Issues with CR- and plasma chemistry modelling for fusion boundary plasmas

Detlev Reiter

25<sup>th</sup> Technical Meeting of the International Atomic and Molecular Data Centre Network (DCN)
IAEA’s Headquarters in Vienna, Austria, from 30 September to 2 October 2019
Detlev Reiter, personal notes:

- Representing Forschungszentrum Jülich in DCN: 2011-2017
- March 2019: Retired from FZ Jülich
- From September 2019:
  Member of ISFN (ITER scientific fellowship network, representing: Heinrich Heine University Düsseldorf, Germany
- Email: reiterd@uni-duesseldorf.de
Tasks in ISFN related to AMS data:

- Radiation transfer: photo-excitation, photo-ionization, photo-dissociation, line broadening
  bidirectional reflectance functions (BDRF)
- Chemical kinetics $\rightarrow$ physical kinetics, e.g. NH$_x$, BeH$_x$ systems
- $(p + e) + H_2$: isotopic effects ($H_2$, $D_2$, $T_2$, HD, HT, DT, and their ions)
  ("on the fly" CR codes embedded in transport models)
IAEA and ITER
Even closer cooperation

Under Practical Arrangements signed in June, the International Atomic Energy Agency and the ITER Organization will be expanding and deepening a long history of cooperation.
The International Atomic Energy Agency (IAEA) fosters international collaboration and coordination to help close the existing gaps in physics, technology and regulation and move forward in developing the peaceful use of fusion energy. The IAEA's activities in this field cover, among others, plasma physics and fusion power, technologies and material, both for magnetic and inertial fusion. The Fusion Portal is dedicated to all these activities, ranging from Conferences, Coordinated Research Projects, Meetings, Workshops and Schools, to providing News Media and Publications related to these projects.

News story

- A history of fusion research and development: Part two
- Pathways to Energy from Inertial Fusion: Materials beyond Ignition – CRP F13016 Successfully Completed
List of the main elements relevant to the ITER plasma

Courtesy: S. Lisgo, 2018
List of the main elements relevant to the ITER plasma

Courtesy: S. Lisgo, 2018
List of the main elements relevant to the ITER plasma

Courtesy: S. Lisgo, 2018
List of the main elements relevant to the ITER plasma

Fe (SS)
Be
C/W
W

Courtesy: S. Lisgo, 2018
List of the main elements relevant to the ITER plasma

- Be
- W
- Fe (SS)
- CORE
- C/W

Courtesy: S. Lisgo, 2018
List of the main elements relevant to the ITER plasma

- Be
- W
- C/W
- Fe (SS)
- H/D/T, He
- CORE

Courtesy: S. Lisgo, 2018
List of the main elements relevant to the ITER plasma

Fe (SS)

N, Ne, Ar

H/D/T, He

CORE

Fe/SS, 2011: armour at diagnostics port plugs
C, in 2013: replaced by all W divertor
But:
C in: W7X (2016), JT-60SA (2019),...
MOLECULAR PROCESSES CONSIDERED IN FUSION:

- $e,p + H_2(v_i) \rightarrow \ldots$, $e+H_2^+(v_i) \rightarrow H + H^*$ divertor detachment dynamics,
- $e, p + C_xH_y \rightarrow \ldots$, $e+C_xH_y^+ \rightarrow \ldots$ C erosion and migration, tritium retention, 
  Excited states of products (CH(A→X))
- $e+H_3^+(v3) \rightarrow \ldots$, DR, DE, \ldots $H_3^+$ probably irrelevant in fusion plasmas
- $e+ BeH/BeH^+ \rightarrow \ldots$ possible role on spectroscopy and on material migration:
  Formation rates ?? 10% of Be sputtering? Volumetric particle exchange reactions?
  Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre, J. Tennyson et al. (Quantemol), R. Celiberto et al. (Bari)
  Multiple aspects solved, but data scattered in literature, not jet compiled into a single comprehensive database.
- $e+ N_2$, $N_2^+ \rightarrow \ldots$ $N_2$-seeding, plasma cooling: Ammonia formation. So far mostly: only resulting atomic ions $N$, $N^+$, $N^{++}$, 
  but first plasma chemistry databases emerge
  See planetary atmospheric entries research, e.g. A. Bultel et al, Universite de Rouen, France
MOLECULAR PROCESSES CONSIDERED IN FUSION:

- $e,p + C_xH_y \rightarrow \ldots$, $e+C_xH_y^+ \rightarrow \ldots$ C erosion and migration, tritium retention,\ldots

Excited states of products ($CH(A \rightarrow X)$) ?


Fusion had not progressed very far until carbon based plasma facing components were used (mid eighties of last century).

Mostly studied then: atomic C spectroscopy and transport, little interest in carbon containing molecules, initially.

This changed in the years following 1997: the tritium experiments at JET
The tritium retention issue:

On JET, operated with tritium (1997), the tritium inventory built up without saturation limit.

Extrapolation to ITER: the permitted in-vessel T inventory, 0.7 kg, could be reached in 100 shots.
Carbon re-deposition, tritium co-deposition in JET

**Location of tritium in JET vessel during the post-DTE1 shutdown**

*The location of the deposition is surprising: only a few mgs were found on typical tiles, but 520 mg were vacuumed up from the cooled, out-of-sight louvers, suggesting up to 3200 mg also that have fallen through to the vessel floor.*

Predictions of fuel retention in ITER
fuel retention in C versus W

Data derived from empirical results obtained at AUG, JET and PISCES and modelling of erosion & re-deposition

Conclusion:
Fuel retention with carbon divertor is unacceptably large

Because of T-retention and migration, Carbon was removed from ITER design in 2013. I.e. the material we knew most about in fusion, and the most forgiving material too (does not melt), was removed.

This puts BeH, BeH$_2$ into focus, wrt. its tritium issues:
- Transport modelling of pathways
- Spectroscopical wall erosion rate quantification

And: Ammonia (NHx) formation in remote subdivertor region, vacuum system, in case of divertor plasma N-cooling

Fe/SS, 2011: armour at diagnostics port plugs
C, in 2013: replaced by all W divertor $\rightarrow$ N, Ne, Ar cooling?
But:
C in: W7X (2016), JT-60SA (2019),…
Release (chem. sputtering) and migration + fragmentation of hydrocarbons

Incoming flux (D⁺, C⁴⁺, O⁵⁺) reflected and eroded particles reflected and eroded particles

Deposition

Re-deposition

To remote areas….

toroidal/ poloidal direction

Courtesy: A. Kirschner, FZ Jülich
C\textsubscript{x}H\textsubscript{y} as a role model for other Hydrides (Be\textsubscript{x}H\textsubscript{y}, NH\textsubscript{x}, HeH\textsuperscript{+},….systems?)

