Ongoing and pending data base activities @ FZ Jülich

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OUTLOOK

- **Generals**: on AM-S data use in fusion plasma models
  “internal consistency”, completeness (competing processes)

- **Surface Data**: Reflection, Sputtering:
  multidimensional distributions: online “TRIM” database
  maintained, and still occasionally upgraded upon demand.

- **AM Data**:
  FZJ: data evaluation, data generation, database compilation “sui generis”
  was initiated by Ratko Janev:
  CₓHᵧ (database is frozen, some low T updates for particle
  rearrangement collisions are pending),
  SiHᵧ (database frozen)
  HₓH₋, H₂, Hₓ₊, Hₓ₊→ ongoing, (now mainly: asymptotics, documentation)
  Be, BeₓHᵧ : unfinished

- **FZJ data activity is now focused on**:
  Data processing/formatting, asymptotics, internal CR modules for transport
  simulations,…,raw data public exposure.
  Sensitivity analysis (uncertainty propagation) on linear CR or chemistry models
Status and purpose of current integrated edge models:

No predictive quality, due to “anomalous” cross field plasma transport (laminar? turbulent? blobby? ....?)

By detailed numerical bookkeeping current edge modelling is the tool to separate the “principal known” (PMI, A&M) from the “principle unknown” (⊥B plasma-transport).

If this is successful, then the latter can be isolated and determined experimentally.
Method: “Operator Splitting”

Advection-diffusion: strongly implicit CFD (macroscopic flows)

Reaction part: explicit (Monte Carlo) (microscopic kinetics)
Simulation of “plasma + wall” – a multi-scale problem

Larger scales in time & space

Transport codes
Adaption of edge transport code for linear devices
(codes: B2, EIRENE, EMC3, ERO,..)

Drift-fluid models
3D Simulations, currents, fields, drifts
Tokam3D (CEA), Bout++, Attempt,…

Gyro-kinetic models
Includes non-Maxwellian effects, ExB nonlinearity and polarization drift retained

Fully kinetic models (PIC/TREE)
Mesh free approach with tree code, particle based, self consistent fields
Goal: ab-initio virtual PMI lab using PEPC

Surface and material simulations
Computational material science: multi-scale in itself:
DFT – QMD – MD - KMC …

Surface and material interface

PEPC (with JSC)
B2: a multi-species plasma fluid code (D+, He++, C4+..,..)

EIRENE:
Monte-Carlo neutral particle, trace ion (He+, C+, C++..) and radiation transport code.

Plasma flow parameters
Source terms (Particle, Momentum, Energy)

MICROSCOPIC

MACROSCOPIC

EDGE CODES
(B2-EIRENE)

processed data

1D core, 0D point reactor STRAHL, ETS

Source terms

(gyro-kinetic, N-body (ERO, PIC))
raw data

2004 -- ...... (ongoing)

HYDKIN
database

toolbox

Spectral (time scale) analysis

Public exposure of data

Sensitivity analysis

Interface

EIRENE
3D Monte Carlo
kinetic transport

KSTAR, TEXTOR, JET,
ASDEX, DIII-D, LHD, W7X, ...
JT-60, LHD, ......
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  $H, H^+, H_2, H_2^+, H_3^+... \rightarrow$ ongoing, (now mainly: asymptotics, documentation)
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A: Basic Processes Induced in Materials by Plasma Particle Impact

- **Void**
- **Sputtering**
- **Reflection**
- **Implantation**
- **Vacancy**
- **Self-interstitial**
- **Dislocation**

**Energy dissipation by elastic (with atoms) and inelastic (with electrons) collisions**

\(10^{-13}\) sec, range \(10^{-7}\) m, 200 eV \(D^+\)

**Elastic collisions**: Creation of vacancies and interstitials

**Diffusion of vacancies and interstitials**

**Recycling**: reflection and thermal re-emission of incident particles at surfaces

**BCA**: Binary collision approximation

- **创造性**
- **变形**
- **扩散**
- **互换**
- **放射**

**Sputtering of surface atoms**

(energy transfer > surface binding energy)

