Atomic, Molecular And PMI Database In Current Edge Plasma Transport Codes, And Forward Sensitivity Analysis

Detlev Reiter, Maarten Blommaert*

Forschungszentrum Jülich GmbH, IEF-4, Association EURATOM – Jülich, 52428 Jülich, Germany
*KU Leuven, Department of Mechanical Engineering, 3001 Leuven, Belgium
ITER: Balance of power

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

D + T → He + neutron

\[ \begin{align*}
\text{PFUS} &= 500 \text{ MW} \\
\text{P}_{\text{He}} &= 100 \text{ MW} \\
\text{PIN} &= 50 \text{ MW}
\end{align*} \]

100 MW

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

400 MW

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

Must be exhausted from the plasma

The “divertor”
List of the main elements relevant to the ITER plasma

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

Be
Fe (SS)
N, Ne, Ar
H/D/T, He
CORE
C/W
W

S. W. Lisgo /
Outline

A: Core plasma:  (beam-) spectroscopy
strongly stripped ions, often: H, He-like

B: Plasma boundary:  spectroscopy plus: powerful plasma flows,
particle exhaust, heat exhaust, machine availability

C: Typical parameters (electron density, temperature)

D: A&M data sensitivity (→ uncertainty propagation)
   ▪ 1: status: A&M data: sensitivity analysis in 0D plasma
      chemistry models.
   ▪ 2: outlook: A&M data: sensitivity analysis in current edge
      plasma flow models ??
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     plasma flow models ???
ITER, 500 MW fusion power, $n_e$, $T_e$

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

- **Plasma density**
  - $n_e$ core: $\approx 10^{14}$ cm$^{-3}$, log scale

- **Electron temperature**
  - $T_{\text{core}}$: 20-25 keV

$10^{14}$ $10^{13}$ $10^{12}$
Relative importance of plasma flow forces over chemistry and PWI

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

\( \text{div}(\mathbf{v}_\parallel) + \text{div}(\mathbf{v}_\perp) = \text{ionization/recombination/charge exchange} \)

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

(advanced plasma scenario development)

\text{ionization/recombination/CX. Atomic data models for hot plasma spectroscopy}
- interpretation,
- line shape modelling:

Spectroscopy : \( nZ^* \)
CR Model : \( nZ^* \rightarrow nZ \)
Transport Model : \( nZ \rightarrow D_\perp, V_\perp \)
W atomic data development requested

Understanding W behaviour in the plasma core is very important for ITER and future high-performance, high-duty cycle devices

- W is a strong radiator at fusion core energies → concentration must be very low (< 0.001% in ITER)
All relevant elements other than W are fully stripped of their electrons, except in the edge region.

In the late 1970’s Afrosimov suggested to inject high energy neutrals (hydrogen) which can pass through the magnetic field, primarily to heat the plasma by momentum transfer, but more importantly, passing electrons to fully stripped plasma ions.
Neutral (H) Beam (100 keV) injection provides electrons to elements, so they can be distinguished by spectroscopy.

All elements (cooling gases, wall materials) become subject to plasma spectroscopy in fusion devices, because they are made “distinguishable” by H-diagnostic beams.

M. von Hellermann
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Relative importance of plasma flow forces over chemistry and PWI: I edge region → II divertor

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

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

I: midplain

parallel vs. (turbulent) cross field flow

II: target

parallel vs. chemistry and PWI driven flow

H, He, Be, W,… dominant process:
vol. recomb., & friction: p + H₂, “detachment”
Atomic & molecular processes: boundary plasma

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

- divertor detachment dynamics, final states? Isotopes?

www.amdis.iaea.org, database & data center network,

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


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

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


\[ e, p + Be, BeH/BeH^+ \rightarrow \ldots \quad \text{possible role on spectroscopy and on} \]

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)

\[ e, p + Ne, Ar, N, N_2, N_2^+ \rightarrow \ldots \quad ?? \]

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

Extensive database exists, See planetary atmospheric entries research, e.g. A. Bultel et al, Universite de Rouen, France
Divertor detachment: ITER, simulation, detached, $T_e$ field. Movie (JET): $T_e$ during $n_e$ ramp up, transition to detachment.