- Already done SiH\textsubscript{y}: Janev, Reiter, Contr. Plasma Physics, 2003,43,401-417

**Chemistry**


Comprehensive set. Cross sections already, but universal fit expression for all types of processes \rightarrow poor asymptotic behaviour

**Physics**


Classification of processes, Asympt. correct fits, separate form for each category of reactions

1987

2002-2004

2012

Plasma chemical rate constants (Arrhenius form) for well stirred, equilibrium, low T conditions

Extensions, evaluations, new exp. and theor. results

APID 16, IAEA AMD unit

[Image of a book cover with the text: "Atmospheric Plasma Interaction Data for Fusion, Volume 15"]
Release (chem. sputtering) and migration + fragmentation of hydrocarbons

- Incoming flux: \( D^+, C^{4+}, O^{5+} \)
- Reflected and eroded particles
- Reflected and eroded particles
- Deposition
- Re-deposition
- Remote areas

Main plasma

Toroidal/poloidal direction

Target-surface
Release (sputtering, volumetric formation/fragmentation) and migration + fragmentation of **beryllium hydrides**

- **Target-surface**
  - **Radial direction**
  - **E** deposition

- **Main plasma**
  - **Radial direction**
  - **B** reflected and eroded particles
  - **Be\textsuperscript{x+}, Be\textsubscript{H\textsubscript{y}}, Be\textsubscript{0}, Be\textsubscript{H\textsubscript{y}0, +}**

- **Reflection and eroded particles**

- **Re-deposition**
  - **To remote areas**
MOLECULAR PROCESSES CONSIDERED IN FUSION:

- $e^+ \text{BeH/BeH}^+ \rightarrow \ldots$. possible role on spectroscopy and on material migration:

Formation rates ?? 10% of Be sputtering? Volumetric particle exchange reactions?

Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre, J. Tennyson et al. (Quantemol), R. Celiberto et al. (Bari)

Multiple aspects solved, but data scattered in literature, not jet compiled into a single comprehensive database.

IAEA Consultancy Meeting, June 2019: review of data status
Available (2019): CR matrix for the Be – BeH$_y$ system in a bath of electrons, protons

<table>
<thead>
<tr>
<th>Educt</th>
<th>H,H$_2$,H$_2^+$</th>
<th>Be</th>
<th>Be$^*$</th>
<th>Be$^+$</th>
<th>BeH</th>
<th>BeH$^*$</th>
<th>BeH$^+$</th>
<th>BeH$^{+*}$</th>
<th>BeH$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>e,H,H$^+$,H$^-$</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be</td>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be$^*$</td>
<td></td>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be$^+$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH$^*$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH$^+$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH$_2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- [7] Ballance 2003; and Bartschat 2016; and Dipti, 2018, ADNDT
- [5] Schneider 2017, 2018
- [6] Laporta 2017
- [9] Celiberto 2013
- [10] Tennyson 2017

- [8] Celiberto 2012; and Tennyson 2012

- Sawada 2016
- Wünderlich 2016
- Janev-Reiter 2013
- Janev 2011, GBB, BB
- "if you must guess", www.hydkin.de

Legend:
- DE: Janev 2011 BB
- DR, DE: IAEA intern. validated dataset
- excitation: Particle exchange: volumetric formation ??
- ionisation: Janev 2011, GBB
- excitation:
Issues:

Many individual data now, spread all over the place.

- Overlapping energy range, temperature range?
- Resolution wrt. vibr., rot., electr. states within each block?
- Detailed balance?
- Near threshold and asymptotic behaviour of cross sections, and rate coefficients?
- Reaction kinetics (KER: kinetic energy releases), branching ratios?
- Heavy particle collisions: particle exchange – charge exchange
- Surface processes: formation of BeH$_y$?
Experiments (fusion relevant)

2008 Plasma Phys. Control. Fusion 50 125007 (PISCES Be, BeH, exp.)

[2] Brezinsek S, Stamp M F et al., 2014, Nucl. Fusion 54 103001 (11pp) and:
Brezinsek S, Widdowson A et al., 2015 Nucl. Fusion 55 063021 (JET, Be wall: exp.)


Codes (fusion relevant)

www.hydkin.de (2011 -2017) and:

2009 Phys. Rev. A 80 012501 (BeH+, DR)

Niyonzima S, ..., Schneider I et al 2018 Plasma Sources Science and Technology (BeD+, calc.)

[6] Laporta V et al
2017 Plasma Phys. Control. Fusion 59 045008 (BeH+, calc.)

and: Zatsarinny, O, Bartschat K et al, 2016, Journal of Physics B: Atomic, Molecular and Optical Physics: 49 235701

Chakrabarti K, Tennyson J 2012 Eur. Phys. J.D 66, 31 (BeH+, X to A,B; calc.)

2013 Plasma Sources Sci. Technol. 22 015008 (BeH, X to A, calc.)

[10] Darby-Lewis D, Mašín Z and Tennyson J

Collision data

Data usage in fusion is now far behind the data availability

Next steps:
• Data processing
• Data evaluation
• Data implementation
Collision data, cont.


Spectroscopic data preliminary, not nearly complete….: tbd (DR)


http://dx.doi.org/10.1088/0741-3335/40/3/002 (BeD)

http://dx.doi.org/10.1006/jmsp.1996.7153 (BeH+)

….. and more ?
The computational plasma boundary science challenge
In most applications of A&M data in low temperature plasma chemistry:

\[
\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot (n_i \vec{V}_i) \approx \frac{n_i}{\tau} = S_{ni}
\]

Plasma transport: known

Well stirred conditions,
Near equilibrium, homogeneous, isotropy

A&M unknown

In magnetically confined fusion plasmas:

\[
\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot (n_i \vec{V}_i) = S_{ni}
\]

Plasma transport: unknown

Anomalous transport
Drifts, electrical currents,
Kinetic corrections

known

“If we are confident in a plasma state, then we can quantify A&M processes in it”.

If we are confident in a plasma state, then we can quantify A&M processes in it.”
Plasma boundary equations: ("transport approx.")

Particle conservation:
\[
\frac{\partial n_i}{\partial t} + \nabla \cdot \left( n_i \mathbf{V}_i^{\text{eff}} \right) = \mathbf{S}_i^n
\]
where \( \mathbf{V}_i^{\text{eff}} = \mathbf{V}_i || \mathbf{b} + \frac{c}{B} \mathbf{b} \times \nabla \varphi + \frac{cT_i}{Z_i e} \nabla \times \left( \frac{\mathbf{b}}{B} \right) - \frac{D_{an}}{n_i} \nabla \perp n_i \)

Parallel momentum conservation:
\[
m_i \frac{\partial n_i V_{i||}}{\partial t} + \nabla \cdot \left( \left( m_i n_i \mathbf{V}_i^{\text{eff}} \right) V_{i||} \right) = -\mathbf{b} \cdot \nabla p_i + Z_i e n_i \mathbf{b} \cdot \nabla \varphi - \mathbf{b} \cdot \nabla \Pi_{i||} + \frac{3}{2} \frac{(\mathbf{b} \cdot \nabla B)}{B} \Pi_{i||} + \nabla \cdot \left( \eta_2 \nabla V_{i||} \right)
\]
\[
\mathbf{S}_{i||} + F_{i||}
\]

Charge conservation:
\[
\nabla \cdot \left( \mathbf{J}^{\text{eff}} \right) = 0 \quad \text{where} \quad \mathbf{J}^{\text{eff}} = J_{i||} \mathbf{b} + c p \nabla \times \left( \frac{\mathbf{b}}{B} \right) + J_{i \perp} \nabla \varphi + \sigma_{an} \nabla \varphi
\]
\[
J_{i||} = \sigma_{i||} \left[ \frac{e}{n_e} \nabla \parallel p_e + \frac{\kappa_{i1}^2}{\kappa_{i2}} \nabla \parallel T_e \right] - \nabla \parallel \varphi
\]

Energy conservation:
\[
\frac{3}{2} \frac{\partial p_i}{\partial t} + \nabla \cdot \mathbf{q}_i^{\text{eff}} = \mathbf{V}_i \cdot \nabla p_i - \Pi_i : \nabla \mathbf{V}_i - \mathbf{Q}_i,
\]
where \( \mathbf{q}_i^{\text{eff}} = -\kappa_{i\parallel} \nabla \parallel T_i - \kappa_{i\perp} \nabla \perp T_i - \chi_{an} n_i \nabla T_i + \frac{5}{2} p_i \mathbf{V}_i^{\text{eff}} \)

\[
\frac{3}{2} \frac{\partial p_e}{\partial t} + \nabla \cdot \mathbf{q}_e^{\text{eff}} = \mathbf{V}_e \cdot \nabla p_e - \mathbf{Q}_e
\]
where \( \mathbf{q}_e^{\text{eff}} = \frac{\kappa_{11}^2}{\kappa_{12}} \left( \frac{T_e}{e} J_{i||} \mathbf{b} - \kappa_{12} \nabla \parallel T_e - \kappa_{11} \nabla \perp T_e - \chi_{an} n_e \nabla T_e + \frac{3}{2} \frac{T_e}{m_e c^2 \tau_e} \nabla \perp p_e + \frac{5}{2} p_e \mathbf{V}_e^{\text{eff}} \right) \)
The generic equation, for all A&M effects „S“ in plasma (or in any other given inhomogeneous medium):

„Boltzmann (linear) transport equation“, solved with conventional Monte Carlo transport codes. In fusion: e.g. EIRENE code, DEGAS-2, NEUT2, etc

\[
\frac{1}{v} \frac{\partial \phi(r, \Omega, E, t)}{\partial t} + \Omega \cdot \nabla \phi(r, \Omega, E, t) + \Sigma(r, E, t) \phi(r, \Omega, E, t) = \int \int \Sigma(r', \Omega', E') \to r, \Omega, E) \phi(r', \Omega', E', t) d\Omega' dE' + Q,
\]

**Neutrons**: nuclear science and engineering → linear, or nonlinear: MC - T- H (e.g.: MCNP)

**Radiation**: astro and laser physics → linear, or nonlinear: MC – temp. fields

**Neutrinos**:

**Electrons**: solid state physics applications

**Neutral atoms/molecules**: magnetic fusion → linear, or nonlinear: MC – plasma (transport) dynamics

And many more….
Here go the data (e.g. nuclear data) 
In fusion: AM&S data 
\[ \frac{1}{v} \frac{\partial \phi(r, \Omega, E, t)}{\partial t} + \Omega \nabla \phi(r, \Omega, E, t) + \Sigma(r, E, t)\phi(r, \Omega, E, t) \]

= \int \int \Sigma(r', \Omega', E') \rightarrow r, \Omega, E \phi(r', \Omega', E', t) d\Omega' dE' + Q,

Neutrons: nuclear science and engineering \rightarrow linear, or nonlinear: MC - T- H 
Radiation: astro and laser physics \rightarrow linear, or nonlinear: MC – temp. fields 
Neutrinos: 
Electrons: solid state physics applications 
Neutral atoms/molecules: magnetic fusion \rightarrow linear, or nonlinear: MC – plasma (transport) dynamics 

And many more....
Ludwig Boltzmann: \( S = k \log W \)

Vienna Central Cemetery, May 2019
Starting from Boltzmann:
Constructing transport models for gases and plasmas
(classical Chapman-Enskog-method, Grad-method, 1930 - 1960
both: series expansions near a Maxwellian distribution)

For a given collision process, cross section \( \sigma(E) \)

Find „collision integrals“

\[
Q^l(T) = \int_{E_{th}}^{\infty} dE \sigma(E) E^l f_{maxw}(E, T), \quad l \geq 1
\]

From those: transport coefficients (viscosity, thermal conductivity)
or source rates \( S, Q \) from particles, momentum and energy

e.g. \( l=1 \): (Maxw. reaction rate coefficient \( k(T) \))
PLASMA CHEMISTRY DATABASES: FAR SOL, SUB-DIVERTOR

C\textsubscript{x}H\textsubscript{y} as a role model for other Hydrides (Be\textsubscript{x}H\textsubscript{y}, NH\textsubscript{x}, HeH\textsuperscript{+},…..systems?)
- Already done SiH\textsubscript{y}: Janev, Reiter, Contr. Plasma Physics, 2003,43,401-417