**Transmutation**

formation of nuclear reaction products (including H isotopes and He)
Backscattering

Reflection of impinging particles at the surface

Reflection coefficient $R$:
$$ R = \frac{\text{number of reflected particles}}{\text{number of incoming particles}} $$

Deposition $= 1 - R$

**Multi-differential recycling coeff.**:
$$ \frac{\partial R}{\partial E} \frac{\partial^2 R}{\partial^2 \Omega} \frac{\partial^3 R}{\partial E \partial^2 \Omega} $$

- In most cases: reflected particles are neutrals
- Reflection coefficient depends on:
  - mass of projectile and target
  - energy and angle of incident particles
Plasma-Wall Interaction Processes

Backscattering

Dependency of reflection coefficient on incident energy

Monte Carlo simulation (BCA): C on C, $\alpha_{\text{in}} = 60^\circ$

At low energies: BCA is not valid $\Rightarrow$ Molecular Dynamic calculations yield $R \neq 0$
Sensitivity of reflection coefficient at low $E_{\text{in}}$ (all within BCA, TRIM)

Particle reflection coefficient, D --> FE, 30 degree

Incident energy, eV

Uncertain MD ?? Quite reliable, BCA

Different choices of “empirical surface binding energy” parameter
Backscattering

Dependency of reflection coefficient on incident angle

Monte Carlo simulation (BCA): C on C, $E_{\text{in}} = 100$ eV

![Graph showing the dependency of reflection coefficient on incident angle. The x-axis represents the incident angle in degrees, and the y-axis represents the reflection coefficient. The graph shows an increasing trend as the incident angle increases.](image-url)
Reasonable assumptions (IYMG*):

Energy: exponential decrease for reflected particles if incoming particle energy is Maxwell-distributed

Angle: cosine distribution for reflected particles if isotropic bombardment

Note: Reflection coefficient $R$ can be very different from Recycling coefficient $R$

Recycling coefficient is typically close to one in magnetic fusion, because wall surfaces are quickly saturated.

* IYMG: If You Must Guess
Surface processes in fusion edge codes:
Jargon in edge modelling talks/papers: “we use TRIM code data....”
(wrt. “physical sputtering and reflection”)
which means: BCA (binary collision approximation)

Full 3V distribution of refl. part.
on: [www.eirene.de/surfacedata](http://www.eirene.de/surfacedata)
Data files with tables of multiple differential reflection distributions, e.g. for particle simulation codes (conditional quantile format)
TRIM.xxx: reflected energy spectra
red: 200,000 TRIM particles,
blue: reconstructed from 10 quantiles

\[ \partial R(E_{in}, \theta_{in}; E) \]
\[ \partial E \]

Energy distribution of reflected particles
H \rightarrow Fe, incident energy: 100 eV, incident angle: 45 degree

what is the minimal dataset that allows to re-sample the full backscattering (and sputtering) distribution?

See: www.eirene.de
Surface data TRIM
Double diff. distr. \[ \frac{\partial R(E_{in}, \theta_{in} ; E, \theta_{out})}{\partial E \partial \theta_{out}} \]

D on C, 10 eV in

D on C, 10 eV, 0 degree incident angle, raw data

D on C, 10 eV, 45 degree incident angle, raw data

D on C, 10 eV, 60 degree incident angle, raw data

D on C, 100 eV in

D on C, 100 eV, 0 degree incident angle, raw data

D on C, 100 eV, 45 degree incident angle, raw data

D on C, 100 eV, 60 degree incident angle, raw data

Data formatting and condensation: G. Bateman, PPPL no. 1 (1980)
Double diff. distr. \[ \partial R(E_{in}, \theta_{in}; E, \theta_{out}) \partial E \partial \theta_{out} \]

D on W, 10 eV in

D on W, 10 eV, 0 degree incident angle, raw data

D on W, 10 eV, 45 degree incident angle, raw data

D on W, 10 eV, 60 degree incident angle, raw data

D on W, 100 eV in

D on W, 100 eV, 0 degree incident angle, raw data

D on W, 100 eV, 45 degree incident angle, raw data

D on W, 100 eV, 60 degree incident angle, raw data

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  \( \text{SiH}_y \) (database frozen)
  \( \text{H}, \text{H}^-, \text{H}_2, \text{H}_2^+, \text{H}_3^+ \ldots \rightarrow \) ongoing, (now mainly: asymptotics, documentation)
  \( \text{Be}, \text{Be}_x \text{H}_y \) : unfinished

- **FZJ data activity is now focused on:**
  Data processing/formatting, asymptotics, internal CR modules for transport simulations,…,raw data public exposure.
  Sensitivity analysis (uncertainty propagation) on linear CR or chemistry models
FZJ homemade “database” for fusion plasma chemistry modelling, is publicly exposed on: www.eirene.de

Reviewed EIRENE database Series 2002-....., (several IAEA CRP’s)
FZ-Jülich (R. Janev, D. Reiter et al.)

Methane (CH_y)  C_2H_y  C_3H_y  Silane (SiH_y)  p,H,H^-,H_2,H_2^+,H_3^+

Ratko Janev, Detlev Reiter: 
H, H₂, H₃⁺... data compilation. 
Mostly cross sections, few rate coefficients 
Today: 471 references, 
New edition: spring 2016 (CRP H, He)

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7.2.1 Photo-absorption

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9.3.3 Dissociative electron capture and fast H_2 production
raw data

HYDKIN database toolbox

2004 -- ……(ongoing)

Spectral (time scale) analysis

fragmentation pathways

Sensitivity analysis

Interface

EIRENE

3D Monte Carlo kinetic transport

TEXTOR, JET, ASDEX, DIII-D, JT-60, LHD, ……
“Battle field” of hydrogen molecule:  
Two-electronic, strongly coupled potential-surfaces of H$_3^+$

H$^+$+H$_2$ is the most fundamental ion-molecule system
We should know all about it  P. Krstic, ORNL, US

**Proton impact of molecule**

\[ p + H_2(v) \rightarrow p + H_2(v') \]

\[ p + H_2(v) \rightarrow H + H_2^+(v') \quad \text{Charge transfer} \]

\[ p + H_2(v) \rightarrow H + H^+ + H \]

\[ p + H_2(v) \rightarrow H + H^+ + H^+ + e \quad \text{Dissoc Double ion} \]

\[ p + H_2(v) \rightarrow p + H_2(n, v') \quad \text{Exc. elec. vib.} \]

**Processes with molecular ion**

\[ H + H_2^+(v) \rightarrow H + H_2^+(v') \]

\[ H + H_2^+(v) \rightarrow p + H_2(v') \]

\[ H + H_2^+(v) \rightarrow p + H + H \]

**Numerous other processes with molecules**

\[ H^- + H_2(v) \rightarrow H + H_2(v') + e \]

\[ H + H_2(v) \rightarrow H + H_2(v') \]

\[ H + H_2(v) \rightarrow H + H + H \]

\[ H_2(v') + H_2(v'') \rightarrow H_2(v''') + H_2(v''') \]

\[ H_2 + H_2(v) \rightarrow H_2 + H + H \]

**Creation of H$_3^+$**

\[ H_2^+(v') + H_2(v) \rightarrow H_3^+(v'') + H \]

\[ H_3^+ \quad \text{Series of interesting reactions:} \]

DE, DR, branching ratios with electrons

D, DCT with H

- “Interplay” of transport and inelastic processes
- Rotational analysis is missing
- Isotopic constitution: D$_2$, T$_2$, HD, HT and DT, sensitive on vib. energy levels
“Battle field” of hydrogen molecule: Two-electronic, strongly coupled potential-surfaces of $H_3^+$