EDGE2D-EIRENE (JET-Detachment) Simulation

hotter than 1 Mill deg.
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

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

Divertor electron temperature

\( \text{eV, lin. scale, } 0 - 500 \text{ eV} \)
Plasma in “weakly detached” ITER divertor
\( n_e: > 1 \times 10^{14}, \ T_e < 5 \text{ eV} \)

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

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

**Divertor electron temperature**
\( \text{eV, lin. Scale, } 0 – 50 \text{ eV} \)
Electron – ion temperature equilibration:
\[ \rightarrow \text{Divertor } T_i \approx T_e \]

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

\[ T_e - T_i \text{ equilibration time} \]
\[ \tau_{eq} \approx 3.16 \times 10^{-10} \frac{A}{Z^2} \left( \frac{T_e}{100 \text{ eV}} \right)^{3/2} \left( \frac{10^{21} \text{ cm}^{-3}}{n_i \log A} \right) \text{ s} \]
\[ \approx 1000 \times \tau_{ee} \text{ (for H plasma), but still fast.} \]

Divertor D\(^+\) ion temperature\[ \text{eV, lin. scale, } 0 - 50 \text{ eV} \]
(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
\[
\frac{\partial}{\partial t} \left( m_i n_i \vec{v}_i \right) + \nabla \cdot \left( m_i n_i \vec{v}_i \vec{v}_i \right) = -\nabla p_i - \nabla \cdot \Pi_i + Z_i e n_i \left( \vec{E} + \vec{v}_i \times \vec{B} \right) + \vec{R}_i + \vec{S}_m \vec{v}_i
\]

Near target pressure gradient balanced by momentum sinks:
- e + H\(^+\) plasma volume recombination
- Neutral gas – plasma friction
ITER divertor detachment:
Plasma pressure gradient [Pa/m] provided by:
MAR < EIR < p+H (CX) < p+H₂ (elastic) friction

\[ p+H₂(v) \rightarrow H^{+} + H \]
\[ \text{e+H}^{+} \rightarrow H + H \]

\[ p + H \rightarrow H + p \]

100 Pa/m
0 Pa/m
-100 Pa/m

100 Pa/m
0 Pa/m
-100 Pa/m
Plasma chemistry is localized in divertor. Provides powerful particle, momentum and energy volumetric sources for plasma flow.

Continuity eq. for ions and electrons

$$\frac{\partial}{\partial \alpha} n_i + \nabla \cdot (n_i\vec{V}_i) = S_{ni}$$

Momentum balance for ions and electrons

$$\frac{\partial}{\partial \alpha} (m_in_i\vec{V}_i) + \nabla \cdot (m_in_i\vec{V}_i\vec{V}_i) =$$

$$-\nabla p_i - \nabla \cdot \Pi_i + Z_i e_n_i (\vec{E} + \vec{V}_i \times \vec{B}) + \vec{R}_i + \vec{S}_{m_i\vec{V}_i}$$

$$-\nabla p_e - e_n (\vec{E} + \vec{V}_e \times \vec{B}) + \vec{R}_e = 0$$

Energy balance for ions and electrons

$$\frac{\partial}{\partial \alpha} \left( \frac{3}{2} n_iT_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) +$$

$$\nabla \cdot \left[ \left( \frac{5}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) \vec{V}_i + \Pi_i \cdot \vec{V}_i + \vec{q}_i \right]$$

$$= \left( e_n Z_i \vec{E} - \vec{R} \right) \cdot \vec{V}_i - Q_{ei} + S^i_E$$

$$\frac{\partial}{\partial \alpha} \left( \frac{3}{2} n_e T_e \right) + \nabla \cdot \left( \frac{5}{2} n_e T_e \vec{V}_e + \vec{q}_e \right) = -e_n \vec{E} \cdot \vec{V}_e + \vec{R} \cdot \vec{V}_e + Q_{ei} + S^e_E$$
Plasma chemistry is localized in divertor. Provides powerful particle, momentum and energy volumetric sources for plasma flow.