<table>
<thead>
<tr>
<th>Chemistry</th>
<th>Physics</th>
</tr>
</thead>
<tbody>
<tr>
<td>1987</td>
<td></td>
</tr>
<tr>
<td>Plasma chemical rate constants (Arrhenius form) for well stirred, equilibrium, low T conditions</td>
<td>Classification of processes, Asympt. correct fits, separate form for each category of reactions</td>
</tr>
</tbody>
</table>

Extensions, evaluations, new exp. and theor. results

2002-2004

APID 16, IAEA AMD unit

Plasma chemical rate constants (Arrhenius form) for well stirred, equilibrium, low T conditions

Comprehensive set. Cross sections already, but universal fit expression for all types of processes \rightarrow poor asymptotic behaviour
# Plasmas Chemistry Databases (Rate Constants)

- **$N_xH_y$** (Nitrogen, Ammonia)

## Chemistry

<table>
<thead>
<tr>
<th>Year</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>2017</td>
<td>Plasma chemical rate constants (Arrhenius) for well stirred, equilibrium, low T conditions</td>
</tr>
<tr>
<td>2017</td>
<td>ITER database, distributed with SOLPS</td>
</tr>
<tr>
<td>2018</td>
<td>0D plasma chemical model, incl. experimental tests, at MAGPIE plasma device, conclusions also about surface mechanisms</td>
</tr>
</tbody>
</table>

## Physics

- If upgrading from 0D reaction kinetics $\rightarrow$ 2D or 3D transport formulations needed ??:
  - Turn this info into comprehensive cross section database, e.g. as in 2002-2004 hydrocarbon database

## Evaluation, Recommended data set
- APID xxx ??, IAEA AMD unit
Transport collision integrals for Arrhenius rates:

- Rate coeff.: 
  \[ K(T) = k' T^\alpha e^{-E_{th}/kT} = k_0 \beta^{-\alpha} e^{-E_{th} \beta} \]
  Well stirred, low T, near equilibrium (not in fusion plasmas)

- Reconstructing cross section from it:

\[ \alpha = -3/2 : \quad \sigma(E) = k_0 \sqrt{\pi \mu / 8} \cdot \frac{\delta(E - E_{th})}{E} \]

\[ \alpha > -3/2 : \quad \sigma(E) = k_0 \sqrt{\pi \mu / 8} \frac{1}{\Gamma(\alpha + 3/2)} \cdot \frac{(E - E_{th})^{\alpha + 1/2}}{E} \]

\[ \Rightarrow Q^l(T) = \int_{E_{th}}^{\infty} dE \sigma(E) E^l f_{maxw}(E,T), \quad l \geq 1 \]

\[ \Rightarrow \text{consistent transport model} \]

E: COM collision energy, \(\mu\): reduced mass
MOLECULAR PROCESSES CONSIDERED IN FUSION:

- $e_p + H_2(v_i) \rightarrow \ldots$, $e + H_2^+(v_i) \rightarrow H + H^*$
  - divertor detachment dynamics,


$e + H_2^+(v)$: Int. Conference series: Dissociative Recombination 1-9 (1988-2012)
**Available (2019): CR matrix for the Be – BeH_y system in a bath of electrons, protons**

<table>
<thead>
<tr>
<th>Educt</th>
<th>H, H_2, H_2^+</th>
<th>Be</th>
<th>Be*</th>
<th>Be^+</th>
<th>BeH</th>
<th>BeH*</th>
<th>BeH^+</th>
<th>BeH^+*</th>
<th>BeH_2…</th>
</tr>
</thead>
<tbody>
<tr>
<td>e, H, H^+, H^-</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be</td>
<td>X</td>
<td></td>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be*</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be^+</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH^+</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH^+*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH_2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**IAEA intern. validated dataset**

DE: Janev 2011 BB

DR, DE

**Excitation**

[7] Ballance 2003; and Bartschat 2016; and Dipti, 2018, ADNDT

[5] Schneider 2017, 2018


[6] Laporta 2017

Sawada 2016

Wünderlich 2016

Jänov-Reiter 2013

Janev 2011, GBB, BB „If you must guess“, www.hydkin.de

[8] Celiberto 2012; and Tennyson 2012


[10] Tennyson 2017

Particle exchange: volumetric formation ??

Ionisation Janev 2011, GBB
Available (2019): CR matrix for the Be – BeH$_y$ system in a bath of electrons, protons

<table>
<thead>
<tr>
<th>Educt</th>
<th>H, H$_2$, H$_2^+$</th>
<th>Be</th>
<th>Be*</th>
<th>Be+</th>
<th>BeH</th>
<th>BeH*</th>
<th>BeH+</th>
<th>BeH+*</th>
<th>BeH$_2$…</th>
</tr>
</thead>
<tbody>
<tr>
<td>e, H, H+, H^-</td>
<td>H, H$_2$, H$_2^+$</td>
<td>Be</td>
<td>Be*</td>
<td>Be+</td>
<td>BeH</td>
<td>BeH*</td>
<td>BeH+</td>
<td>BeH+*</td>
<td>BeH$_2$…</td>
</tr>
<tr>
<td>Be</td>
<td>IAEA intern. validated dataset</td>
<td>DE</td>
<td>Janev 2011 BB</td>
<td>DR</td>
<td>DE</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Be+</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH+</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH+*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BeH$_2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- [7] Ballance 2003; and Bartschat 2016; and Dipti, 2018, ADNDT
- [5] Schneider 2017, 2018
- [6] Laporta 2017
- Sawada 2016
- Wünderlich 2016
- Janev-Reiter 2013
- Janev 2011, GBB, BB
- “if you must guess“, www.hydkin.de
- [8] Celiberto 2012; and Tennyson 2012
- [9] Celiberto 2013
- [10] Tennyson 2017
\[(e, p) + H/\text{H}_2/\text{H}_2^+\]

\[\text{CR model}\]
\[(e, p) + H/H_2/H_2^+ \text{ CR model}\]

