414 (https://doi.org/10.1016/j.adt.2021.101414)

[12] E. Safi, G. Valles, A. Lasa, K. Nordlund, "Multi-scale modelling to relate beryllium surface temperature, deuterium concentration and erosion in fusion reactor environment", *J. Phys. D* **50**, 204003 (2017).

Appendix 1

List of Participants

Ghassan ANTAR, American University of Beirut, Riad El-Solh, P.O. Box 11-0236, 1107 2020 BEIRUT, LEBANON

Dmitriy BORODIN, Forschungszentrum Jülich, Insititute of Energy and Climate Research, 52425 JÜLICH, GERMANY

Kalyan Kumar CHAKRABARTI, Department of Mathematics, Scottish Church College, 1 & 3 Urquart Square, 700006 KOLKATA, INDIA

DIPTI, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

FUJII Keisuke, Oak Ridge National Laboratory, One Bethel Valley Road, P. O. Box 2008, 37830-6010 OAK RIDGE, UNITED STATES OF AMERICA

Dmitry FURSA, Department of Physics and Astronomy, Curtin University, G.P.O. Box 1987 U, PERTH, WA 6845, AUSTRALIA

Kalle HEINOLA, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

Christian HILL, IAEA Division of Physical and Chemical Sciences, Nuclear Data Section, Vienna International Centre, A-1400 VIENNA, AUSTRIA

KAWATE Tomoko, National Institute for Fusion Science, 322-6 Oroshi-cho, 509-5292 TOKI, GIFU, JAPAN

Åsa LARSON, Department of Physics, Alba Nova University Centre, Stockholm University, Roslagstullsbacken 21, 106 91 STOCKHOLM, SWEDEN

Stefan MIJIN, United Kingdom Atomic Energy Authority, Culham Science Centre, ABINGDON, OX14 3DB, UK

Nicolina POP, The Polytechnic University of Timişoara, Piaţa Victoriei 2, 300006 TIMIŞOARA, ROMANIA

Ioan F. SCHNEIDER, Le Havre Normandy University, 25, rue Philippe Lebon, POB 540, 76058 LE HAVRE CEDEX, FRANCE

Jonathan TENNYSON, Department of Physics and Astronomy, University College London, Gower Street, LONDON WC1E 6BT, UNITED KINGDOM

Kevin VERHAEGH, United Kingdom Atomic Energy Authority, Culham Science Centre, ABINGDON, OX14 3DB, UK

Appendix 2

Agenda

Wednesday, 6 December 2023

10:00 – 10:30	**Arjan KONING**, **Kalle HEINOLA**, **Christian HILL** (IAEA): Meeting Opening and Welcome
10:30 – 11:00	**Dmitry FURSA**, *Faculty of Science and Engineering, Curtin University, Australia* An update on MCC calculations: molecular hydrogen, its isotopologues and beyond *[online presentation]*
11:00 – 11:30	Coffee Break
11:30 – 12:00	**Kalyan Kumar CHAKRABARTI**, *Scottish Church College, India* Electron collision studies on some molecular species in edge plasmas
12:00 – 12:30	**Jonathan TENNYSON**, *University College London, United Kingdom* Molecule physics at the edge of fusion plasmas: BH and WH
12:30 – 14:00	Lunch
14:00 – 14:30	**Åsa LARSON**, *Stockholm University, Sweden* Theoretical studies of scattering processes involving H_2 and BH reaction complexes
14:30 – 15:00	**Ioan F. SCHNEIDER**, *Université du Havre, France* Electron-induced recombination, excitation and dissociation of molecular cations in edge plasmas
15:00 – 15:30	**Nicolina POP**, *Politehnica University of Timișoara, Romania* Modeling of the kinetics of H_2^+, BeH^+, NH^+ and isotopologues at high energy of the incident electron in fusion plasmas
15:30 – 16:00	Coffee Break
16:00 – 17:00	All: Discussion and planning
19:00 – 21:00	Social Dinner: L'Asino Che Ride, Augustinerstrasse 12, 1010 Wien.

