Status of A&M database and data analysis for fusion edge plasma transport

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The vision of nuclear fusion research: A miniature star in a solid container.

The Sun: T=15 Mill. degrees in the center

Fusion Reactor: T=100 Mill. degrees

\[ p + p \rightarrow d, \quad d+p \rightarrow \text{he-3}, \quad \ldots, \quad \ldots \rightarrow \text{he-4} \]

Reaction time \(1/(n_p \langle \sigma v \rangle_{\text{fus}}) = t_{\text{fus}}\) approx. \(10^9\) years
The vision of nuclear fusion research: A miniature star in a solid container.

Hydrogen burn $\rightarrow$ Helium accumulation $\rightarrow$ Collaps

Sun: $\approx 10$ Billion years
The vision of nuclear fusion research: A miniature star in a solid container.

Hydrogen burn → Helium accumulation → Collaps

Sun: \( \approx 10 \text{ Billion years} \)

Fusion flame on earth: \( \approx 100 - 200 \text{ s} \)
The largest fusion reactor today: JET (Joint Europ. Torus):
Ø 8.5 m, 2.5 m high, 3.4 T, 7 MA, 1 min

Key area for “plasma wall interaction science”:
Particle exhaust and Q < 10 MW/m²


The challenge: remove Helium ash and maintain
peak power load < 10 MW/m² steadily
ITER – the biggest tokamak ever built

ITER is twice as big as the world’s largest currently operating tokamak (JET)

TEXTOR (FZJ)
- \( V_{\text{plasma}} = 7 \text{ m}^3 \), \( I_p \approx 0.5 \text{ MA} \)
- \( P_{\text{fusion}} = 0 \text{ MW} \)
- \( t_{\text{plasma}} \approx 12 \text{ s} \)

JET (EU)
- \( V_{\text{plasma}} = 80 \text{ m}^3 \), \( I_p \approx 3 \text{ MA} \)
- \( P_{\text{fusion}} \approx 16 \text{ MW, 1 s} \)
- \( t_{\text{plasma}} \approx 30 \text{ s} \)

ITER
- \( V_{\text{plasma}} = 830 \text{ m}^3 \), \( I_p = 15 \text{ MA} \)
- \( P_{\text{fusion}} \approx 500 \text{ MW, 300 – 500 s} \)
- \( t_{\text{plasma}} \approx 600 – 3000 \text{ s} \)
ITER platform, Cadarache (Fr), April 2014
ITER: Balance of power

\[ Q = \frac{\text{Fusion power}}{\text{Input power}} = \frac{500}{50} = 10 \]

\[ \text{D} + \text{T} \rightarrow \text{He} + \text{neutron} \]

100 MW

400 MW

\( P_{\text{FUS}} = 500 \text{ MW} \)
\( P_{\text{He}} = 100 \text{ MW} \)
\( P_{\text{IN}} = 50 \text{ MW} \)

Trapped by the magnetic field (He\(^{2+}\)) \rightarrow gives its energy up to the plasma \rightarrow maintains the fusion reactions

Escapes from the plasma (no electric charge) \rightarrow absorbed in the blanket surrounding the plasma

Must be exhausted from the plasma

The “divertor”
Molecular Processes considered in fusion:

e,p + H\textsubscript{2}(v\textsubscript{i}) \rightarrow \ldots, e+H\textsubscript{2}\textsuperscript{+}(v\textsubscript{i}) \rightarrow H + H^*

- divertor detachment dynamics, final states? DR, DE?

www.amdis.iaea.org, database & data center network, Wuenderlich, Fantz, IPP Garching,...


e,p + C\textsubscript{x}H\textsubscript{y} \rightarrow \ldots., e+C\textsubscript{x}H\textsubscript{y}\textsuperscript{+} \rightarrow \ldots. C erosion and migration, tritium retention in remote areas,... Excited states of products (CH(A→X))? 


e+H\textsubscript{3}\textsuperscript{+}(v\textsubscript{3}) \rightarrow \ldots, DR, DE,...

- H\textsubscript{3}\textsuperscript{+} probably irrelevant in fusion plasmas


e+ BeH/BeH\textsuperscript{+} \rightarrow \ldots. possible role on spectroscopy and on material migration: Formation rates ?? 10% of Be sputtering?


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

e+ N\textsubscript{2}, N\textsubscript{2}\textsuperscript{+} \rightarrow \ldots. NN

- N\textsubscript{2}-seeding, edge plasma cooling: not yet studied in fusion plasmas, only resulting atomic ions N, N\textsuperscript{+}, N\textsuperscript{++},...

See planetary atmospheric entries research, e.g. A. Bultel et al, Universite de Rouen, France
This talk:

\[ e, p + H_2(v_i) \rightarrow ..., \quad e + H_2^+(v_i) \rightarrow H + H^* \]

- divertor detachment dynamics, final states? DR, DE?


\[ e, p + C_xH_y \rightarrow ..., \quad e + C_xH_y^+ \rightarrow ... \] C erosion and migration, tritium retention in remote areas, ... Excited states of products (CH(A→X))?


\[ e + BeH/BeH^+ \rightarrow ... \] possible role on spectroscopy and on material migration: Formation rates?? 10% of Be sputtering?


Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre, J. Tennyson et al. (Quantemol), R. Celiberto et al. (Bari),…
Relative importance of plasma flow forces over chemistry and PWI

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

div(nv_∥)+div(nv_⊥)= ionization/recombination/charge exchange

- All chemical bonds broken,
- (turbulent) cross field flow, D_⊥, V_⊥

(advanced plasma scenario development)

ionization/recombination/CX.

Atomic data models for hot plasma spectroscopy
- interpretation,
- line shape modelling:

Spectroscopy : nZ*
CR Model : nZ* \rightarrow nZ
Transport Model : nZ \rightarrow D_⊥, V_⊥
Relative importance of plasma flow forces over chemistry and PWI: I edge region → II divertor

\[
\text{div}(n\nu_{||}) + \text{div}(n\nu_{\perp}) = \text{ionization/recombination/charge exchange}
\]

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

I: midplain

parallel vs. (turbulent) cross field flow

II: target

parallel vs. chemistry and PWI driven flow

This talk: dominant process: friction: p + H₂, detachment
Relative importance of plasma flow forces over chemistry and PWI: I: edge region \(\rightarrow\) II: divertor

$$\text{div}(n_{v_{||}}) + \text{div}(n_{v_{\perp}}) = \text{ionization/recombination/charge exchange}$$

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

**I: midplain**
- SOL plasma (50-300 eV), absence of neutrals and molecules, electron-impurity ion processes, radiative plasma cooling

**II: target (divertor)**
- Divertor region, 50 - 1 eV, \(10^{14} - 15\) cm\(^3\), H, H\(_2\) dominant, He, He\(^+\), impurities; neutral particle transport, helium removal, recombination, plasma – surface interaction:
  - Key for thermal power and helium exhaust problem

Planetary science is in a lower, partially overlapping region of collision energies!
Relative importance of plasma flow forces over chemistry and PWI: I edge region $\rightarrow$ II divertor

\[
\text{div}(nv_{\parallel}) + \text{div}(nv_{\perp}) = \text{ionization/recombination/charge exchange}
\]

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

In tokamak edge, all three phenomena are active everywhere

“Diffusion-advection-reaction” problem
(Fusion edge plasmas: Hybrid finite volume/Monte Carlo method)

“edge transport codes” to do the “bookkeeping” between these three processes.

Linear plasma devices often operate in the advection-reaction dominated regime

Dominant friction: $p + H_2$, detachment

paral\(\text{lell\right vs. (turbulent) cross field flow\right)

\begin{align*}
\text{I: midplain} & \quad \text{parallel vs.} \\
\text{II: target} & \quad \text{cross field flow}
\end{align*}
JET (Joint European Torus): Ø 8.5 m, 2.5 m high, 3.4 T, 7 MA, 1 min

Key area for plasma wall interaction
Plasma chemistry is localized in divertor. Provides powerful particle, momentum and energy volumetric sources for plasma flow.

**Continuity eq. for ions and electrons**

\[
\frac{\partial}{\partial \alpha} n_i + \vec{v} \cdot (n_i \vec{v}) = \mathcal{S}_{n_i}
\]

**Momentum balance for ions and electrons**

\[
\frac{\partial}{\partial \alpha} \left( m_i n_i \vec{v} \right) + \vec{v} \cdot \left( m_i n_i \vec{v} \vec{v} \right) =
\]

\[
-\vec{v} P_i - \vec{v} \cdot \vec{I}_i + Z_i n_i \left( \vec{E} + \vec{v} \times \vec{B} \right) + \vec{R}_i + \mathcal{S}_{m_i \vec{v}_i}
\]

\[
-\vec{v} P_e - en_e \left( \vec{E} + \vec{v} \times \vec{B} \right) + \vec{R}_e = 0
\]

**Energy balance for ions and electrons**

\[
\frac{\partial}{\partial \alpha} \left( \frac{3}{2} n_i T_i + \frac{m_i n_i}{2} \vec{v}_i^2 \right) +
\]

\[
\vec{v} \cdot \left[ \left( \frac{5}{2} n_i T_i + \frac{m_i n_i}{2} \vec{v}_i^2 \right) \vec{v}_i + \vec{I}_i \cdot \vec{v}_i + \vec{q}_i \right]
\]

\[
= \left( en_i Z_i \vec{E} - \vec{R}_i \right) \cdot \vec{v}_i - Q_{ei} + \mathcal{S}_{E_i}^i
\]

\[
\frac{\partial}{\partial \alpha} \left( \frac{3}{2} n_e T_e \right) + \vec{v} \cdot \left( \frac{5}{2} T_e \vec{v}_e + \vec{q}_e \right) =
\]

\[
- en_e \vec{E} \cdot \vec{v}_e + \vec{R} \cdot \vec{v}_e + Q_{ei} + \mathcal{S}_{E_e}^e
\]
B2: a 2D multi species (D+, He++, C4+...6+, ...) plasma fluid code.

