Tracking of internal states in collisional-radiative models employed in the transport codes

D.V.Borodin, F.Cianfrani, B.Küppers, J.Romazanov, M.Groth, P.Boerner, S.Brezinsek, Y.Marandet
Monte-Carlo edge plasma transport codes: EIRENE and ERO
Plasma flow parameters
Source terms (Particle, Momentum, Energy)

Macroscopic:

CFD codes (computational fluid dynamic):
B2, Edge2D, EMC3, SOLEdge3X, etc...

Volume grid
2D or 3D Volume grid (e.g. tetraeder) adopted for current magnetic configuration

Microscopic:

EIRENE-NGM: a 3D3v MC multi-species transport code incl. radiation transfer, kinetic or F-K hybrid.

Source terms (Particle, Momentum, Energy)

CRMs (HYDKIN, AMJUEL, ADAS, …)
for atomic and molecular neutrals
H, H*, H₂, H₂(v), H₂*, H⁻,
H₂⁺, …, impurities
Ionisation, CX, recombination etc.

What is EIRENE in a nutshell (e.g. in SOLPS)?..
ERO code: concept and design

Significant code upgrade ERO2.0:
Based on same principles, but allows extending the simulation volume significantly (using HPC)

3D full orbit simulation in test particle approximation

Plasma-Wall-Interaction (PWI)

Be wall

D, Be

D, Be

D, Be

BeD

Be wall

Impurity Transport

Be\(^0\)

Be\(^{Z+}\)

Lorentz force ionization/recombination/dissociation

friction, diffusion

light emission

physical sputtering

chemical erosion, chemically assisted physical sputtering (CAPS)

(co-)deposition

reflection

Based on same principles, but allows extending the simulation volume significantly (using HPC)
### Transport code variations and commons: CRMs

<table>
<thead>
<tr>
<th>Property</th>
<th>EIRENE</th>
<th>ERO, ERO2.0</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Ab initio</strong></td>
<td>Yes (iterations with fluid code, e.g. with B2.5 → “SOLPS-ITER”)</td>
<td>No, test-particle approximation on a given plasma BG (e.g. from SOLPS)</td>
</tr>
<tr>
<td><strong>Gyro-motion</strong></td>
<td>Guiding centre approximation</td>
<td>Full-resolved, detailed 3D wall elements, surface sheath</td>
</tr>
<tr>
<td><strong>Plasma-wall interaction</strong></td>
<td>Less detailed locally, often no 3D</td>
<td>More detailed: 3D, sheath, etc.</td>
</tr>
<tr>
<td><strong>PWI impact on plasma</strong></td>
<td>Yes, also “advanced fluid neutrals”, “wall reservoirs” etc.</td>
<td>In general NO (certain effects were introduced…)</td>
</tr>
</tbody>
</table>

Both approaches have clear advantages and range of appropriate tasks, both packages are highly demanded by ITER, EU-DEMO and other fusion-relevant devices!

*Moreover, they often support each other (plasma BGs from various CFD-EIRENE used and tested in ERO)*

However, the subtasks for treatment of atomic and molecular processes in plasma are very similar!

- Break-up of the molecular species in plasma
- Ionisation and other processes affecting charge and energy, thus transport
- Synthetic spectroscopy for comparison with diagnostics

**Similar A&M process treatment challenges!**
Collisional-radiative models (CRMs):
→ treating none-stationary
→ metastables (MS) in atoms
→ vibrational states in molecules
CRM solvers available

CRM (technically) = reaction data + SOLVER

- Most solvers solve algebraic stationary system of equations \( \frac{dN_i}{dt} = 0 \)

- in such cases the solver is much less valuable than the A&M data collection
- this statement is underlined even by the developers of the very well established and mostly up-to-date YACORA model

- CRM containing molecular species is even more complex, e.g. one needs to track more processes and more states (vibrational, rotational).

- Tracking all the states as separate species demands enormous CPU and memory resources.

- EIRENE pre-calculates rates for each volume cell. It also allows to pre-calculate values for various \( T_i/T_e \) ratios.