Thursday, 7 December 2023

10:00 – 10:30	**Ghassan ANTAR**, *American University of Beirut, Lebanon* Spectroscopic measurements and analyses of water and air molecules in glow plasma discharges for fusion applications
10:30 – 11:00	**Kevin VERHAEGH**, *UK Atomic Energy Authority, United Kingdom* Study of molecular hydrogen data and their impact on CRMs and exhaust simulations for detached plasmas
11:00 – 11:30	Coffee Break
11:30 – 12:00	**KAWATE Tomoko**, *National Institute for Fusion Science, Japan* Calculation and experimental studies on the formation and emission processes of boron hydride molecules
12:00 – 12:30	**Dmitriy BORODIN**, *Forschungszentrum Jülich (FZJ), Germany* Providing the flexible CRM usable standalone and inside edge transport codes including EIRENE
12:30 – 14:00	Lunch
14:00 – 14:30	**Christian HILL**, *IAEA, Austria* Atomic and Molecular Databases and Data Services at the IAEA
14:30 – 16:00	All: Discussion

Friday, 8 December 2023

10:00 – 13:00	Discussion: Workplan Summaries, potential Code Comparison and Benchmarking Activities; Meeting Close

Appendix 3

Presentation Abstracts

Molecules formation during air or water leaks in tokamaks and their behavior during glow discharges

Ghassan Antar
American University of Beirut, Lebanon

Air or water leaks occur in all tokamaks and, while it is rather easy to know that there is a leak, it remains very difficult to identify its spatial location without important loss of time and dedicated resources. This problem, which occurs on all present-day tokamaks will be even more important for future ones like ITER and DEMO because of the large vacuum vessel dimensions and the various components. Leaks may occur for a variety of reasons: Air leaks could result from the misalignment of flanges, whereas water leaks could be caused by the various cooling circuits inside the tokamak. The goal of this project is to identify the spatial location of a leak by exciting the molecules using glow discharges. Adequate characterization of the molecular spectra will allow adequate imaging in the visible domain to be developed. Glow discharges are frequently used for wall cleaning on all tokamaks where the ions bombard the vessel walls with high energy thus removing the molecules that are stuck on the surface. On the other hand, imaging inside the vacuum vessel is now done routinely for a variety of reasons using fast visible cameras. Since our goal is to investigate the spatial localization of leaks by combining adequate imaging techniques during glow discharges, we need to search for the emission spectra of molecules that are common to air and water like H_2O, H_2, O_2, and N_2 molecules. We propose to study the spectra of these molecules in a glow-discharge environment under different conditions. We will also investigate the introduction of test molecules that could enhance the light emission thus making it easier to identify the spatial position of the leak inside the vacuum vessel. The glow discharge and the impurities coming from the wall form a high level of light that could mask the signature of the leak. Specific tools need to be implemented to get the signal of the leak out of the background noise. The main outcome of this research is thus to identify the filter(s) that would be installed in front of the camera so that spatial identification can be made despite the high level of background radiation.

Providing the Flexible CRM Usable Standalone and Inside Edge Transport Codes Including EIRENE

D. Borodin, D. Harting, S. Brezinsek

Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung – Plasmaphysik, Partner of the Trilateral Euregio Cluster (TEC), 52425 Jülich

The presentation has covered the main ideas as well as motivation for the contribution proposal with the same title. It has also give a flavour of related EIRENE (and CFD-EIRENE packages) development in the frame of international TSVV-5 project based in FZ Jülich.

The presentation has demonstrated the key role the CRMs are playing in the edge-transport modelling in fusion-related plasma devices. It was demonstrated that despite only the unified by Monte-Carlo (MC) approach treatment of CRM and transport effect can possibly allow obtaining the full picture, the stand-alone CRM simulations are really useful for assembling and checking of the underlying atomic and molecular (A&M) data. It was demonstrated that tracing of highly resolved (by vibration states and isotopes at least) molecular data is necessary even for "global" parameters: ~40 % of error in effective total dissociation rate of H_2 and isotopomers if neglected. The concept of the new module "ModCR" was presented which can be used both standalone and insider the EIRENE. Moreover, it can provide a smooth transition between the particles states being tracked as separate MC species and as population variables. The latter can significantly improve performance and improve cancelation error due to the limited statistics in MC on the price of a small bias error. In addition it uses the very same JSON-based format for the CRMs allowing creating the production pipelines for the particular purpose CRMs via several intermediate stages e.g. at first just uniting all the relevant basic data. Obliviously such pipelines allow repeating all the stages automatically at necessity e.g. if the basic data is updated. The proposal suggests using this approach it systematic creation of the practice-use data in the interest of the CRP based on MCCC and R-matrix produced basic datasets allowing validation and applications requested by the other participants.

Electron Collision Studies on Some Molecular Species in Edge Plasmas

K. Chakrabarti
Department of Mathematics, Scottish Church College, India

Collision processes in plasmas play a very important role in the dynamics and in determining the characteristics of the plasma. Collision processes may lead to the formation of new species in the plasma which can not only alter plasma characteristics but also affect the dynamics. In this talk we review our recent works on the electron collision with the BeO and BeN molecules and their ions BeO+ and BeN+. Beryllium is chosen to be the plasma facing material in ITER and JET. Oxygen can enter into the edge plasma either due to presence of trace gases in the fuel or in the case of a leak which allows entry of air. Nitrogen is also often used as an injected impurity to attenuate the heat load on plasma facing components. In both cases, interaction with the wall material with oxygen and nitrogen can lead to the formation of BeO, BeN and their positive ions. We have studied electron collision with BeO, BeN, BeO^+ [1,2,3] in the framework of the R-matrix method, which is now considered as a state of the art in electron molecule collision calculations. Calculations of electron collision with BeN^+ is underway and will be reported soon.

References

1. N. Mukherjee and K. Chakrabarti, Theoretical study of low energy electron collisions with the BeO molecule, *J. Phys. B: At. Mol. Opt. Phys.* **56** (2023) 015202.

2. K. Chakrabarti and S. Dinda, Calculated cross sections for electron collisions with the BeN molecule, *Plasma Phys. Control. Fusion* **65** (2023) 085017.

3. N. Mukherjee, A. Bhattacharyya and K. Chakrabarti, R- matrix Calculation of Electron Collision
with the BeO^+ Molecular Ion, *Atoms* (2023) *Submitted*.

An update on MCC calculations: molecular hydrogen, its isotopologues and beyond

D. V. Fursa
Department of Physics and Astronomy, Curtin University, Perth, Australia

Molecular hydrogen and its isotopologues are present in a range of vibrationally excited states in fusion, atmospheric, and interstellar plasmas. Electron-impact excitation cross sections resolved in both the target's final and initial vibrational levels are required for modeling the properties and dynamics and controlling the conditions of many low-temperature plasmas. The molecular convergent close-coupling (MCCC) method has been utilised to provide a comprehensive set of accurate excitation, ionization, and grand total cross sections for electrons scattering on H_2 in the ground electronic state resolved in all initial and final vibrational levels. This dataset is currently being extended to scattering from electronically excited states and obtaining rotationally resolved cross sections. In this talk, I will review the available e-H_2 collision data and discuss their application to modeling electron impact dissociative processes for molecular hydrogen and its isotopologues. Planned application of the MCCC method to more complex molecules will be discussed.

Calculation and Experimental Studies on the Formation and Emission Processes of Boron Hydride Molecules

Tomoko Kawate
National Institute for Fusion Science, Japan

Toward real-time wall conditioning, impurity powder dropping experiments with boron powder were performed in the 22nd experimental campaign of the Large Helical Device. To examine the deposition and desorption process of boron, we focus on boron hydride (BH) molecules which presumably populate near plasma-facing components. We performed spatially-resolved spectroscopic measurements of emission by boron ions and BH molecules. From the measurement, we found that BH and B^{+} were concentrated on the divertor viewing chord, which suggest boron deposition in the divertor region. Although emissions from BH and B^{+} increased linearly, emissions by B^{0} and B^{4+} became constant after the middle of the discharge. Continuous reduction of carbon density in the core plasma was confirmed even after B^{0} and B^{4+} became constant. The results may show facilitation of impurity gettering by boron in the divertor region and thus effective real-time wall conditioning.

Aiming at the quantitative diagnostics of boron monohydryde, BH, in fusion plasmas, we present elastic, electronic excitation, and ionization cross sections of BH for the first time. The calculations were performed by the R-matrix and Binary Encounter Bethe methods utilized by Quantemol-EC software. To examine the uncertainty due to the calculation conditions, we compared the results by different basis sets and internuclear distances of the target model. We found that the uncertainties are typically within ~10%. Rate coefficients were derived and fitted to an Arrhenius function. The derived decay rate per photon, S/XB, agreed with the value presented by Lieder et al. (1994).