EIRENE: a 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)

1D core, 0D point reactor STRAHL, ETS

processed data

Data use in Microscopic

gyro-kinetic, N-body (ERO, PIC)
Divertor detachment: ITER, simulation, detached, $T_e$ field. Movie (JET): $T_e$ during $n_e$ ramp up, transition to detachment.
Evolution of ITER divertor design:
design goal: “partial detachment” plus He removal

1996: big ITER
“wings”
to brake the gas
(“momentum removal”)
dome
to support wings
baffles
to confine neutrals
sealing
between cassettes

2001: FEAT
no “wings”
dome
to prevent neutrals reaching X-point
baffles
to confine neutrals
grill
to catch carbon

2009: final design
no “wings”
dome
to compress neutrals
baffles
to support targets
no sealing

See essay by: A.K. Kukushkin,
Molecular processes considered in fusion:

\[ e, p + H_2(v_i) \rightarrow \ldots, \quad e + H_2^+(v_i) \rightarrow H + H^* \]

- **divertor detachment dynamics, final states? DR, DE?**

www.amdis.iaea.org, database & data center network, Wuenderlich, Fantz, IPP Garching,.....


\[ e, p + C_xH_y \rightarrow \ldots, \quad e + C_xH_y^+ \rightarrow \ldots \]

C erosion and migration, tritium retention in remote areas,..... Excited states of products (CH(A\rightarrow X)) ?


\[ e + H_3^+(v_3) \rightarrow \ldots, \quad DR, DE,\ldots \]

- \( H_3^+ \) probably irrelevant in fusion plasmas


\[ e + BeH^+ \rightarrow \ldots \]

possible role on spectroscopy and on material migration: not yet clearly demonstrated. Formation rates ??


\[ e + N_2, N_2^+ \rightarrow \ldots \]

- \( N_2 \)-seeding, edge plasma cooling: \( N_2 \) not yet studied in fusion plasmas, only resulting atomic ions \( N, N^+, N^{++},\ldots \)

See planetary atmospheric research
ITER, 500 MW fusion power, $n_e$, $T_e$

$P_{FUS} = 500$ MW
$P_{He} = 100$ MW
$P_{IN} = 50$ MW

Plasma density cm$^{-3}$, log scale

Electron temperature eV, lin. scale

$n_e$ core: $\approx 10^{14}$

$T$ core: 20-25 keV
Narrowing down on the divertor plasma

Electron thermalization time

\[ \tau_{ee} \approx 3.3 \times 10^{-13} \left( \frac{T_e}{100 \text{ eV}} \right)^{3/2} \left( \frac{10^{21} \text{ cm}^{-3}}{n_i \log \Lambda} \right) \text{ s} \]

→ Electrons well thermalized in divertor
→ no need for EEFD considerations there

Divertor plasma density cm\(^{-3}\), log scale, \(10^{12} - 10^{14}\)

Divertor electron temperature eV, lin. scale, 0 – 500 eV

ITER, case 2011, single fluid, medium density
Plasma in weakly detached ITER divertor
\( n_e > 1 \times 10^{14} \), \( T_e < 5 \) eV

Tokamak Divertor Detachment:
- Self sustained dense, cold plasma layer (≈ 1 – 3 eV) formed in front of high heat flux components.
- Plasma flux drops, despite increased density

Divertor plasma density
\( \text{cm}^{-3} \), log scale, \( 10^{12} - 10^{14} \)

Divertor electron temperature
\( \text{eV} \), lin. Scale, 0 – 50 eV
Electron – ion temperature equilibration:

$\rightarrow$ Divertor $T_i \approx T_e$

$T_e - T_i$ equilibration time

$$\tau_{eq} \approx 3.16 \times 10^{-10} \frac{A}{Z^2} \left( \frac{T_e}{100 \text{ eV}} \right)^{3/2} \left( \frac{10^{21} \text{ cm}^{-3}}{n_i \log \Lambda} \right) \text{ s}$$

$\approx 1000 \times \tau_{ee}$ (for H plasma), but still fast.

Divertor $D^+$ ion temperature

eV, lin. scale, 0 – 50 eV

Divertor plasma density

$\text{cm}^{-3}$, log scale, $10^{12} - 10^{14}$
(static) plasma pressure (Pa)

- Inside separatrix (confined plasma): constant on magn. flux surf.
- In divertor: pressure drop along B-field

Momentum balance for H\(^+\) ions

\[
\frac{\partial}{\partial t} \left( m_i n_i \vec{v}_i \right) + \vec{\nabla} \cdot \left( m_i n_i \vec{v}_i \vec{v}_i \right) = -\vec{v}_p i - \vec{\nabla} \cdot \vec{\Pi}_i + Z_i e n_i \left( \vec{E} + \vec{v}_i \times \vec{B} \right) + \vec{R}_i + \vec{S}_m \vec{v}_i
\]

Near target pressure gradient balanced by momentum sinks:
- e + H\(^+\) plasma volume recombination
- Neutral gas – plasma friction
Self sustained neutral gas cushion H, H₂, H₂⁺

In ITER: neutral gas – plasma exchange is a narrow boundary layer effect
Self sustained neutral gas cushion H, H₂, H₂⁺

Neutral H density
Log color scale
$10^{10} - 10^{13}$ cm$^{-3}$

Neutral H₂ density
Log color scale
$10^{10} - 10^{13}$ cm$^{-3}$

H₂⁺ ion density
Log color scale
$10^{9} - 10^{12}$ cm$^{-3}$

Scale: x 1/10

$n_{H_2}^{+} << n_{H_2} \rightarrow \text{no significant } H_3^{+} \text{ formation}$

(competing electron collisions on $H_2^{+}$ are too strong)

(Distinct from some linear plasma devices operated at low $n_e/n_{H_2}$ ratios)
H₂ molecule, status in present SOLPS-ITER code

initially compiled 1997

13.6 eV Resonance!

More complete models are available → identify „as simple as possible“ model for fusion plasma

H₂ molecule, status in present SOLPS-ITER code

Several dedicated CR models have been constructed. see: IAEA, Nucl. Data Section www.amdis.iaea.org

- Mostly: electron collisions
- Databases: several coordinated projects (all ITER member states) by IAEA, A&M data unit, since 1977 (R. Janev → R. Clark → B. Braams, H. Chung)
- Full models are challenged at small linear plasma (divertor simulator) devices
- Fusion plasmas: strongly reduced, condensed, but underlying raw (cross section) data are publicly exposed e.g.: www.hydkin.de for the EIRENE Monte Carlo code in SOLPS-ITER edge code package.

More complete models are available → identify „as simple as possible“ model for fusion plasma.
“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**

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

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

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

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

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

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

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

**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 \( \text{H}_3^+ \)

\( \text{H}^+ + \text{H}_2 \) is the most fundamental ion-molecule system

We should know all about it  P. Krstic, ORNL, US

**Proton impact of molecule**

\[
p + \text{H}_2(v) \rightarrow p + \text{H}_2(v')
\]

\[
p + \text{H}_2(v) \rightarrow \text{H} + \text{H}_2^+(v') \quad \text{Charge transfer}
\]

\[
p + \text{H}_2(v) \rightarrow \text{H} + \text{H}^+ + \text{H}
\]

\[
p + \text{H}_2(v) \rightarrow \text{H} + \text{H}^+ + \text{H}^+ + e \quad \text{Dissoc Double ion}
\]

\[
p + \text{H}_2(v) \rightarrow p + \text{H}_2(n, v') \quad \text{Exc. elec. vib.}
\]

**Processes with molecular ion**

\[
\text{H} + \text{H}_2^+(v) \rightarrow \text{H} + \text{H}_2^+(v')
\]

\[
\text{H} + \text{H}_2^+(v) \rightarrow p + \text{H}_2(v')
\]

\[
\text{H} + \text{H}_2^+(v) \rightarrow p + \text{H} + \text{H}
\]

**Numerous other processes with molecules**

\[
\text{H}^- + \text{H}_2(v) \rightarrow \text{H} + \text{H}_2(v') + e
\]

\[
\text{H} + \text{H}_2(v) \rightarrow \text{H} + \text{H}_2(v')
\]

\[
\text{H} + \text{H}_2(v) \rightarrow \text{H} + \text{H} + \text{H}
\]

\[
\text{H}_2(v') + \text{H}_2(v'') \rightarrow \text{H}_2(v''') + \text{H}_2(v''')
\]

\[
\text{H}_2 + \text{H}_2(v) \rightarrow \text{H}_2 + \text{H} + \text{H}
\]

**Creation of \( \text{H}_3^+ \)**

\[
\text{H}_2^+(v') + \text{H}_2(v) \rightarrow \text{H}_3^+(v'') + \text{H}
\]

\( \text{H}_3^+ \) Series of interesting reactions:

DE, DR, branching ratios with electrons

D, DCT with \( \text{H} \)

- “Interplay” of transport and inelastic processes
- Rotational analysis is missing
- Isotopic constitution: \( \text{D}_2, \text{T}_2, \text{HD}, \text{HT} \) and \( \text{DT} \), sensitive on vib. energy levels
ITER divertor detachment:
Plasma pressure gradient [Pa/m] provided by:
MAR < EIR < p+H (CX) < p+H₂ (elastic) friction

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

EIR:
\[ e + p \rightarrow H + h\nu \]
\[ e + p + e \rightarrow H + e \]

CX:

Elast.
\[ p + H \rightarrow H + p \]
\[ p + H_2 - \text{elastic} \]

-100 Pa/m
0 Pa/m
100 Pa/m
Competition between processes:
(outcome in fusion divertors is sometimes quite distinct from that in linear plasma “divertor simulators”)
• \(p^+ H_2 \rightarrow H_2^+ + \ldots, e + H_2^+ \rightarrow p + H + e \) “DE wins over DR”: \(\ldots e + H_2^+ \rightarrow H + H\)
• \(e + H_2^+ \rightarrow \ldots \) fragments “wins over PR”: \(H_2 + H_2^+ \rightarrow H_3^+ + H\)
  (very low \(H_2^+, H_3^+\) concentrations)

\(H_2(v)\) vibrational kinetics is involved in a controlling way (resonance IC)

Isotopomerese? \(D^+ + HD(v) \rightarrow \ldots\) vs. \(H^+ + D_2(v) \rightarrow \ldots\), and DT, \(T_2\)?

unknown territory (in fusion edge plasma science)?

Isotopomerese: Currently only simple scalings of cross sections with transition energies
Molecular Processes considered in fusion:

e, p + H\(_2\)(v\(_i\)) \rightarrow \ldots, \ e + H\(_2\)^+(v\(_i\)) \rightarrow H + H^*

- divertor detachment dynamics, final states? DR, DE?

e, p + C\(_x\)H\(_y\) \rightarrow \ldots, \ e + C\(_x\)H\(_y\)^+ \rightarrow \ldots C erosion and migration, tritium retention in remote areas, \ldots Excited states of products (CH(A\rightarrow X))? 

e + H\(_3\)^+(v\(_3\)) \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??

e + N\(_2\), N\(_2^+\) \rightarrow \ldots NN

- N\(_2\)-seeding, edge plasma cooling: not yet studied in fusion plasmas, only resulting atomic ions N, N\(^+\), N\(^{++}\), \ldots
  See planetary atmospheric research
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

JET, Joint European Torus

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.

Hydride e,p collision cross section ($\sigma(E)$) databases for technical plasmas and fusion plasmas

Database Series 2002-..., (several IAEA coord. research projects “CRP’s”)
FZ-Jülich

Methane (CH$_y$) C$_2$H$_y$ C$_3$H$_y$

Silane (SiH$_y$) p,H,H$^-$,H$_2$,H$_2^+$,H$_3^+$


www.eirene.de & www.amdis.iaea.org
Release (chem. sputtering) and migration of hydrocarbons

Radial direction

Main plasma

Incoming flux \((D^+, C^{4+}, O^{5+})\)

Reflected and eroded particles

Reflected and eroded particles

Deposition

\(E\)

\(B\)

\(C^0\)

\(C^x^+\)

\(C\ Ki\)

\(CD_4\)

\(CD_{y,0,+}\)

Re-deposition

To remote areas...

Target-surface

Toroidal/Poloidal direction
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

Proposed ITER divertor strategy: decision at the end of 2013

H/He

D/DT

CFC/W

Full-W

Full-W

CFC monoblocks at 10 MW m⁻², W monoblocks at 5 MW m⁻²

21.11.2013; The ITER Council approved the IO proposal and decided to commence operations with a full tungsten divertor...
Proposed divertor strategy: decision at the end of 2013

- **H/He**
  - **BASELINE**
    - CFC monoblocks at 10 MW m\(^{-2}\),
    - W monoblocks at 5 MW m\(^{-2}\)
  - **FULL-W START**
    - W monoblocks at 10 MW m\(^{-2}\)

- **D/DT**
  - ~10 years
Molecular Processes considered in fusion:

\[ e, p + H_2(v_i) \rightarrow \ldots, \quad e + H_2^+(v_i) \rightarrow H + H^* \]

- divertor detachment dynamics, final states? DR, DE?

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\[ e, p + C_x H_y \rightarrow \ldots, \quad e + C_x H_y^+ \rightarrow \ldots \]
C erosion and migration, tritium retention in remote areas,….
Excited states of products (CH(A→X))?

\[ e + H_3^+(v_3) \rightarrow \ldots, \quad DR, \quad DE, \ldots \]
- \( H_3^+ \) probably irrelevant in fusion plasmas


\[ e + BeH/BeH^+ \rightarrow \ldots \quad \text{possible role on spectroscopy and on material migration:} \quad \text{Formation rates ?? 10% of Be sputtering as BeD?} \]
Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre, J. Tennyson et al. (Quantemol), R. Celiberto et al. (Bari)

\[ e + N_2, \quad N_2^+ \rightarrow \ldots \quad NN \]
- \( N_2 \)-seeding, edge plasma cooling: not yet studied in fusion plasmas, only resulting atomic ions \( N, \quad N^+, \quad N^{++}, \ldots \).

See planetary atmospheric entries research, e.g. A. Bultel et al, Universite de Rouen, France
Variation of BeD with plasma conditions

BeD contribution to total Be yield in PISCES and MD simulations

BeD detected over a wide range of accessible plasma conditions with JET-ILW


JET BeD limiter data in good agreement with yields deduced from PISCES exp. and MD simulations
Summary:

• Current magnetic confinement is powerful enough to contain a burning fusion flame

• But: exhaust of heat, ash, steady state operation of the system “plasma – vessel” (nuclear conditions) require significant attention.

• Since about mid 90th of last century we have the “makings of” a solution to this exhaust (“divertor”) problem: detached plasma state in a divertor, with a chemical richness not otherwise encountered in fusion

Detached divertors:
• Major molecular processes: e,p + H₂, e + H₂⁺, isotopomeres,
• inelastic vs. transport

Machine operation/lifetime: Material migration, tritium retention, spectroscopy:
• e,p + CₓHᵧ fusion database has been set up,
• but e,p + BeHₓ still only fragments of a database, apparently largely unknown territory

N₂ plasma cooling:
• molecular database used in fusion: obsolete, perhaps not critical (?)
Current Nucl. Fusion N$_2$ database: obsolete
see e.g.: Planetary Atmospheric Entries

**Nitrogen**
Species, states and elementary processes

\[ N_2, N_2^+, N, N^+ \text{ and } e^- \]

**CR Model Database – CoRaM – N$_2$**
Forward rate coefficient

\[ k_i(T_{A,e}) = \sqrt{\frac{8 k_B T_{A,e}}{\pi \mu}} \int_{x_0}^{+\infty} x e^{-x} \sigma_i(x) \, dx \]

with \( \sigma_i(x) \) the cross section and

\[ x = \frac{e}{k_B T_{A,e}} \] the reduced collision energy

Backward rate coefficient from **Detailed Balance**

⇒ 100 000 elementary processes

A. Bultel et al., UNIVERSITÉ DE ROUEN, UNIVERSITÉ DE AIX-MARSEILLE (FRANCE)
• Fusion edge codes: The ITER (DEMO) divertor design challenge

• Evaluation of data by experimental checks on code results (→ very indirect consistency checks only, but best one can do with codes re. data evaluation)

• → Edge codes can not evaluate (validate) data by comparison with experiments: too many other unknowns

• Format of “evaluated” edge code “reference” data

• Marc Kushner’s guidelines: databases for plasma chemistry (→ HYDKIN → data sensitivity analysis)
Particle flux determination

\[ \varepsilon = \frac{1}{4\pi} n^*_A A_{ij} \]

\[ n^*_A \sum_{k \leq i} A_{ik} = n_A n_e < \sigma_{Exg} \nu_e > \]

Particle flux \( \leftrightarrow \) number of ionisation events

\[ \frac{d\Gamma_A}{dr} = \frac{d(n_A \nu_A)}{dr} = -n_A(r)n_e(r) < \sigma_I \nu_e > \]

\[ \Gamma_A = \int_{r_1}^{r_2} n_A(r)n_e(r) < \sigma_I \nu_e > dr \]

For an exact solution one has to know the local values of \( n_e, T_e \), the rates as \( f(T_e, n_e) \)!

Assumption of a fully ionising plasma & almost constant local plasma conditions in the region of emission

\[ \Gamma_A = 4\pi \frac{I_{tot}}{B h \nu} \frac{\int_{r_1}^{r_2} n_A(r)n_e(r) < \sigma_{Exg} \nu_e > (r) dr}{\int_{r_1}^{r_2} n_A(r)n_e(r) < \sigma_{Exg} \nu_e > (r) dr} \]

\[ \Gamma_A = 4\pi \frac{I_{tot}}{B h \nu} \frac{S}{B X} \]
The kinetic equation solved by EIRENE:  www.EIRENE.de

Generic kinetic (transport) equation (L. Boltzmann, ~1870)

• for particles travelling in a background (plasma) between collisions
• with (ions) or without (neutrals, photons) forces (Lorentz)
• acting on them between collisions

Basic dependent quantity: distribution function \( f(\mathbf{r}, \mathbf{v}, t) \)

\[
\frac{\partial f(E, \Omega)}{\partial t} + \mathbf{v} \cdot \nabla f(E, \Omega) + \text{Forces} = S(E, \Omega) - \mathbf{v} \sigma_a(E) f(E, \Omega)
\]

Free flight External source Absorption

\[
+ \int_{0}^{\infty} \int_{4\pi} dE' d\Omega' \left[ \nu' \sigma_s(E' \rightarrow E, \Omega' \cdot \Omega) f(E', \Omega') - \nu \sigma_s(E \rightarrow E', \Omega' \cdot \Omega') f(E, \Omega) \right]
\]

microscopic collision kinetics, microscopic boundary conditions

Altogether, just a balance in phase space
Kinetic (transport) equation, one for each species

\[
\frac{\partial f(E, \Omega)}{\partial t} + v \nabla \cdot \nabla f(E, \Omega) + \text{Forces} = S(E, \Omega) - v \sigma_a(E) f(E, \Omega)
\]

Transport, External source, Absorption

\[
+ \int_0^\infty dE' \int_0^{4\pi} d\Omega' \left[ v' \sigma_s(E' \rightarrow E, \Omega' \cdot \Omega) f(E', \Omega') - v \sigma_s(E \rightarrow E', \Omega \cdot \Omega') f(E, \Omega) \right]
\]

Collisions, Boundary Conditions

From partial integro-differential (Boltzmann) eg. to
→ Ordinary Integral equation (0D 3V, t)
(“kinetically correct CR model”, multidimensional, retains collision Kinetics, energy exchanges, \(\rightarrow\) multiparametric CR model)

Next: remove 3d velocity space physics (0D-one-speed transport),

EIRENE \((3D3V,t)\)
Kinetic (transport) equation, one for each species

\[ \frac{\partial f(E, \vec{\Omega})}{\partial t} + v \frac{\partial f(E, \vec{\Omega})}{\partial t} \neq \text{Forces} = S(E, \vec{\Omega}) - v \sigma_a(E) f(E, \vec{\Omega}) \]

Transport

External source

Absorption

\[ + \int_0^\infty dE' \int_0^{4\pi} d\Omega' \left[ v' \sigma_s(E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega}) f(E', \vec{\Omega}') - v \sigma_s(E \rightarrow E', \vec{\Omega} \cdot \vec{\Omega}') f(E, \vec{\Omega}) \right] \]

Collisions, Boundary Conditions

System then becomes analogous to:

\[ \frac{\partial \vec{f}}{\partial t} = \vec{S} + \vec{M} f, \quad \vec{M} = \vec{C} + \frac{1}{\tau} \]

Ordinary (0D0V) CR model, “Plasma chemistry Model”

for those \( f_i \), for which the transport has been removed from kinetic equation
raw data

2004 -- ……(ongoing)

HYDKIN
database toolbox

Spectral (time scale) analysis
Public exposure of data
Sensitivity analysis

Interface

EIRENE
3D Monte Carlo kinetic transport

TEXTOR, JET, ASDEX, DIII-D, JT-60, LHD, …..

ITER
Verify Interface: HYDKIN --- EIRENE
(check for correct transfer of chemistry, correct integration of cross sections)

Make one grid cell, homogeneous plasma, source of CH4 somewhere in box, run Monte Carlo

- Mostly H from CH4 fragmentation
- \( \rightarrow \) focus stat. weights on C containing fragments

(3D3V,t) kinetic transport

(0D3V,t) kinetically correct CR model
Choose in HYDKIN and in EIRENE:
same Influx: CH₄, density: 5e12 cm⁻³, Te=Ti=1 eV, same [0,t_max] time period

Density of CHₓ vs. time
HYDKIN: closed form analytical solution, t-dep or 1D-stationary
EIRENE: Monte Carlo solution, same equation.

EIRENE: $3D3V,t \rightarrow 0D3V,t \rightarrow 0D0V,t$ exact CR model, by Monte Carlo transport
The data evaluation (e.g. for an ITER reference AM&S data set) should be on an as microscopic as possible level (plus, perhaps, provide simple toolbox to process/condense).

This is the task of atomic/molecular/surface science experts. Modeling codes can not contribute.

But: Codes are very good at reducing data, multidimensional to averaged, on a “case-by-case” basis as appropriate, based on other model time scales (transport time scale, surface saturation,…discharge time scale)
• Fusion edge codes: The ITER (DEMO) divertor design challenge

• Evaluation of data by experimental checks on code results (→ very indirect consistency checks only, but best one can do with codes re. data evaluation)

• Format of “evaluated” edge code “reference” data

• Marc Kushner’s guidelines: databases for plasma chemistry (→ HYDKIN → data sensitivity analysis)
“plasma chemistry modeling for magnetic fusion devices”

STRATEGIES FOR RAPIDLY DEVELOPING PLASMA CHEMISTRY MODELS*

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October 1999

* Work supported by NSF, SRC and AFOSR/DARPA
BEFORE YOU WERE TASKED: A TOOLBOX

- In preparation of your task, you should have assembled a flexible computational toolbox.

**Databases →**

**DataBase Processor →**

**Reaction Mechanisms →**

A "basic" global plasma model →

**Visualizer and post-processor**

Many, external resources

**“Evaluated reference data” for ITER?**

www.hydkin.de

B2-EIRENE

Many, often Matlab

University of Illinois
Optical and Discharge Physics
COMPONENTS OF YOUR TOOLBOX

**Databases:**

- Ion and Neutral transport coefficients
- Electron-impact cross sections
- Heavy particle reaction coefficients
- Gas/plasma-surface reaction probabilities

*Data should be in as "unprocessed" a form as possible. (e.g., cross sections are preferred over Townsend coefficients)*

**DataBase Processor:**

- Method to convert "raw" database to "model usable" coefficients (e.g., cross sections to rate coefficients)
  - Boltzmann solver
  - Maxwellian "integrator" of cross sections

---

**University of Illinois**  
Optical and Discharge Physics

www.eirene.de/A+Mdata  
www.eirene.de  
www.hydkin.de
Basic input for ITER divertor code: 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, H₂, H₃⁺, ....
• W, W⁺, ....W ⁷₄⁺
• N, N₂

Next GOAL: BeH, BH, .......
HYDKIN: select a number of species, and a set of reactions. Then:

The online solver automatically builds the master rate equation:

$$\frac{d\vec{y}}{dt} + \bar{A}\vec{y} = \vec{b} - \vec{y}_{\text{loss}}$$

$\bar{A}$ : master operator

$A$: constructed from reaction rates for losses and gains of population $y$

(Maxw. reaction rates are obtained by integration of reaction cross sections, “on the fly”)

\[ \begin{align*}
\vec{y} &= \begin{pmatrix}
  n_C \\
n_{CH} \\
\vdots \\
n_{CH_4}
\end{pmatrix}
\text{vector of species concentrations involved in reaction kinetics [particles/unit volume, mol/unit volume]}
\end{align*} \]

\[ \begin{align*}
\vec{b} &= \begin{pmatrix}
  \Gamma_C \\
\Gamma_{CH} \\
\vdots \\
\Gamma_{CH_4}
\end{pmatrix}
\text{influx (external source, reservoir) [injected particles/s/unit volume, injected mol/s/unit volume]}
\end{align*} \]

\[ \begin{align*}
\vec{y}_{\text{loss}} &= \begin{pmatrix}
  n_C / \tau_C \\
n_{CH} / \tau_{CH} \\
\vdots \\
n_{CH_4} / \tau_{CH_4}
\end{pmatrix}
\text{loss of species to external reservoir [loss particles/s/unit volume, loss mol/s/unit volume]}
\end{align*} \]

Gas puff, chem. sputtering

Transport losses
Error propagation and sensitivity analysis

Atomic structure → collision codes → experimental data

Velocity distribution: Boltzmann solver, Maxwellian

fundamental data

Processed data (rate coef.)

CR transition matrix $A = A_{\text{excit}} + A_{\text{radiative}} + A_{\text{ionis}} + A_{\text{cx}} + A_{\text{recomb}} + \ldots$

effective rates, population coefficients, cooling rates, beam stopping rates, \ldots

Linear algebra, ODE solvers
Error propagation and sensitivity analysis

A&M experts

Evaluation, …
Data centers

 Atomic structure
 collision codes
 experimental data

fundamental data

Process data (rate coeff.)
CR transition matrix $A = A_{\text{excit}} + A_{\text{radiative}} + A_{\text{ionis}} + A_{\text{cx}} + A_{\text{recomb}} + \ldots$

effective rates,
population coefficients
cooling rates,
beam stopping rates,….

Data centers
and/or
user community

PMI, and kinetic models

near edge plasma
far

core plasma
Error propagation and sensitivity analysis

Atomic structure

collision codes

experimental data

fundamental data

CR transition matrix $A = A_{\text{excit}} + A_{\text{radiative}} + A_{\text{ionis}} + A_{\text{cx}} + A_{\text{recomb}} + \ldots$. 

effective rates, population coefficients, cooling rates, beam stopping rates, \ldots 

reduced chemistry models

Monte Carlo, C. Ballance

Lin. Algebr. D. Reiter
Error propagation and sensitivity analysis

Atomic structure
- collision codes
- experimental data

fundamental data

Monte Carlo, C. Ballance

Processed data (rate coef.)

CR transition matrix \( A = \)
- \( A_{\text{excit}} + \)
- \( A_{\text{radiative}} + \)
- \( A_{\text{ionis}} + \)
- \( A_{\text{cx}} + \)
- \( A_{\text{recomb}} + \ldots \)

effective rates,
- population coefficients
- cooling rates,
- beam stopping rates,
- reduced chemistry models

ODEq.
Lin. Algebr.
D. Reiter

Sensitivity, error propagation to final model results:
PDEq, IDEq, …
leave to modelers, spectroscopists
Questions

Error propagation for processed data:

At which level to specify “propagated errors” in a database?
(Connor: reduced pop. coeffs., effective rates)
or : at individual rates (before CR modeling) ?
or : at (differential) cross section level ?

Perhaps (?) separate issues of “Data” (“error analysis”, propagation from atomic structure → fundamental data) and “Data processing toolbox” (linear sensitivity analysis, or Monte Carlo)
How sensitive is a result to particular process reaction rates (or transport losses)?

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.

HYDKIN.de: online sensitivity analysis


Breakup of CH₄ @ 40 eV
(143 parameters)

Analytic solution for sensitivity, online

\[ Z_{jk}(t) = \frac{d(\ln[n_j])}{d(\ln<rate_k>)} \]

Identify, print and plot the most sensitive parameters:

If \(<rate_k>\) changes by x %
Then \(n_j\) changes by x * \(Z_{jk}\) %

At 40 eV (TEXTOR)
Only DE, I, DI processes are relevant,
(nearly) no dependence on transport at all
HYDKIN.de: online sensitivity analysis


Breakup of CH4 @ 2 eV (143 parameters)

Identify, print and plot the most sensitive parameters:

If $<\text{rate}_k>$ changes by x %
Then $n_j$ changes by x * $Z_{jk}$ %

Analytic solution for sensitivity, online

$Z_{jk}(t)=d(ln[n_j])/d(ln<\text{rate}_k>)$

At 2 eV (detached divertor, PSI-2)
Only CX, DR processes are relevant, strong dependence on transport details
SENSITIVITY, uncertainty propagation

B2-fluid (2D,t) ↔ AM&S kinetic (3D3V,t) ↔ HYDKIN (0D0V,t)

(adjoint) HYDKIN sensitivity (0D0V,-t)

Adjoint B2-fluid (2D, -t) ↔ AM&S kinetic (3D3V, -t)

Available since 30 years
Recent development
Missing link

for “adjoint” automated divertor design
Probably needs detailed microscopic balance
Thank you for your attention!
Reserve slides