<table>
<thead>
<tr>
<th>(H(1s))</th>
<th>(+H^+)</th>
<th>(+H^-)</th>
<th>(+H)</th>
<th>(+3^+)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(H^*(n), n = 2, 30)</td>
<td>(e, H^+)</td>
<td>(H_2(X \ ^1\Sigma^+_g, v = 0))</td>
<td>(H_2(X, v = 1, 14))</td>
<td>(H^- \to H + H^-)</td>
</tr>
<tr>
<td>(H_2(N \ ^1\Lambda_\sigma, v))</td>
<td>(H_2(b^3\Sigma^+_u) \to H + H)</td>
<td>(H_2(N \ ^3\Lambda_\sigma, v))</td>
<td>(H_2^+(v'))</td>
<td>(H_2 + H_2^+ \to H_3^+)</td>
</tr>
</tbody>
</table>
\((e, p) + H/H_2/H_2^+\) CR model

- H(1s)
- \(H^*(n), n = 2, 30\)
- \(e, H^+\)
- \(H_2(X^1\Sigma_g^+, v = 0)\)
- \(H_2(X, v = 1, 14)\)
- \(H_2^+ \rightarrow H + H^-\)
- \(H_2(N^1\Lambda_\sigma, v)\)
- \(H_2(b^3\Sigma_u^+) \rightarrow H + H\)
- \(H_2(N^3\Lambda_\sigma, v)\)
- \(H_2^+(v')\)
- \(H_2 + H_2^+ \rightarrow H_3^+\)

H - atom CR Codes
Since 1960th,
Johnson-Hinnow

\(H_3^+:\) non-linear part.
Probably not needed
in fusion plasmas
(but:
in small technical
plasma devices)
Warm up: H-atom, CR model: H(1), H*(2), ..., H*(30), H^+

(i,k-excitation, i-ionization A_ik, and k,i de-excitation)

Eigenvalues of Hydrogen CR Rate Matrix
Non-zero Eigenvalues. 0 Eigenvalues are zero.

@ Te = 10 eV, ne = 1e13

One, out of the 30 eigenvalues of H-CR Matrix, is order of magnitudes smaller than the others. Ground state H(1s)

Very disparate time scales → Model reduction possible → Use effective CR rates, with only H and H^+ kept separate in transport equations.
Coupled H-H⁺-H₂-H₂⁺ CR model, @ 10 eV, 1e13 cm⁻³
134 species/states, 16 final states, 117 non-zero eigenvalues

16 eigenvalues are orders of magnitude smaller than all the others.

These correspond to H(1s) and the H₂(v, v=0,14) vibr. states in electronic ground state

→ 16 ("metastables"), 16 coupled transport (Boltzmann) eqs. for them.

All the other ≈100 states can be condensed, in effective CR rates and hence be removed from transport problem.
The curse of dimensionality:
eff. Rates (Te, ne, Ti, ni, E, opacity, loss times), \(\rightarrow\) multidim. tables?

Solution: brute force computing power: solve CR models “on the fly”, rather than lookup in precomputed tables (done in EIRENE code for H (2001), He (2018), next: H\(_2\), Be, 

Same trend in fission (neutronics):
Massive distributed computing vs. complex

---

**MC Neutron: Cross Sections**

- Take up 80% of overall computing time:
  - This time is mostly spent in the Binary Search to locate \(E\) in the energy grid:
    - \(E_0\) to \(E_N\)
    - Bouncing binary search \(\rightarrow 65\%\) LLC misses


- Analysis shows that:
  - The energy grid is **accessed randomly**
  - The floating point unit is mostly idle because of **cache misses**
  - The vector unit does **nothing**

---

**The addressed problems**

**Optimization of the cross-section lookup:**
- Both in terms of CPU performances and memory footprint
- We focus on many core architecture (multilevel parallelism and vectorization)
- Try to find efficient approaches for many core architecture: from memory bound problem \(\rightarrow\) CPU-bound problem

2 approaches:
- Classical one: cross-sections are pre-computed and stored into memory – Find an optimal energy lookup algorithm
- One-the-fly cross sections calculations, minimize memory footprint – But what about performances?
Remove species, for which we solve transport equations. (here: 18)

Solve for CR

Population of the rest, taking the former as Known (here: 120)
Rapid progress in molecular H₂ data, often tested against experimental results in small (linear) plasma devices

Recommended entry point to the data-bases used here (and in other edge codes): 3 recent reviews (2016) from an IAEA “coordinated research project” (CRP) 2011-2016

First ab initio electron-molecule CCC calculations now become available (one of the golden standards for electron collision processes in small systems) for the e+H₂ and e+H₂⁺ systems: Curtin Univ. Perth, Australia

Data usage in fusion is now far behind the data availability
• The most sophisticated tokamak divertor ever built
  ▪ 54 individual cassettes, fully water cooled, designed to handle up to ~100 MW in steady state
  ▪ Now entering the procurement phase → design essentially complete
The ITER divertor

Courtesy: S. Lisgo, 2019
The ITER divertor

Courtesy: S. Lisgo, 2019
The ITER divertor

Recall: a 5 mm $\lambda_q$ at the outer mid-plane is assumed for the power channel.

Courtesy: S. Lisgo, 2019
Also, the current DEMO reference involves large modular components

In ITER, the entire cassette is thrown away if the strike-point surface is damaged.

(Replacement time of 6 months, and only 4 spare cassettes. 5 years to make new ones.)

Courtesy: S. Lisgo, 2019
Dissipation – Divertor detachment

ION STREAMING TO SURFACE

Courtesy: S. Lisgo, 2019
Dissipation – Divertor detachment

SHEATH ACCELERATION TO THE TARGET

[Image 460x0 to 838x449]

[Image 134x3 to 388x478]

[Stangeby ...]

Courtesy: S. Lisgo, 2019
Dissipation – Divertor detachment: Stability and control issues?

“GAS TARGET” FOR DETACHED PLASMA

[LaBombard, McLean 2015, PPCF 2017, Krasheninnikov and Kukushkin 2017]

break confinement

Courtesy: S. Lisgo, 2019
Dissipation – Plasma-surface interaction can be a mess

IMPURITY PRODUCTION (AND A LOT MORE...)

Courtesy: S. Lisgo, 2019
Most important molecular processes (reaction channels): attached plasmas

*Attached, high recycling*

Te ≈ 5 -10 eV

*Attached, low recycling*

Te ≥10 eV

Janev et al., (1987)

**Electron collisions**
Most important molecular processes (reaction channels)

Detached

\[ \text{Te} \approx 1 - 3 \text{ eV} \]

\[ \rightarrow \text{H} + \text{H}^+ \]

\[ \rightarrow \text{H} + \text{H}^* \]

\[ \rightarrow \text{H} + \text{H} \]

Attached, high recycling

\[ \text{Te} \approx 5 - 10 \text{ eV} \]

\[ \rightarrow \text{H} + \text{H}^+ \]

\[ \rightarrow \text{H} + \text{H}^* \]

\[ \rightarrow \text{H} + \text{H} \]

Attached, low recycling

\[ \text{Te} \geq 10 \text{ eV} \]

\[ \rightarrow \text{H} + \text{H}^+ \]

\[ \rightarrow \text{H} + \text{H}^* \]

\[ \rightarrow \text{H} + \text{H} \]
Most important molecular processes (reaction channels)

Detached

Realm for “dissociation recombination community”,
(mostly: cosmology, astrophysics, ….applications)
9 International conferences “Dissociative recombination”
held (1988, Alberta, Canada -- 2012 Paris, France)

Bridgehead to fusion community:
Late Prof. Hidedazu Takagi, Kitasato Univ. Jp.

Multi step process:

But:
removes an ion-electron pair from the plasma flow
and replaces it by a thermal particle (atom or ion) taken
from former $\text{H}_2$

$\rightarrow$ Relevance for particle balance: puff $\rightarrow$ divertor $\rightarrow$ pump
$\rightarrow$ (density control, stability, ….)

MITTAG DER HELmholtz-Gemeinschaft
ISOTOPE EFFECTS? H → D → D/T

H2(v) vibrational kinetics is involved in a controlling way, resonance effects in ion conversion (IC) Isotopomers? D+ + HD(v) → ... vs. H+ + D2(v) → ... , and DT, T2, DT...? unknown territory (in fusion edge plasma science)?
Vibrational kinetics, electron dynamics and elementary processes in H$_2$ and D$_2$ plasmas for negative ion production: modelling aspects

M. Capitelli$^{1,2}$, M. Cacciatore$^2$, R. Celiberto$^3$, O. De Pascale$^2$, P. Diomede$^1$, F. Esposito$^2$, A. Gicquel$^1$, C. Gorse$^{1,2}$, K. Hassouni$^4$, A. Laricchiuta$^2$, S. Longo$^{1,2}$, D. Pagano$^1$ and M. Rutigliano$^2$

$^1$ Dipartimento di Chimica, Università di Bari, Italy
$^2$ IMIP-CNR, Bari, Italy
$^3$ Dipartimento di Ingegneria Civile ed Ambientale, Politecnico di Bari, Italy
$^4$ LIMHP-CNRS, Université Paris Nord, Villetaneuse, France

Received 30 June 2005, accepted for publication 3 March 2006
Published 22 May 2006
Online at stacks.iop.org/NF/46/S260
vibr. quantum number vs. vibrational eigenvalue

the behaviour of, respectively, the total and dissociative cross section for transitions to the members of the spectroscopic series $^1\Pi_u[n\pi\pi]$, as a function of the principal quantum number $n$ of the excited molecular state, for a given electron impact energy. The cross-sections decrease, due to increase in transition energy, scaling approximately with $n$ as $n^{-4}$, a result which can be used in the improvement of the collisional radiative model for Rydberg states.

In [19] the dependence of the total excitation cross section on the molecular mass has been widely discussed. The observed shift to higher vibrational quantum numbers in the vibrational profile of heavier isotopes seems to be connected to existence of an isotopic effect; however, this is only apparent and depends on the different level density in the same transition energy range for different isotopes; in fact the cross-sections collapse when plotted as a function of the vibrational eigenvalues. In the case of an e–V processes [20], plotting the monoquantic ($v_f = v_i + 2$) and biquantum ($v_f = v_i + 2$) resonant vibrational excitation cross sections, at a fixed incident energy, for $H_2$, $D_2$ and $T_2$ molecules, as a function of either the vibrational quantum number (figure 2(a)) or the corresponding vibrational eigenvalue, the same cross-section collapse has been observed, suggesting an energy-based scaling law.

The database reported in [18] has been enriched by the electron–molecule cross sections for transitions involving triplet states of $H_2$ molecule [21]:

$$H_2(a^3\Sigma_g^+, v_i) + e \rightarrow H_2(d^3\Pi_u) + e, \quad (6)$$

$$H_2(c^3\Pi_u, v_i) + e \rightarrow H_2(g^3\Sigma_g^+) + e, \quad (7)$$

$$H_2(c^3\Pi_u, v_i) + e \rightarrow H_2(h^3\Sigma_g^+) + e, \quad (8)$$

in particular the Fulcher band has been considered; this system is important in spectroscopic diagnostic methods, providing information about the vibrational and translational temperatures of $H_2$ under non-equilibrium conditions [22].
e-V processes in $H_2(^1X_g, v)$

Figure 2. Cross section for the process $H_2(^1\Sigma_g^+, v_f) + e \rightarrow H_2^- \rightarrow H_2(^1\Sigma_g^+ , v_f) + e$, for a fixed collision energy, $E = 5$ eV, as a function of (a) the vibrational quantum number $v_f$ and (b) vibrational eigenvalue, for $H_2$ and its isotopic variants (close diamonds—$H_2$, open diamonds—$D_2$, open circles—$T_2$).
Also for other electron collision processes?

Presentation by Roberto Celiberto, at FZ-Juelich, sometime in summer 2006
Talk starts: 30 pictures like this

- Audience getting tired....
Wow!

That, if not an artifact of the computational method used, would be of key importance for data implementation.
Talk continues with 25 pictures like this......

Almost falling asleep again....
Slide 59: the key result, again....

This was for electron impact excitation on H2, D2, T2, HD, HT, DT
Collapsing isotopic effects: BeH⁺, BeD⁺, BeT⁺, DR

Priv. comm. Aug. 2019: Ioan Schneider, Université du Havre, (follow up discussions from AMD unit CM meeting in June 2019)

Vibrational energy, 17 lowest levels of BeH⁺, fake continuum
H2(v) vibrational kinetics is involved in a controlling way, resonance effects in ion conversion (IC) Isotopomeres? D+ + HD(v) → … vs. H+ + D2(v) → …, and DT, T2, DT…?
unknown territory (in fusion edge plasma science)?