Theoretical studies of scattering processes involving H_2 and BH reaction complexes

Åsa Larson, Johan Hörnquist, Ann E. Orel
Department of Physics, Stockholm University, Sweden

With *ab initio* structure and electron scattering calculations on H_2, a diabatic representation of the excited bound and resonant electronic states have been developed[1]. The model allows for inclusion of an arbitrary number of Rydberg states as well as rotational couplings, autoionization and a correct treatment of non-vanishing non-adiabatic couplings. The model is used to perform quantum mechanical studies of different scattering processes involving the same set of electronic states. Total and differential cross section and branching ratios are computed for processes such as mutual neutralization[1]

$$H^+ + H^- \rightarrow H^* + H$$

associative ionization[2]

$$H^* + H \text{ (or } H^+ + H^-) \rightarrow H_2^+(v,J) + e^-$$

and dissociative recombination

$$H_2^+(v,J) + e^- \rightarrow H^* + H \text{ (or } H^+ + H^-)$$

The calculated results are compared with measurements. The processes are computed for different hydrogen isotopes and different ro-vibrational states of the molecular ion relevant for the fusion plasmas.

A similar diabatization method will be used to study processes involving the BH reaction complex. Electron structure calculations using the MRCI method have been performed to compute adiabatic potential energy curves of the excited states of BH and BH^+. The extracted effective quantum numbers are compared with quantum defects obtained from the structure calculations on BH by Petsalakis *et al*.[3] Preliminary results from electron scattering calculations using the Complex Kohn variational method was presented. Using the diabatic potentials and couplings, dissociative recombination of BH^+ will be studied using the MQDT method in collaboration with the groups of I. F. Schneider and Z. Mezei.

---

[1] J. Hörnquist, P. Hedvall, Å. Larson and A E Orel, Phys. Rev. A, **106**, 062821 (2022).

[2] J. Hörnquist et al. Phys. Rev. A, **108**, 052811 (2023).

[3] I. D. Petsalakis, G. Theodorakopoulos, Mol. Phys. 104, 103, (2006).

Modelling of the kinetics of H_2^+, BeH^+, NH^+ and isotopologues at high energy of the incident electron in fusion plasmas

Nicolina Pop
Politehnica University of Timișoara, Romania

The Multichannel Quantum Defect Theory (MQDT) has been employed in computing cross sections and Maxwell rate coefficients for electron-driven reactions involving molecular cations. These data are usefully in the modelling of the kinetics of various cold ionized media of fundamental and applied interest. Rotational and vibrational transitions (RVT) and dissociative recombination (DR) rate coefficients, an extension of our previous studies [1-2] and outline several important features, like isotopic and resonant effects are presented for H_2^+ , HD^+ and D_2^+.

For the fusion plasma edge, extensive cross sections and rate coefficients have been produced for BeH^+ [4], BeD^+ [5] and BeT^+ [6] cations. The isotopic effects demonstrates the quasi-independence of the rate coefficients on the isotopologue, if they are represented with respect to the vibrational energy of the target, at a given electron temperature. The energy of the incident electron is below the dissociative threshold, 2.7eV. New computations on extended energy/temperature range, up to 12 eV/30000 K, are ongoing.

References

1. O. Motapon N. Pop, F. Argoubi, J. Zs Mezei, M. D. Epee Epee, A. Faure, M. Telmini, J. Tennyson, and I. F. Schneider, *Phys. Rev. A* **90**, 012706(2014)
2. M. D. Epée, J. Zs Mezei, O. Motapon, N. Pop, I. F. Schneider, *MNRAS* **455**, 27(2016)
3. M. D. Epee´ Epee, O. Motapon, N. Pop et al., *MNRAS* **512**, 424–429 (2022).
4. S. Niyonzima, S. Ilie, N. Pop, et al., *Atomic Data and Nuclear Data Tables*, **115-116**, 287-308 (2017).
5. S Niyonzima, N Pop, et.al, *Plasma Sources Sci. Technol.* **27**, 025015 (2018).
6. N. Pop, et. Al., *Atomic Data and Nuclear Data Tables*, **139**, 101414 (2021).

Electron-Induced Recombination, Excitation and Dissociation of Molecular Cations in Edge Plasmas

J. Zs. Mezei, J. Boffelli, R. Hassaïne, E. Djuissi, N. Pop, F. Iacob, S. Niyonzima,M. D. Epée Epée, O. Motapon, V. Laporta, K. Chakrabarti, M. Ayouz, V. Kokoouline,J. Tennyson, F. Argoubi, M. Telmini, D. Reiter, A. Bultel, I. F. Schneider

The mechanisms driving the dynamics of the dissociative recombination of molecular cations is discussed, in the frame of a stepwise version of the Multichannel Quantum Defect Theory. It is shown that they strongly depend on the energy of the incident electron: at very low energy, very often (with notable exceptions), prominent narrow resonances are superposed on a 1/energy dependence. They are due to the resonant capture into ro-vibrationally excited Rydberg states (indirect process via closed channels). At intermediate energy, rotational effects loose relevance, and the resonances are important but less numerous, except in the case of capture into core-excited Rydberg states. And finally, above the dissociation threshold of the target cation, the narrow resonances disappear, but the autoinization of the dissociative states (more and more numerous) results not only in vibrational (de-)excitation, but also in dissociative excitation. Examples are given for electron collisions with H_2^+, BeH^+, ArH^+ and their isotopologues, as well as for N_2^+.

An alternative MQDT approach, based on the use of the R-matrix theory via the package Quantemol, has been employed for the study of diatomic and triatomic systems - in collaboration with University of Central Florida and CentralSupélec Paris Saclay, and we illustrate this for CF^+, N_2H^+, C_2H^+, CH_2^+ .

The perspectives of advancement are finally given.

Molecule physics at the edge of fusion plasmas: BH and WH

Jonathan Tennyson
Department of Physics and Astronomy, University College London, UK

Previous studies of molecules resulting from plasma facing surfaces have considered BeH. Vibrationally resolved electron impact electronic excitation cross sections were computed for BeH, BeD and BeT which are available in CollisionDB. A spectroscopic model was developed for all 3 isotopologues which gave excellent agreement with spectra observed in plasma experiments. For BH electron impact excitation cross sections are available from Kawate et al (2023 *Plasma Sources Sci. Technol.* **32** 085006) so we are building a corresponding spectroscopic model. Future work will consider WH for which it will be necessary to implement effective core potentials (ECPs) in the *R*-matrix scattering programs (work in progress) and for which there are plasma observations of emission spectra but rather sparse laboratory data.

Study of Molecular Hydrogen Data and Their Impact on CRMs and Exhaust Simulations for Detached Plasmas

K. Verhaegh, S. Mijin, D. Moulton, et al.

United Kingdom Atomic Energy Agency, UK

Divertor detachment is a key requirement for mitigating the target heat loads to develop fusion reactors in magnetic confinement devices. Plasma-molecular chemistry can play a key role in reducing the target particle loads, a key feature of plasma detachment, as well as power exhaust [1,2,3]. This arises from vibrationally excited molecules undergoing interactions with the plasma, forming molecular ions (D_2^+ and $D_2^- \rightarrow D^- + D$), which interact with the plasma – leading to power losses, particle losses, additional dissociation channels as well as hydrogenic emission, impacting diagnostic measurements. Such interactions have been shown to be relevant for reactors [4], particularly for tightly baffled alternative divertor designs that are employed in the STEP [5] and SPARC [6] reactor designs.

The work focuses on understanding plasma-molecular interactions in tokamak divertors, particularly regarding the impact of molecular hydrogen on plasma detachment. The project aims achieve this by first compiling experimental data from tokamak divertors for investigating plasma-molecular interactions, which can be used for benchmarking interpretive simulations. Secondly, molecular rates will be evaluated through collisional-radiative modelling and their impact on the divertor state will be investigated through plasma-edge modelling. Thirdly, the combination of the first and second point enables an assessment of the molecular hydrogen data requirements for interpreting tokamak divertor experiments and simulations.

The goal is to enhance the accuracy of exhaust simulations and reactor designs by improving the understanding and modelling of plasma-molecular interactions. This includes addressing the underestimation of molecular charge exchange in current simulations [1,4] and evaluating the impact of various rates on power exhaust physics, diagnostic analysis, and detachment control strategies.

References

1) Verhaegh, *et al*. 2021, *Nucl. Fusion*
2) Verhaegh, *et al*. 2021, *Nucl. Mater. Energy*
3) Verhaegh, *et al*. 2023, *Nucl. Fusion* **63**, 126023
4) Verhaegh, *et al*. 2023, IAEA FEC 2023, ArXiV, 2311:08580
5) Osawa, *et al*. 2023, *Nucl. Fusion*
6) Kuang, *et al*. 2020, *Journal of Plasma Physics*
7) Verhaegh, et al. 2023, *Nucl. Fusion* **63**, 076015

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

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600-21725
Web: http://nds.iaea.org