Effective rates:

1,2) transitions $<\text{Ex}..>$ between "GS" and "MS"

3,4) ionizations $<\text{Iz}..>$ from "GS" and "MS"

5,6) line intensity (PEC – photon emission coefficient), contributions from "GS" and "MS"

- MS-population tracking was introduced into ERO and demonstrated to be of significance by applications to PISCES-B, PSI-2 and JET-ILW (neutral Be, He, W)
- For WI dedicated ADAS dataset was developed; various lower states bundling options (~10) tested etc.
**MS-effect for WI (PSI-2 linear plasma device, JET)**

A. Eksaeva PhD-thesis, 2020

MS population exchange

- Ionization
- Recombination
- Excitation
- Line emission

Test in tokamak (JET ITER-like Wall): MS tracking reduces simulated line intensity by x1.7!

Dedicated ADAS’18 dataset

Multiple options for state bundling are worth considering
CRM FOR MOLECULES

\[ H_2 + H^+ \to H_2^+ + H \]

\[ H_2 + e \to H_2^+ + 2e \]

\[ H_2 + H_2^+ \to H \]

\[ H + e \to H^+ + 2e \]

\[ H_2^+ + e \to 2H^+ + 2e \]

\[ H^+ + e \to H + H^+ + e \]

\[ H_2 + e \to H + H^+ + 2e \]

\[ H + e \to H^+ + 2e \]

Plasma parameters:
- \( T_e = T_i = 0.2 \pm 30 \text{eV} \)
- \( n_e = n_i = 10^{19} \text{m}^{-3} \)
- \( n_e = n_i = 10^{21} \text{m}^{-3} \)

Databases:
- AMJUEL, HYDHEL
- JET
- EU-DEMO
\[ H_2 + H^+ \rightarrow H_2^+ + H \]

\[ H_2 + e \rightarrow H_2^+ + 2e \]

\[ H_2 + e \rightarrow 2H + e \]

\[ H_2 + e \rightarrow H + H^+ + 2e \]

\[ H_2 + e \rightarrow H_2^+ + e \]

\[ H_2^+ + e \rightarrow 2H^+ + 2e \]

\[ H_2 + e \rightarrow H + H^+ + 2e \]

\[ H + e \rightarrow H^+ + 2e \]

\[ H_2(X) \]


**H_2(X)**

\[ v=5 \]

\[ v=4 \]

\[ v=3 \]

\[ v=2 \]

\[ v=1 \]

\[ v=0 \]

**SOURCE**

**H_2(X)**

**Databases:**

- AMJUEL
- H2VIBR

**Plasma parameters:**

- \( T_e = T_i = 0.2 \pm 30 \text{eV} \)
- \( n_e = n_i = 10^{19} \text{m}^{-3} \)
- \( n_e = n_i = 10^{21} \text{m}^{-3} \)

**JET**

**EU-DEMO**
Standalone CRM vs EIRENE: Effective source (JET)

- CRM in each simulation cell: molecule density scales linearly with the source →
  with isotope rescaling

\[
\frac{\text{density}(\text{edge2D})}{\text{density}(\text{CRM})} = \frac{\text{effective source}(\text{edge2D})}{\text{reference source}(\text{CRM})}
\]

Effective source

Gas puffing

- divertor region: iny → novel physical conditions (dominance of CX reactions at low temperature)

Based on EDGE2D-EIRENE simulations
JET shot 81472

M Groth et al. NF 2013
SOLPS-ITER basic simulation case for EU-DEMO

Below X-point:
1) $T_e = T_i = 10\text{eV}$
2) $T(H) = T(H_2) = 10\text{eV}$
3) $N_e \sim 10^{18}\ \text{m}^{-3}$
4) $N(H) = 10^{20}\ \text{m}^{-3}$
5) . . .

We can do the following:

a) run full EIRENE: SOLPS with a “frozen” fluid side (B2.5)

b) try to get some results from the standalone approach (mostly neglecting transport)
low temperature (T < 2eV) leading reaction chains:

\[ \text{MAR/MAD} \]

competition at very low temperature

**CRM FOR MOLECULES: leading reactions**
EU-DEMO – effect of resolution by vibrostates

Fully in line with the EIRENE and other CRMs:

JET modelling: “Up to 40% reduction in effective dissociation rate due to transport of vibrational states”

A.Holm, M.Groth, et al., PET, CPP 2021

F.Cianfrani et al., EPS-2022
Larger molecular density (factor $\approx 2 - 3$) along the separatrix with vibr. resolution.

Resolved vs. unresolved on vibrostates CRM in EIRENE
CRM underestimates excited state population at large temperature.

CRM overestimates excited state population at low temperature.