$H^+ + H_2$ is the most fundamental ion-molecule system

We should know all about it. P. Krstic, ORNL, US, talk @ IAEA, DCN, 2013

Proton impact of molecule

\[ p + H_2(v) \rightarrow p + H_2(v') \]
\[ p + H_2(v) \rightarrow H + H_2^+(v') \text{ Charge transfer} \]
\[ p + H_2(v) \rightarrow H + H^+ + H \]
\[ p + H_2(v) \rightarrow H + H^+ + H^+ + e \text{ Dissoc Double ion} \]
\[ p + H_2(v) \rightarrow p + H_2(n, v') \text{ Exc. elec. vib.} \]

Processes with molecular ion

\[ H + H_2^+(v) \rightarrow H + H_2^+(v') \]
\[ H + H_2^+(v) \rightarrow p + H_2(v') \]
\[ H + H_2^+(v) \rightarrow p + H + H \]

Numerous other processes with molecules

\[ H^- + H_2(v) \rightarrow H + H_2(v') + e \]
\[ H + H_2(v) \rightarrow H + H_2(v') \]
\[ H + H_2(v) \rightarrow H + H + H \]
\[ H_2(v') + H_2(v'') \rightarrow H_2(v'''') + H_2(v''''') \]
\[ H_2 + H_2(v) \rightarrow H_2 + H + H \]

Creation of $H_3^+$

\[ H_2^+(v') + H_2(v) \rightarrow H_3^+(v'') + H \]

$H_3^+$ Series of interesting reactions:
DE, DR, branching ratios with electrons
D, DCT with H

- “Interplay” of transport and inelastic processes
- Rotational analysis is missing
- Isotopic constitution: $D_2, T_2, HD, HT$ and $DT$, sensitive on vib. energy levels
“Battle field” of hydrogen molecule:
Two-electronic, strongly coupled potential-surfaces of H₃⁺
H⁺+H₂ is the most fundamental ion-molecule system
We should know all about it.

Proton impact of molecule

\[ p + H_2(v) \rightarrow p + H_2(v') \] 
Also large σ

\[ p + H_2(v) \rightarrow H + H^+_2(v') \] 
Charge transfer

\[ p + H_2(v) \rightarrow H + H^+ + H \]

\[ p + H_2(v) \rightarrow H + H^+ + H^+ + e \] 
Dissoc Double ion

\[ p + H_2(v) \rightarrow p + H_2(n, v') \] 
Exc. elec. vib.

Processes with molecular ion

\[ H + H_2^+(v) \rightarrow H + H_2^+(v') \]

\[ H + H_2^+(v) \rightarrow p + H_2(v') \]

\[ H + H_2^+(v) \rightarrow p + H + H \]

Numerous other processes with molecules

\[ H^- + H_2(v) \rightarrow H + H_2(v') + e \]

\[ H + H_2(v) \rightarrow H + H_2(v') \]

\[ H + H_2(v) \rightarrow H + H + H \]

\[ H_2(v') + H_2(v'') \rightarrow H_2(v'''') + H_2(v'''') \]

\[ H_2^+(v') + H_2(v) \rightarrow H_3^+(v'') + H \]

Creation of H₃⁺

\[ H_2^+(v') + H_2(v) \rightarrow H_3^+(v'') + H \]

H₃⁺ Series of interesting reactions:
DE, DR, branching ratios with electrons
D, DCT with H

• “Interplay” of transport and inelastic processes
• Rotational analysis is missing
• Isotopic constitution: D₂, T₂, HD, HT and DT, sensitive on vib. energy levels

P. Krstic, ORNL, US, talk @ IAEA, DCN, 2013
Spectral analysis in CR models: \(\rightarrow\) model reduction

Build \(v\)-\(v'\) transition rate matrix, for \(e\) and \(p\) collisions on \(H_2 \rightarrow HYDKIN\)
\(\rightarrow\) slowest timescale (smallest eigenvalue): relaxation of \(T_{\text{vib}}\) to \(T_e\) or \(T_i\)

Cross section database is scanty (very, very scanty, to say the least)
result from (spectral) analysis:
p+\(H_2(v)\) cross sections large, effect on fusion plasma negligible compared to e+\(H_2(v)\) (still good to have, "reserve of knowledge", but: main focus elsewhere)
HYDKIN: spectral analysis for reaction kinetics

Warm up: H-atom, CR model: H(1), H*(2),…., H*(30), H^+

(l,k-excitation, i-ionization $A_{ik}$, and k,i de-excitation

@ $Te = 10 \text{ eV}$, $ne = 1e13$
HYDKIN: spectral analysis for reaction kinetics

Coupled H-H\(^+\)-H\(_2\)-H\(_2\)^+ CR model, @ 10 eV, 1 e13 cm\(^{-3}\)
134 species/states, 16 final states, 117 non-zero eigenvalues
H, H+, H2, H3+, ..., database for fusion edge plasma modelling:

**Status:** cross sections, CR models, “ok, up 2011..” (at least: compiled, fitted....)

**Main issues in transport modelling:**
- Multi-parametric dependencies of eff. rates: $T_e$, $T_i$, $n_e$, $n_{i1}$, $n_{i2}$, $E0$, .....  
- Asymptotic behavior of either: fits or tables  
  (what do complex codes really do with the data ??)  
- Our current tendency: integrate CR model solvers inside transport solvers,  
  evaluated CR rates on the fly, cell by cell,  
  fully parallelized (domain decomposition) $\rightarrow$ very little CPU penalty  
Available for H, soon for He (W7X) , H2/H (?) ,  
and we would hope for: BeH/BeH+/Be...  
- current applications are:
  1. e.g.: ITER diagnostic beam (100 keV) plus Halo  
     (thermal gas cloud around 100 keV beam that forms from charge exchange)  
  2.) main chamber erosion by neutral CX sputtering, power plant studies

SIMILAR ISSUES: He – He+ – He++
W7X, Greifswald, Germany:
start of plasma operation: October 2015: He-plasmas

Current FZJ activity:

EMC3-EIRENE:
Fully 3D,
Helium plasmas
He -- He$^+$ -- He$^{++}$
by Oct. 2015 ??
EDGE MODELLING EXPRESSIONISM......

W7X: 3 D grid (trilinear hexahedrons): EMC3-EIRENE, 1-3 Mill cells

Full He CR model, 65 states, MS resolved, cell by cell, about extra 1-3 sec. CPU cost on 1028 compute cores (typical value)
EDGE MODELLING EXPRESSIONISM......

W7X, Te profile, 3D.
Possible future relevance of these developments also for SOLPS-ITER (?)

- Pure He plasmas ??
- Gas flows in full 3D sub-divertor structures, based on detailed tetrahedral discretization?
Starting Hypothesis at W7X Team: Edge Model for He, He+, ignore He++ (until June 2014)

Spring 2015: **FLYCHK, (AMDU): case study: must build He – He++ model, with He+ only as tracer.**

→ Use EMC3-EIRENE in hybrid fluid-kinetic mode. (M.Rack, D.Reiter, EPS 2015)

Consequences for He - He+ + He++ database:

From a consistent set of cross sections: many datasets are derived:
- MS resolved, MS condensed, S/XB, rad. loss, Elect. energy loss rates, opacity, etc…
- A single transition cross section upgrade → replace the full set of CR data files.

**Solution:** Similar to H-COL (built in CR model into transport code)
- Also build He-COL (a He-CR Model, with matrix solver inside transport code, Condensation, data processing: on the fly.

**Database:** provide all individual He collision processes needed to build a CR matrix.
- Issues: asymptotics in rates or cross sections! detailed balancing!

Transport code does not need fits or tables (and their asymptotics) to multidimensional CR data vs.: Te, Ti, E0, ne, ni1,ni2…..)
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  rearrangement collisions are pending),
  SiH\textsubscript{y} (database frozen)
  H, H\textsuperscript{−}, H\textsubscript{2}, H\textsubscript{2}\textsuperscript{+}, H\textsubscript{3}\textsuperscript{+}… ongoing, (now mainly: asymptotics, documentation)
  Be, Be\textsubscript{x}H\textsubscript{y} : unfinished

• **FZJ data activity is now focused on:**
  Data processing/formatting, asymptotics, internal CR modules for transport simulations,…, raw data public exposure.
  Sensitivity analysis (uncertainty propagation) on linear CR or chemistry models
Basic input for EIRENE: A&M data, ( & surface data)
Goal: publicly expose raw data used in any modelling

www.hydkin.de

Online data base and data analysis tool-box:

- CR model condensation
- Sensitivity analysis
- Fragmentation pathway analysis
- Reduced models
  - Hydrocarbons
  - Silanes
  - \(H, H_2, H_3^+,\ldots\)
  - \(W, W^+,\ldots\) \(W^{74+}\)
  - \(N, N_2\), activity stopped, rely on other communities…

Be-BeH-BeH\(^+\), …… attempted, but expert help needed for cases of doubt
Towards a Be – Be$^+$ CR modul for transport simulations

Various sets of CCC cross section data provided by I. Bray, 2013
Complementary set of R Matrix cross section data from C. Balance (2014)
$e + \text{Be}(1) \rightarrow e + \text{Be}(4)$

2 datasets (CCC and R-Matrix), 2 set of fits (2 tasks, c & k, independent): positive example. Easy decision
Less clear examples: CCC or R-Matrix, and poor fits... → evaluation (experts)
So: bring on Be – Be+ evaluated cross section database:

with:

- either asymptotically correct fits
- or recommendations re threshold and high E asymptotics
- consistent forward and reverse processes
- double excited states?
- recombination (radiative, threebody, dielectronic…)


Current Nucl. Fusion N\textsubscript{2} database: obsolete!
see e.g.: Planetary Atmospheric Entries

Dissociative Recombination in Reactive Flows
Relative to Planetary Atmospheric Entries

Nitrogen
Species, states and elementary processes

\[ N\textsubscript{2}, N\textsubscript{2}^+, N, N^+ \text{ and } e^- \]

\begin{align*}
N\textsubscript{2} & \quad V, X^1\Sigma\textsubscript{g}^+ (v = 0 \rightarrow v_{max} = 67), A^3\Pi\textsubscript{u}, B^3\Pi\textsubscript{g}, W^3\Sigma\textsubscript{u}^-, B^3\Sigma\textsubscript{u}^-, \text{a}^1\Sigma\textsubscript{g}^-, \text{a}^1\Pi\textsubscript{g}, \text{w}^1\Delta\textsubscript{u}, G^3\Delta\textsubscript{g}, \text{O}^3\Pi\textsubscript{g}, E^3\Sigma\textsubscript{g}^+ \\
N\textsubscript{2}^+ & \quad X^2\Sigma\textsubscript{g}^+, A^2\Pi\textsubscript{u}, B^2\Sigma\textsubscript{u}^+, \text{e}^3\Pi\textsubscript{u}, D^2\Pi\textsubscript{g}, \text{c}^2\Sigma\textsubscript{g}^+ \\
N & \quad 4\text{S}_{1/2}, 2\text{P} = \left(2\text{D}_{5/2} + 2\text{D}_{3/2}, 2\text{P}^0 = \left(2\text{P}_{1/2} + 2\text{P}_{3/2}, 4\text{P}_{1/2, 3/2} \ldots \text{ (63 states)} \right)
\end{align*}

150 states

CR Model Database – CoRaM – \( N\textsubscript{2} \)
Forward rate coefficient
\[ k_i(T\text{A.e}) = \sqrt{\frac{8k_B T\text{A.e}}{\pi \mu}} \int_{x_0}^{+\infty} x e^{-x} \sigma_i(x) \, dx \]
with \( \sigma_i(x) \) the cross section and
\[ x = \frac{e}{k_B T\text{A.e}} \] the reduced collision energy

Backward rate coefficient from Detailed Balance

\[ \Rightarrow 100,000 \text{ elementary processes} \]

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Thank you