Currently:
Electron collisions: use vibrational energy, rather than vibrational quantum number (for H2(v), D2(v), T2(v),….)
→ collapse to a single set (of isotope independent) rates.
Heavy particle collisions: scaling of cross sections to same collision velocity, rather than collision energy
→ collapse to a single set (of isotope independent) rates
(as we have already seen in resonant charge exchange).
Collapsing isotopic effects

- When can we always rely on such simplifications?
- Not always.....
Isotope effects? $H_2^+$ or $H^-$ mitigated recombination channel:
From various code - experiment comparisons:
Looking for further (collisional) channels that might enhance cross field plasma losses (such as MAR). A. Kukushkin, ..., D. Reiter 22nd PSI (Rome), NME 2017

Other channels with similar effects?

e + H2(v) → H + H^-

Enhanced D^- MAR over H^- MAR (loc cit.)? This was the wrong conclusion.
A “true” isotope effect in dissociative attachment (caused by nuclear motion in molecule)

Dissociative attachment in $\text{D}_2$ is strongly reduced, compared to $\text{H}_2$

→ many theoretical and exp. confirmations since…, latest:
E. Krishnakumar, S. Denifl, I. Cadez et al.
PRL 106, 243201 (2011)

$$e + \text{H}_2(v) \rightarrow \text{H} + \text{H}^-$$
$$e + \text{D}_2(v) \rightarrow \text{D} + \text{D}^-$$
A “true” isotope effect in dissociative attachment

Wrapping this up: a plasma chemical approach (0D, rate constants, … loss times, …)

- Long list of reactions → …
- estimate isotopically correct MAR rates, etc…

No enhanced “MAR”, but isotope separation in molecular cloud

Lighter isotope enhanced in neutralized channel (→ pump)
(same trend in D-T mixture)
Thank you for your attention!
Preface: A little bit of history….

1990: R.A. Hulse: ALADDIN atomic physics database system → IAEA AM data unit

https://www-amdis.iaea.org/ Accessed: June 2018
Define sensitivity $Z$ of density $n_j$ wrt. reaction rate $R_k$ as logarithmic derivative:

$$Z = \frac{d (\ln n_j)}{d (\ln R_k)}$$

For $n$ species in the system, and $m$ different processes active, there are $n \times m$ such sensitivity functions.

Fortunately: the system of DGL for these $Z$ has the same form as that for the densities $n$, and can also be solved in closed form using the known eigenvalues and eigenvectors.

If this option is activated, HYKIN prints and plots the $s$ (input) largest (at $t=t_{\text{max}}$) such sensitivity functions.

Sensitivity study: H-H2-H2+ CR model: @1 eV

\[ spec - 131 - H2^+ \]
Sensitivity study: H-H2-H2+ CR model: @10 eV

\[ \text{spec} - 131 - H2^+ \]
\[ \frac{dn(p)}{dt} = - \left\{ \sum_{q \neq p} C(p,q)n_e + \sum_{q < p} A(p,q) + S(p)n_e \right\} n(p) \\
+ \sum_{q \neq p} \{C(q,p)n_e + A(q,p)\} n(q) + \{\alpha(p)n_e + \beta(p) + \beta_d(p)\} n_i n_e. \]

\[ \dot{n} = M(T_e, n_e) \cdot n + \Gamma(T_e, n_e, n_i), \text{ where} \]

\[ M_{pq} = \begin{cases} 
C(q,p)n_e + A(q,p), & \text{if } p \neq q \\
- \sum_{j \neq p} C(p,j)n_e - \sum_{j < p} A(p,j) - S(p)n_e, & \text{if } p = q 
\end{cases} \]

and \[ \Gamma_p = [\alpha(p)n_e + \beta(p) + \beta_d(p)] n_i n_e. \]
2.1 Reducing the dimensionality

Equation (3) can be solved via e.g. eigenvalue decomposition or Laplace transformation. But in practice, the computational effort can be drastically reduced since the timescales for the development of different atomic states are very different. So, if diagnostics with finite temporal resolution are used, and no processes other than those in (1) are relevant on faster time scales, some of the states can be assumed stationary. The vector space of $\mathbf{n}$ can then be split in three,

$$
\begin{pmatrix}
\dot{n}_P \\
\dot{n}_Q \\
\dot{n}_S
\end{pmatrix} = \begin{pmatrix}
M_P & M_{PQ} & M_{PS} \\
M_{QP} & M_Q & M_{QS} \\
M_{SP} & M_{SQ} & M_S
\end{pmatrix}
\begin{pmatrix}
n_P \\
n_Q \\
n_S
\end{pmatrix} + \begin{pmatrix}
\Gamma_P \\
\Gamma_Q \\
\Gamma_S
\end{pmatrix},
$$

where $\mathbf{n}_S$ is given by (2) and hence $\dot{n}_S = 0$. We assume $\dot{n}_Q = 0$ and immediately derive

$$
n_Q = -M_Q^{-1}(M_{QP}n_P + M_{QS}n_S + \Gamma_Q),
$$

(5)

$$
\dot{n}_P = (M_P - M_{PQ}M_Q^{-1}M_{QP})n_P + (M_{PS} - M_{PQ}M_Q^{-1}M_{QS})n_S + \Gamma_P - M_{PQ}M_Q^{-1}\Gamma_Q
$$

(6)

$$
= M_{\text{eff}}n_P + \Gamma_{\text{eff}},
$$

which reduces the dimension of the ODE system to the dimension of the $P$ space. In the last step we have used that both $\Gamma$ and $\mathbf{n}_S$ are proportional to $n_i$ and hence represent a source.
2.2 Formulation I ("meta-stable resolved")

Taking only the ground and the two meta-stable states into the $P$ space, hence assuming $\dot{n} = 0$ for all the other states, eq. (5) can be written for a state $q$ as

$$n_Q|_q = n(q) = r_0(q)n_en_i + r_1(q)n_en(1^1S) + r_2(q)n_en(2^1S) + r_3(q)n_en(2^3S).$$  \hspace{1cm} (7)

$r_j(q)$ are called population coefficients and depend on $T_e$ and $n_e$. The subscripts $j \in \{0, 1, 2, 3\}$ stand for the ion, the ground state $1^1S$, and the meta-stable $2^1S$ and $2^3S$ states, respectively. For the $P$ space, hence $p \in \{1, 2, 3\}$, eq. (6) becomes

$$\frac{d}{dt}n(p) = \sum_{j \neq p, j \neq 0} k_{jp}n(j)n_e - k_p n(p)n_e + k_{0p}n_i n_e.$$ \hspace{1cm} (8)

Notice that the constraint on ion density $n_i$ in [1, eq. (25)] is only valid in a closed system. In EiRENE, it is usually additionally modified by plasma transport (on larger time scales) and other collision terms.

The $k$'s are the CR coupling coefficients and are given explicitly in terms of the population coefficients in [1]. From (6) we see that $(M_{eff})_{pp} = -k_p n_e$, $(M_{eff})_{pj} = k_{jp} n_e$ and $\Gamma_{eff}|_p = k_{0p} n_i n_e$. 

2.3 Formulation II ("meta-stable unresolved")

If the quasi-steady-state (QSS) assumption also holds for the meta-stable states, they may be also moved into the $Q$ space. The $P$ space becomes one dimensional - it is the most simple choice. The excited level population is then given by

$$n_{Q|q} = n(q) = R_0(q)n_e n_i + R_1(q)n_e n(1^1S).$$  \hspace{1cm} (9)

$R_0(q)$ and $R_1(q)$ are also called population coefficients. They are associated with the recombining and the ionizing plasma component, respectively. The time evolution of the ground state is written in the reduced form as

$$\dot{n}_P = \frac{d}{dt} n(1^1S) = -\frac{d}{dt} n_i = -S_{CR} n(1^1S)n_e + \alpha_{CR} n_i n_e.$$  \hspace{1cm} (10)

$S_{CR}$ and $\alpha_{CR}$ are the CR ionization and recombination rate coefficients, respectively. $S_{CR}$, $\alpha_{CR}$, $R_0(q)$ and $R_1(q)$ can be obtained directly from (5) and (6) or from $k$’s and $r$’s according to expressions given in [1, eq. (31-38)]. They are therefore functions of $T_e$ and $n_e$. 

6 Electron cooling rates

Often, EIRENE [7] is coupled to a plasma fluid code like B2 [9] or EMC3 (edge Monte Carlo 3D) [10] to describe the coupling of the plasma to neutrals. It acts then as a source (and sink) of the fluid due to neutrals, e.g. due to ionization (and recombination) - calculated with a CR model.

It also provides a source (and sink) for the fluid energy and momentum due to the exchange with neutrals. Here, only electron collisions are considered for helium: since $m_e \ll m_i$, momentum exchange can be neglected. The change in energy is expressed with the electron cooling rate density

$$W = \sum_{p} \left\{ \chi(p)S(p)n_en(p) + \sum_{q \neq p} [\chi(q) - \chi(p)]C(q, p)n_en(q) \right\}$$

$$-\chi(p)\alpha(p)n_i^2n_i + W_{\beta}(p)n_en_i + W_{\beta\alpha}(p)n_en_i \right\}. \quad (46)$$

It has the dimension “energy per time and volume”. $p$ and $q$ are hereby energy states of the helium atom as in (1) and $\chi$ the ionization potential. $W_{\beta}(p)$ and $W_{\beta\alpha}(p)$ are the rate coefficients associated with the radiative and dielectronic recombination into state $p$. 
6.2.1 Derivation

Having the expression in (46) fully defined, we notice that it depends on the helium population (and ion) density. Hence, a solution for the rate equation (1) is required. Naturally, we want to use the approximate solutions from formulation I or II: we insert (2) for \( n \geq 21 \) (Saha states), for \( n < 21 \) and \( q \notin \{1^1S,2^2S,2^3S\} \) we use (7) in form. I or (9) for \( q \neq 1^1S \) in form. II. We obtain

\[
W = W_0^I n_e n_1 + W_1^I n_e n(1^1S) + W_2^I n_e n(2^1S) + W_3^I n_e n(2^3S)
\]

(56)
in formulation I and

\[
W = W_0^I n_e n_1 + W_1^I n_e n(1^1S)
\]

(57)
in formulation II.

Explicitly, in form. I the cooling rate coefficients are

\[
W_j^I = \sum_p \left\{ \chi(p)S(p)n_e r_j(p) + \sum_{q \neq p \atop n < 21} \left[ \chi(q) - \chi(p) \right] C(q,p)n_e r_j(p) \right\} \text{ for } j \in \{1,2,3\},
\]

(58)

and

\[
W_0^I = \sum_p \left\{ \chi(p)S(p)n_e r_0(p) + \sum_{q \neq p \atop n < 21} \left[ \chi(q) - \chi(p) \right] C(q,p)n_e r_0(p) - \chi(p) \alpha(p)n_e + W_\beta(p) + W_\beta_0(p) + \sum_{q \neq p \atop n > 21} \left[ \chi(q) - \chi(p) \right] C(q,p)n_e Z(q) \right\}.
\]

(59)

In form. II, \( W_0^I \nLeftarrow W_0^I \) with \( R_0(p) \) instead of \( r_0(p) \), and \( W_1^I \nLeftarrow W_j^I \) with \( R_1(p) \) instead of \( r_j(p) \).
6.3 Radiative loss rates

Similarly to the cooling rate, we can define the radiative loss rate

\[
W_{\text{rad}} = \sum_p \left\{ \sum_{q > p} [\chi(q) - \chi(p)] A(q, p)n(q) - \left( \frac{1}{2} m_e v^2 + \chi(p) \left( \sigma_\beta + \sigma_\beta_0 \right) v \right) \right\}.
\]  

(60)

$q > p$ means that state $q$ lies energetically higher than state $p$. The second term accounts for the photons mentioned in chapter 6.1. Note: $W_{\text{rad}} < 0$. Like the cooling rate, it can be computed using formulation I or II, hence

\[
W_{\text{rad}} = W_{\text{rad}_0} n_e n_i + W_{\text{rad}_1} n_e n(1^1S) + W_{\text{rad}_2} n_e n(2^1S) + W_{\text{rad}_3} n_e n(2^3S)
\]

(61)

and

\[
W_{\text{rad}} = W_{\text{rad}_0} n_e n_i + W_{\text{rad}_1} n_e n(1^1S).
\]

(62)

Due to energy conservation, the plasma’s thermal energy change (cooling/heating) must be balanced by change of the internal state (atomic level transition) and radiation. This also holds in the reduced formulations, hence

\[
W_i = \sum_{j \neq i} [\chi(i) - \chi(j)] k_{ij} - W_{\text{rad}_i}.
\]

(63)