SIMULATIONS: SOURCE υ=0

EIRENE: 793'300 histories
EIRENE×10: 7'933'000 histories
EIRENE×100: 79'330'000 histories
The deviations from CRM are determined by molecular sources:

\[
\hat{S}_v = \sum_{\nu=\nu_0}^{N} S_{\nu}^{EIR} \left( \frac{n_{\nu}}{n_{\nu+1}} \right)^{CRM} \left( 1 - \frac{\hat{S}_v}{k_v^{exc} n_e n_\nu} \right)
\]

Positive deviations at sinks

Negative deviations at sources

\[
\left( \frac{n_{\nu+1}}{n_\nu} \right)^{EIR} = \left( \frac{n_{\nu+1}}{n_\nu} \right)^{CRM} \left( 1 - \frac{\hat{S}_v}{k_v^{exc} n_e n_\nu} \right)
\]
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\]

\[
\hat{S}_\nu = \sum_{\nu=\nu+1}^{N} S^{EIR}_\nu \left( \frac{n_{\nu}}{n_{\nu+1}} \right)_{CRM} \frac{k^{dex}_{\nu} \cdot \ldots \cdot k^{dex}_{\nu+2}}{k^{exc}_{\nu+1} \cdot \ldots \cdot k^{exc}_{\nu-1}} \frac{1}{\nu - \nu - 1}
\]

Positive deviations at sinks

Negative deviations at sources

\[ k^{exc/dex}_\nu \] : excitation/de-excitation rate

EIRENE:

\[ S^{in}_{\nu} + S^{EIR}_{\nu} \]

diss./ion. /transp.

CRM:

\[ S^{ref}_{\nu} \]

diss./ion.

Standalone CRM vs EIRENE - 3
EXCITED MOLECULAR STATES

Model for excited states on top of ground state distribution:

- population coeff. excited state $d^3\Pi_u$: $n_i = n(d, \nu=i)$

\[
\begin{align*}
\text{n}_1/\text{n}_0 & \quad 1 & \quad 1 \\
\text{n}_2/\text{n}_1 & & 1 \\
\text{n}_3/\text{n}_2 & & \\
\text{n}_4/\text{n}_3 & & \\
\end{align*}
\]

\[
\begin{align*}
\nu = 0 & \quad \nu = 1 & \quad \nu = 2 & \quad \nu = 3 & \quad \nu = 4 & \quad \nu = 5 \\
@ & & & & & \\
\end{align*}
\]

- e-impact exc.
- spont. decay
- MCCC database: Scarlett ADT 2021
- Fantz Wünderlich ADT 2006

ratio of Fulcher band intensities as a proxy for ground state vibr. distribution
EIRENE: exited molecular states in divertor

Excited state $d\ 3\Pi_u$: Deuterium (D) divertor population coefficients $\approx 1.6$

Vibro-state population ratio $n_1/n_0$: Deuterium (D) divertor population coefficients $\approx 1.6$

Hydrogen (H) exited molecular states in divertor

EIRENE: exited molecular states in divertor

Vibro-state population ratio $n_1/n_0$: Hydrogen (H) divertor population coefficients $\approx 1.2$
New (or updated) modelling tools:

→ Ploutos
→ ModCR
Standalone CRM - Ploutos: what is inside?..  

Earlier known as “HydKin”

1) CRM solver (transport excluded, pure A&M side of the problem) with extensive features
   ➔ Stationary and non-stationary solution (assuming velocity and plasma pars)
   ➔ Any specie can be treated as “Reservoir”
   ➔ “Spectral analysis” based on eigenvalue approach (which reactions are most important?)
   ➔ Sensitivity analysis – vary the plasma parameters, solver settings, reactions, etc.

2) Plotting, solver results visualisation
   ➔ Useful for fast consistency checks and trivial analysis while constructing the CRMs
   ➔ Good for physics analysis in case one follows established routines

3) Flexible reaction tables interconnected with the solver and plotting
   ➔ Optimised for consistency checks and trivial analysis while constructing the CRMs
   ➔ Input/output in various formats (new: JSON) including directly for EIRENE
   ➔ Critical things are highlighted, level of information detail controlled by the user.
   ➔ Data is grouped by the reactions (even if from various sources).
   ➔ Standard or custom initial configurations
PLOUTOS can be used to

- to import/export data (JSON, tabular, etc.)
- to produce input data for EIRENE and for other codes with CRMs
  
  load/improve/save the developed configuration (selected reactions and parameters) including starting from the standard pre-sets
- to check data for consistency and abnormal features
- do sensitivity studies:

  understand A&M side of the problem and identify the most significant processes (among the selected ones)

Both statues are at Glyptothek, Munich.

www.eirene.de

EIRENE
### PLOUTOS – (H$_2$ 2022/23 case)

<table>
<thead>
<tr>
<th>Collision with e</th>
<th>Number reaction</th>
<th>Range</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>e + H(1s) → H(2p) + e</td>
<td>$E_{\text{min}}$: 1.08e+01, $E_{\text{max}}$: 2.00e+04</td>
<td>JanevEtAl(1987)</td>
</tr>
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<td>$T_{\text{min}}$: 1.26e+00, $T_{\text{max}}$: 2.00e+04</td>
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<tr>
<td></td>
<td>e + H(n) → H(n') + e</td>
<td>$E_{\text{min}}$: 1.00e-01, $E_{\text{max}}$: 1.00e+03</td>
<td>SawadaFujimoto(1995)</td>
</tr>
</tbody>
</table>

Visibility columns:
- reaction: switch to off
- range: switch to off
- reference: switch to off
- data type: switch to off
- Peculiar properties: switch to on
- generation: switch to on
- data origin: switch to on
- File/chapter: switch to off

Buttons to adjust table content:
- show only selected reactions (Groups)
- show only selected reactions (rows)
New CRM Solver for EIRENE concepted

- This CRM is aimed to precompute rate coefficients accounting for all parametric dependences \((n_e, T_e, \text{but also } T_i, \ldots)\) in contrast with currently used polynomial fits (AMJUEL, ...) + add a number of levels/processes not accounted for at this time.

- The internal states (e.g., rovibrational states in molecular species) are to be tracked with a flexible control over this resolution (as separate species or variable).

- The nonstationary solution for balance equations should be the default one (with the stationary only as a useful option).

- The solver should be modular, thus usable standalone or even in various codes.

- The improved A&M data input should be readable and structured (for starters JSON, potentially also HDF5). It should be pre-processed mostly automatic and easily exchanged with other codes and tools. We need tools for visualisation and testing.
  - The only way to meet the exploding amounts of data from RMPS and CCC for molecules (with resolution by rovibrational states)
  - IAEA GNAMPP assists, but also reveals the challenges

Not only performance and reliability to be improved, but additional physics can be provided!
New code (also library for EIRENE): “ModCR”

- Should provide **BOTH** standalone and build-in CRM for EIRENE
  - Therefore written in modern Fortran
  - Linked with Ploutos (uses the same JSON files for I/O)
    - *(AMJuel, HydHel, H2Vibr, etc are already inside, moreover under flexible web-powered control)*
  - Non-stationary approach utilising up-to-date Sundails solver (CVODE) for stiff ODE systems
    - *(algebraic stationary option also available for control)*

- The whole specie-state and reaction basis is inside, however the code should form the list of “active states”
  - Determined by user in JSON parameter file (for a few simulations)
  - Provide different resolution on states being tracked
  - Provide **flexible** border for tracking of MC species and internal state populations as variables

(This is unique and justifies creation of the new code)
ODE Solver for ModCR

- **SUNDIALS**: SUite of Nonlinear and DIfferential/ALgebraic Equation Solvers

Developed at LLNL - awarded the 2023 SIAM/ACM Prize in Computational Science and Engineering

[![git repository](https://github.com/LLNL/sundials)](https://github.com/LLNL/sundials)

<table>
<thead>
<tr>
<th>Package</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>CVODE</td>
<td>solves initial value problems for ordinary differential equation (ODE) systems.</td>
</tr>
<tr>
<td>CVODES</td>
<td>solves ODE systems and includes sensitivity analysis capabilities (forward and adjoint).</td>
</tr>
<tr>
<td>ARKODE</td>
<td>solves initial value ODE problems with additive Runge-Kutta methods, including support for IMEX methods.</td>
</tr>
<tr>
<td>IDA</td>
<td>solves initial value problems for differential-algebraic equation (DAE) systems.</td>
</tr>
<tr>
<td>IDAS</td>
<td>solves DAE systems and includes sensitivity analysis capabilities (forward and adjoint).</td>
</tr>
<tr>
<td>KINSOL</td>
<td>solves nonlinear algebraic systems.</td>
</tr>
</tbody>
</table>

Modern, powerful and flexible – still it is available in FORTRAN (so suits to EIRENE)
Summary and outlook

1) CRMs are essential and potentially common part of the plasma MC transport codes

2) Transport and A&M sides of MC transport codes are NOT separable, however using the standalone approach is often extremely useful
   - Gives insight into the A&M physics
   - Allows more control, looking into details and straightforward answers
   - Particular valuable if standalone and external CRM would be just the same
   - Isotope (D vs. H) effect demonstrates the significance of vibro-resolved MCCC data

3) New CRM (ModCR) is concepted and under development
   - PLOUTOS will keep and even strengthen its role as data pre-processor
   - It is aimed to provide flexible “border” between particles treated as MC species or variables characterising the internal state

4) Opacity and other effects should be available in ModCR, but it is too early to talk about that at the current stage.

Further details at [www.eirene.de](http://www.eirene.de)
Thanks for the attention!

Special thanks to
1) ADAS (M.O’Mullane et al.) for constant support
2) YACORA developers (U.Fanz, D.Wunderlich, et al.) for consultations
3) MCCC developers (D.V.Fursa et al.) for providing the database
Collisional-Radiative Models (CRM)

Grotrian diagram for atomic H (D, T)

Ry=13.6eV

**Balance equations:**
\[
\frac{dN_i}{dt} = \sum_{j \neq i} A_{ji} N_j + n_e \cdot (EXCIT + IZ + CX + REC) 
\]

**EXCIT** = \[\sum_{j \neq i} \langle v \sigma_{ji} \rangle N_j \]

**IZ** = \[\sum_{m} \langle v \sigma_{mj} \rangle N_m^- + \sum_{z} \langle v \sigma_{zi} \rangle N_z^{2-} + \ldots \]

**REC** = \[\sum_{k} \langle v \sigma_{ki} \rangle N_k^+ + \sum_{l} \langle v \sigma_{li} \rangle N_l^{2+} + \ldots \]

\[ \ldots \]

\[ j, k, l, m, z, \ldots \] states can be fine-superfine resolved or, opposite, bundled into few quasi-metastables (MS)

CRM = list of states + transition data

Often used:
\[ \langle v \sigma_{ji} \rangle (T_e, n_e) \] - effective Maxwellian averaged rates
These are semi-detached conditions (1 point)

- Attached vs. detached + 2-3 semidetached cases would be wishful to have!
- We use EIRENE or standalone CRM to identify spectral features useful for the degree of detachment control for this plasma conditions

We can run (and mean to in future!) full EIRENE: SOLPS with a “frozen” fluid side (B2.5)

- This option is not mature enough for meaningful physics results
- We use standalone CRM and vary constant plasma conditions around

Below X-point:
1) \( T_e = T_i = 10\text{eV} \)
2) \( T(H) = T(H_2) = 10\text{eV} \)
3) \( N_e \sim 10\text{e}^{18} \text{m}^{-3} \)
4) \( N(H) = 10\text{e}^{20} \text{m}^{-3} \)
• **SUNDIALS**: SUite of Nonlinear and DIfferential/ALgebraic Equation Solvers

written in C++: **Modern Fortran interface** (modules)

\[ \dot{y} = f(t, y), \quad y(t_0) = y_0 \]

- **CVODE**: solution of IVP variable-step multistep methods:
  - ADAMS-MOULTON FORMULAS
  - BACKWARDS DIFFERENTIATION FORMULAS \( \rightarrow \) stiff problems

**Nonlinear solve**:
- default: Newton iteration based on linear solver
- user-defined

**Linear solver families**:
- *direct* for dense, banded, or sparse matrices
- *spils*: scaled preconditioned iterative (Krylov) linear solvers.
YACORA: inclusion molecular source term

• Stationary run vibrationally resolved:

\[ p, H^+_2, Z \]
\[ H_2(v = 0), \ldots, H_2(v = 14) \]

- Electron impact:
  \[ H_2 + e \rightarrow H_2(b_{\text{triplet}}) \rightarrow H^+ + H^+ + e + e \]
  \[ H_2 + e \rightarrow H^+_2 + e + e \]
  \[ H_2 + p \rightarrow H^+_2 + p + e \]
  \[ H_2 + e \rightarrow H^+ + H^+ + e + e \]

- Vibrational transitions:
  \[ H_2(v = 0) \rightarrow H_2(v = 1) \]
  \[ H_2(v = 1) \rightarrow H_2(v = 2) \]

- Proton impact:
  \[ H_2(p = 0) \rightarrow H_2(p = 1) \]

- Electron impact:
  \[ H_2(v = 13) \rightarrow H_2(v = 14) \]

\[ Z \rightarrow H_2(v = 0) \]