Continuity eq. for ions and electrons

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

Momentum balance for ions and electrons

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

\[ - \vec{\nabla} p_i - \vec{\nabla} \cdot \vec{\Pi}_i + Z_i e n_i (\vec{E} + \vec{v}_i \times \vec{B}) + \vec{R}_i + \vec{S}_{m_i \vec{v}_i} \]

\[ - \vec{\nabla} p_e - e n_e (\vec{E} + \vec{v}_e \times \vec{B}) + \vec{R}_e = 0 \]

energy balance for ions and electrons

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

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

\[ = (e n_i Z_i \vec{E} - \vec{R}) \cdot \vec{v}_i - Q_{ei} + S_E^i \]

\[ \frac{\partial}{\partial t} \left( \frac{3}{2} n_e T_e \right) + \vec{\nabla} \cdot \left( \frac{5}{2} n_e T_e \vec{v}_e + \vec{q}_e \right) = -en_e \vec{E} \cdot \vec{v}_e + \vec{R} \cdot \vec{v}_i + Q_{ei} + S_E^e \]

In magnetic fusion:

focus is on plasma flow, turbulence,…..

(unknown, and computational challenge),

taking the S terms (A&M data) as „known“, and computationally „in hand“

Selection:

Non atomic physics experts

Disconnection between „fusion“ and atomic physics communities

Implementation:

Very time consuming

Software duplication

Results:

Comparison of results from different groups is often highly dependent on the atomic data used

See: Enrico Landi (CHIANTI), on atomic database for astrophysical plasmas (IAEA-NFRI, 2012, Daejeon)
Atomic & molecular processes: boundary plasma

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

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


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


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

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


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


\[ e+ N, N_2, N_2^+ \rightarrow .... \text{ NN} \]

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

See planetary atmospheric research
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/W monoblocks at 10 MW m⁻², W monoblocks at 5 MW m⁻²

FULL-W START

H/He

~10 years

W monoblocks at 10 MW m⁻²

D/DT

Full-W

Full-W

Full-W
Tokamak/Stellarator boundary: hybrid plasma (fluid) neutral/impurity (kinetic)

- **Status:**
  transition from computational science to computational engineering currently ongoing (e.g. divertor design for ITER, DEMO, W7X, JT-60SA…)
  despite many deficits still

- **But: long list of deficient understanding:**
  In particular: plasma material interaction (empirical laws only)
  but also: sources, parallel flows, cross field turbulent fluxes….

- **Goal:** separate all known (ab initio) model parts from the still unknown (ad hoc) parts, often by detailed computational bookkeeping.
  Ultimately: isolate anomalous cross field transport as only remaining unknown, to make it accessible experimentally.

  ➔ sub-Goal: at least: turn A&M&S data issues from unkown to known (at least to: “evaluated”, “publicly exposed”, “ITER reference data set”)
Thank you for your attention!
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Uncertainty propagation and sensitivity analysis

Atomic structure
  ↓
collision codes
  ↓
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

Velocity distribution: Boltzmann solver, Maxwellian

Linear algebra, ODE solvers

experimental data
Uncertainty propagation and sensitivity analysis: journey of data…

Atomic structure

collision codes

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, …

Experimental data

A&M experts

Evaluation, …

Data centers

Data centers and/or user community

PMI, and kinetic models

near edge plasma

far

core plasma

Machine design and operation
Uncertainty propagation and sensitivity analysis

Atomic structure

collision codes

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,

cooling rates,

reduced chemistry models

Monte Carlo

Lin. Algebr.

experimental data

pde, CFD, spectroscopy

Machine design and operation

Fusion plasma science
Uncertainty propagation and sensitivity analysis

Atomic structure

collision codes

experimental data

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,........

reduced chemistry models

Monte Carlo

ODEq. Lin. Algebr.

Sensitivity, error propagation to final model results:
PDEq, IDEq,........leave to modelers, spectroscopists
A&M sensitivity, uncertainty propagation in fusion reactor design and operation: How do uncertainties in A&M data propagate to divertor target heat load

Available since 30 years
Recent development
By-product from “adjoint” based automated divertor design approaches (adaptations from methodology in automotive and aeronautic applications)
Introducing adjoint sensitivities

Coils & transformers

Magnetic equilibrium

Grid generator

Plasma edge simulation

Target heat load

www.efda.org

Adjoint plasma edge Simulation

Desired change
Sensitivities from adjoint flow simulation

\[ \phi + t \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \]

\[ \nabla_{\phi} \hat{I} = \begin{pmatrix} 2 \\ -1 \\ 1 \\ 3 \\ -2 \end{pmatrix} \]
Sensitivities in practice

\[ \text{cost}(\nabla_\phi \hat{I}) \approx 2 \text{cost}(\hat{I}) \]

Details: