The EIRENE.DE online database for surface and A+M data in fusion edge modelling

Detlev Reiter | Institute of Energy Research – Plasma Physics |
OUTLINE

I  Motivation (very short)

II  Current plasma chemistry modeling activities in FZJ (short)

III  Hydrogen and Helium Chemistry in Fusion Plasmas:
     the EIRENE code and the HYDKIN online toolboxes
Relative importance of plasma flow forces over chemistry and PWI

I core plasma \(\rightarrow\) II edge region \(\rightarrow\) III divertor

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

II: midplain

parallel vs. (turbulent) cross field flow

III: target

parallel vs. chemistry and PWI driven flow

Dominant friction: \(p + H_2\)
Integrated edge plasma simulation: “From the barrier to the target”

Drift-Fluid turbulence: Attempt


EMC3 (& B2) CFD, 2D & 3D
Charged fluid parcels
m – 100 m scale

Mostly ITER contractual work

EIRENE
3D kinetic
Gyro centers,
Entire SOL and Core
mm - m scale

ERO, PEPC
“Real” ions (and electrons)
PSI in plasma, near solid
(sub-) cm scale

Input: Kinetic boundary conditions

PMI inside solid: TRIM.xxx,
Material science etc…,
nm-scale

Iter

ITER

MACRO

MICRO
ITER, B2-EIRENE simulation, fully detached, $T_e$ field hotter than 1 Mill deg.
Atomic, Molecular and Surface physics is mainly integrated into fusion edge plasma codes via kinetic (Monte Carlo) solvers: DEGAS-2 (US), NIMBUS (stopped), NEUT2D (JP), EIRENE (EU), ...

B2 – EIRENE (ITER, since 1991, TEXTOR, ASDEX,…many more ) (FV, 2D)

OSM – EIRENE (D-IIID, ITER,….)

EDGE2D – EIRENE (JET, since 2007) (FD, 2D)


FIDAP – EIRENE (Philips Lighting, finished, lamps marketed in 2008) (FEM, 3D)

+….many stand alone applications to specific physics questions
Numerical tool for the edge plasma transport: B2-EIRENE code package

SOLPS4.3: ITER.org (Cadarache) – FZ Juelich
jointly developed and applied: since about 15 years

Self-consistent description of the magnetized plasma, and neutral particles produced due to surface and volume recombination and sputtering

see www.eirene.de

**B2**: a 2D multi species (D\(^+\), He\(^{+;++}\), C\(^{4+;6+}\),...) 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)

**CR codes**: HYDKIN

Computational Grid
ITER contractual edge modelling

Goal: quantify PWI, when RMPs are applied in ITER
(EMC3-EIRENE 3D tokamak edge transport application)

F4E-GRT-055 (PMS-PE)
FZJ-IPP-CEA
(since July 2010)

Goal: diagnostic mirror lifetime assessment
(closing the gap between SOL and wall in B2-EIRENE)

ITER.CT.09.4300000034
FZJ (since Oct. 2009)

SOLPS4.x (ITER, FZJ) vs. SOLPS 5.y (IPP)

F4E-OPE-258
FZJ, Univ. St. Petersburg, (Dec. 2010)
FZJ activities:
Plasma Chemistry Modeling for Fusion

I) CAD design
II) grid generation ANSYS
III) 3D EIRENE
Monte Carlo Simulation
Erosion, Deposition (lifetime) of mirrors

PMI data: TRIM.xxx

BES, CXRS, Data: O.Marchuk et al.

Color: erosion rate inside port plug by Be wall impurities

Data: HYDKIN B2-EIRENE
The ITER design review found that PF coil set would not support range of operating space for 15 MA, $Q_{DT} = 10$ inductive scenario goals to be met when more realistic assumptions used:

- Excessive V-s consumption during $I_p$ ramp-up $\rightarrow$ restrictions on flattop time
- Peaked current profiles during ramp-up $\rightarrow$ instability
- Broader current profiles due to H-mode pedestal $\rightarrow$ PF6 coil current and field limits exceeded
- Central solenoid separation forces restricting operational space

Divertor dome and slot clearances of 2007 design too small for nominal operating points and during disturbance transients

- Modification of PF system $\rightarrow$ Change in equilibrium
The geneology of ITER divertors
2007-2009: New reference design
B2-EIRENE: main ITER edge plasma design tool

Kukushkin A., Lisgo, S. et al. (ITER IO)
Kotov. V., Reiter D. et al., (FZ-J)
Pacher G. et al. (INRS-EMT, Varennes, Québec, Canada)

2004 reference

Calculations slow \(\rightarrow\) so use the previously studied variants to see the progression
Extend parallelization of EIRENE to B2-EIRENE (2008), + HPC-FF, ….
This work: “plasma chemistry modeling for magnetic fusion devices”

STRATEGIES FOR RAPIDLY DEVELOPING PLASMA CHEMISTRY MODELS*

Mark J. Kushner
University of Illinois
Dept. of Electrical and Computer Engineering
Urbana, IL, 61801, USA

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 → Many, external ressources

DataBase Processor

Reaction Mechanisms

A "basic" global plasma model →

Visualizer and post-processor

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
CONSTRUCTING YOUR DATABASE

- The most reliable, most understood, most readily available, best formatted and most "comfortable" databases available are those you build *yourself*

- Take FULL advantage of all external resources in building your database however devise a method of formatting, keeping track of references, revisions and updates which best suits *your* needs.

- *(DON'T ALLOW YOUR ABILITY TO ACCOMPLISH YOUR GOAL BE LIMITED BY SOMEONE ELSE'S DECISION TO UPDATE THE FORMAT OF THEIR DATABASE...)*

- In constructing your database, you will need to make value judgements on the goodness, appropriateness and validity of primary data sources or other databases.

- Make these decisions with some deliberate forethought as to what the database (or subsets of the database) will be used for.

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*University of Illinois*

Optical and Discharge Physics*
www.eirene.de → A&M Data → HYDHEL, AMJUEL

Atomic & Molecular Database

Choose one of the A&M databases from the menu. For questions refer to the FAQ or contact us.

HYDK
Reaction kinetics for Hydrocarbon catalysis
Plasm

Hydride Database:

Methane family:
Ethane/Propane family:
Silane family:
Hydrogen family:

Juel-Report 3966:
Collision Processes of Hydrocarbon Species in Hydrogen Plasmas: I. Methane Family
(by R. Janev & D. Reiter)

Juel-Report 4005:
Collision Processes of Hydrocarbon Species in Hydrogen Plasmas: II. Ethane & Propane Families
(by R. Janev & D. Reiter)

Juel-Report 4038:
Collision Processes of Hydrocarbon Species in Hydrogen Plasmas: III. Silane Family
(by R. Janev & D. Reiter)

Juel-R...

All data, figs, and references: HERE
Our own homemade “database” for fusion plasma chemistry modelling, in this sense described by M. Kushner, 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 (CH₃)  C₂H₃  C₃H₃
Silane (SiH₃)  p,H,H⁻,H₂,H₂⁺,H₃⁺

JUEL 3966, Feb 2002

JUEL 4005, Oct. 2002

JUEL 4038, Mar. 2003

JUEL 4105, Dec. 2003
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, H₂, H₃⁺,….
• W, W⁺, ….W 74⁺
• N, N₂

Next GOAL: BeH, BH, ……
raw data → 2004 -- ...... (ongoing)

HYDKIN database toolbox → Spectral (time scale) analysis

HYDKIN database toolbox → fragmentation pathways

HYDKIN database toolbox → Sensitivity analysis

Interface → EIRENE

EIRENE 3D Monte Carlo kinetic transport → TEXTOR, JET, ASDEX, DIII-D, JT-60, LHD, ...... → ITER
## Example: Hydrocarbon cross section database

Molecular Data analysis (www.HYDKIN.de):

IAEA, Data centers (ORNL, NIFS, …)

<table>
<thead>
<tr>
<th></th>
<th>CH$_4$</th>
<th>C$_2$H$_6$</th>
<th>C$_3$H$_8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>DE</td>
<td>RKJ 2009</td>
<td>JR 2004</td>
<td>JR 2004</td>
</tr>
<tr>
<td>I-DI</td>
<td>RKJ 2009</td>
<td>RKJ 2009 #</td>
<td>JR 2004 ##</td>
</tr>
<tr>
<td>DI$^+$</td>
<td>RKJ 2009</td>
<td>JR 2004 #</td>
<td>JR 2004 #</td>
</tr>
<tr>
<td>CX-PR</td>
<td>2011 Upgrade ongoing: more low T reactions: Particle exchange</td>
<td>JR 2004</td>
<td>JR 2004</td>
</tr>
<tr>
<td>R-DR</td>
<td>JR 2002</td>
<td>RKJ 2009</td>
<td>RKJ 2009</td>
</tr>
</tbody>
</table>


- **DE**: Dissociative excitation of neutral molecules
- **DE$^+$**: Dissociative excitation of molecular ions
- **I-DI**: Ionisation and Dissociative Ionisation of neutral molecules
- **DI$^+$**: Dissociative Ionisation of molecular ions
- **CX-PR**: Charge exchange and particle re-arrangement
- **R-DR**: Recombination, Dissociative Recombination

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# new experiments planned Univ. Louvian la Neuve, P. Defrance et al.
# # Revision planned in 2011, Univ. Innsbruck, S. Huber et al., CPP 2011, in printing
Major difference to other online A@M toolboxes:

Not COL. RAD., but SPECTRAL A@M modelling (needed in transport codes for time-scale analysis)

→ Online sensitivity analysis possible !

Perhaps in the future:
Revised data reduction scheme (ILDM rather than CR):
Dauwe, Tytgadt, Reiter, JUEL 4229, Nov. 2006,
Available on www.eirene.de/html/relevant_reports
HYDKIN.de: online sensitivity analysis


Breakup of CH4 @ 40 eV (143 parameters)

Analytic solution for sensitivity, online

\[ Z(t) = \frac{d(\ln[n_Y])}{d(\ln<\text{rate}>)} \]

Identify, print and plot the most sensitive parameters:

If \(<\text{rate}> \) changes by \( x \) %
Then \( n_Y \) changes by \( x \times Z \) %

At 40 eV (TEXTOR)
Only DE, I, DI processes are relevant,
(nearly) no dependence on transport at all
Analytic solution for sensitivity, online

\[ Z(t) = \frac{d(\ln[n_Y])}{d(\ln<\text{rate}>)} \]

Identify, print and plot the most sensitive parameters:

If \(<\text{rate}>\) changes by \(x\) %
Then \(n_Y\) changes by \(x \times Z\) %

At 2 eV (detached divertor, PSI-2)
Only CX, DR processes are relevant, strong dependence on transport details
TRIM-codes family, online database for fully kinetic reflection velocity space PDFs

Legend:
- Eirene Reflection Database (TRIM-Code, section 1.1)
- W. Eckstein, "Calculated sputtering, reflection and range values", IPP-Report IPP 9/113, 2002
Storing full 3D pdf of reflected particles, for given incident energy (12) and angle (7) i.e. 84 tables for each target-projectile combination

Next: similar database for sputtering.

TRIM database (www.eirene.de)

Figure 1: Sample reflection data table, for D on Fe, 200 eV, 30 degrees incident energy and angle, respectively. Marked are the reflection energy, polar and azimuthal angles for the triple of random number (0.3, 0.5, 0.9)
Goal: replace various scalings (e.g. Yamamura for incident angle dependence) by full database, same format as for EIRENE-reflection database

Still not decided: how to parameterize
a) Surface roughness,
b) Material mixing

Universal sputtering law: Janev, Ralchenko, et al. for normal incidence yield.
Backup slides
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, or guiding center) acting on them between collisions

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

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

Free flight  \hspace{1cm} \text{External source}  \hspace{1cm} \text{Absorption}

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

Collisions, boundary conditions

Altogether, just a balance in phase space
CR Models in Transport Codes

1) System of N kinetic (or fluid) equations (PDE, IDE), one for each species: H, H*, Ly_α…

2) Select M species, remove transport term and explicit time derivative
   (Interpretation: their lifetime is short compared to transport time)

3) System reduced to N – M transport equations plus one linear algebraic system (CR Model), of order M

The M states are in quasi steady state with the N – M transported species.
CR models are QSS models
Kinetic (transport) equation IDE, one for each species

\[ \frac{\partial f(E, \Omega)}{\partial t} = \text{EIRENE:} \]

NFOL\(_i\)=-1 option

0 = \( S(E, \Omega) - \nu \sigma_a(E) f(E, \Omega) \)

External source  Absorption

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

Collisions, Boundary Conditions

Provides fully user controlled condensation of plasma chemistry into CR model, retaining all parametric dependencies in multidimensional reduced rates but, of course is also a patently foolish way to build CR models (by “Monte Carlo matrix inversion”).
N-M coupled Boltzmann eqs. for: \( f_i, \ i=1,...,N-M \)

\[ \frac{\partial f}{\partial t} = \vec{M}f + \vec{S} \]

for: \( f_i, \ i=N-M+1,...,M \)

- No general rules for “condensation” of chemistry matrix \( M \) exist.
- Optimal condensation is highly cases dependent.
- Transport codes do not need CR-Model data (eff. rate coeff.), but the Master Matrix \( M \) and a solver “on the fly” embedded as sub-module into them.
- No a-priory “bundling” of states.
e.g. $\bar{y} = \begin{pmatrix} n_{CH_4} \\ n_{CH_4} \end{pmatrix}$ vector of species concentrations involved in reaction kinetics [particles/unit volume, mol/unit volume]

$\bar{b} = \begin{pmatrix} \Gamma_C \\ \Gamma_{CH} \end{pmatrix}$ influx (external source, reservoir [injected particles/s/unit volume, injected mol/s/unit volume]

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


Contact: b.kueppers@fz-juelich.de
### Corrections, addition

<table>
<thead>
<tr>
<th>Date</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feb., 28, 2007</td>
<td>Revision: energy depending branching ratios</td>
</tr>
<tr>
<td>June, 25, 2006</td>
<td>Memo added re. definition of D/XB values.</td>
</tr>
<tr>
<td>June, 9, 2006</td>
<td>partial cross sections for C&lt;sub&gt;2&lt;/sub&gt; ionization and dissociative ionization channels added</td>
</tr>
<tr>
<td>April 28, 2006</td>
<td>Implemented: the (thermal) particle rearrangement channels (see plotform, under CX-PR)</td>
</tr>
<tr>
<td>Dec. 21, 2005</td>
<td>Implemented: excitation rates for Swan, Mulliken and 390nm HC-band, for S/XB evaluations</td>
</tr>
<tr>
<td>Dec. 19, 2005</td>
<td>Implemented: CAD (Capture auto dissociation channels) (could be relevant at energies well below threshold for DE&lt;sup&gt;+&lt;/sup&gt; channels)</td>
</tr>
<tr>
<td>Dec. 14, 2005</td>
<td>Implemented: ADAS charge exchange recombination rates for atomic carbon ions, neutral H-density added as parameter</td>
</tr>
<tr>
<td>Dec. 10, 2005</td>
<td>Implemented: ADAS ionization and recombination rates for atomic carbon ions</td>
</tr>
<tr>
<td>Nov. 3, 2005</td>
<td>print all values of rates as used in transition matrix, see under matrix elements</td>
</tr>
<tr>
<td>Nov. 3, 2005</td>
<td>Sample case added, C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;4&lt;/sub&gt; source</td>
</tr>
<tr>
<td>Nov. 2, 2005</td>
<td>thermal CX, PR components removed for ethane, propane families to avoid double counting was ok for methane family</td>
</tr>
</tbody>
</table>

**Revisions 04-09:** APID Vol. 16 (2011)

### Issue: backward compatibility
NEW: added after Juel-Reports and PoP papers

NEW: surface reflection database
Choose plasma background
Integration time
Graphical presentation
### Printout:

Reflect input as selected

(composition, initial condition, influx, transport losses, per species)

### Printout in tabular form

<table>
<thead>
<tr>
<th>number</th>
<th>species</th>
<th>init.cond (#/unit volume)</th>
<th>influx (#/unit volume)</th>
<th>losstime (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H⁺</td>
<td>0</td>
<td>0</td>
<td>1e+300</td>
</tr>
<tr>
<td>2</td>
<td>H</td>
<td>0</td>
<td>0</td>
<td>1e+300</td>
</tr>
<tr>
<td>3</td>
<td>H₂⁺</td>
<td>0</td>
<td>0</td>
<td>1e+300</td>
</tr>
<tr>
<td>4</td>
<td>H₂</td>
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<td>0</td>
<td>1e+300</td>
</tr>
<tr>
<td>5</td>
<td>C²⁺</td>
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<td>0</td>
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</tr>
<tr>
<td>6</td>
<td>C⁺</td>
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<tr>
<td>7</td>
<td>C</td>
<td>0</td>
<td>0</td>
<td>1e+300</td>
</tr>
<tr>
<td>8</td>
<td>CH⁺</td>
<td>0</td>
<td>0</td>
<td>1e+300</td>
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<tr>
<td>9</td>
<td>CH</td>
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<td>10</td>
<td>CH₂⁺</td>
<td>0</td>
<td>0</td>
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<tr>
<td>15</td>
<td>CH₄</td>
<td>0</td>
<td>1</td>
<td>1e+300</td>
</tr>
</tbody>
</table>

C⁺(3H) lost to external reservoir
H₂ final (absorbing) state (Eigenvalue = 0)
H₂⁺ final (absorbing) state (Eigenvalue = 0)
H⁺ final (absorbing) state (Eigenvalue = 0)
H final (absorbing) state (Eigenvalue = 0)

### Printout in tabular form

- matrix elements
- Table reactions - species
- Output for EIRENE
- printout of solution in tabular form

### Output for interface to EIRENE

All individual rates used
Solution, vs. time (distance)

Here: $0 \rightarrow 1 \times 10^{-4}$ s

Species selected for printout and plotting
Online solution of time-dep. (1D) Hydrocarbon breakup, for any prescribed divertor plasma conditions, up to C$_3$H$_8$
Diagnostics from this run at $t = t_{\text{max}} = 1.0 \times 10^{-3}$ s

$T_e$ [eV] = 25
$T_p$ [eV] = 25
$T_H$ [eV] = 10
$n_0$ [#/cm$^3$] = $1.0 \times 10^{13}$
$n_p$ [#/cm$^3$] = $1.0 \times 10^{13}$
$n_H$ [#/cm$^3$] = $1.0 \times 10^{13}$

$E_0$ [eV] = 1
total influx [#/s/unit volume] = $1.00 \times 10^0$

production and loss rates at $t = t_{\text{max}} = 1.0 \times 10^{-3}$ s

<table>
<thead>
<tr>
<th>Species</th>
<th>external source</th>
<th>production rate</th>
<th>loss rate</th>
<th>$dy/dt$</th>
<th>abs. error at $t = t_{\text{max}}$</th>
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<tbody>
<tr>
<td>reservoir p</td>
<td>0.000000e+00</td>
<td>0.000000e+00</td>
<td>-2.669383e-01</td>
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<td>1.082178e+01</td>
<td>-6.726742e+00</td>
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<td>$H^+$</td>
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<td>0.000000e+00</td>
<td>1.314818e+00</td>
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<tr>
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<td>1.990817e+00</td>
<td>0.000000e+00</td>
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<tr>
<td>$H_2^+$</td>
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<td>4.985027e-02</td>
<td>0.000000e+00</td>
<td>4.985027e-02</td>
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<td>-2.639000e-13</td>
<td></td>
</tr>
<tr>
<td>CH$_2$</td>
<td>0.000000e+00</td>
<td>3.835393e-01</td>
<td>-3.835393e-01</td>
<td>1.370015e-13</td>
<td></td>
</tr>
<tr>
<td>$CH_3^+$</td>
<td>0.000000e+00</td>
<td>5.341870e-01</td>
<td>-5.341870e-01</td>
<td>5.551115e-15</td>
<td></td>
</tr>
<tr>
<td>CH$_3$</td>
<td>0.000000e+00</td>
<td>3.812394e-01</td>
<td>-3.812394e-01</td>
<td>-1.238789e-14</td>
<td></td>
</tr>
</tbody>
</table>
Spectral analysis of reaction kinetics

- Non-zero eigenvalues: 11, \(|\lambda_{\text{min}}| = 1.049495 \times 10^4\), \(|\lambda_{\text{max}}| = 2.231726 \times 10^6\)
- Stiffness parameter: \(\lambda_{\text{max}} / \lambda_{\text{min}} = 2.126476 \times 10^2\)
- Number of non-zero eigenmodes with \(|\lambda| \leq 1000 \times 1.049495 \times 10^4\): 11
- Used non-zero eigenvalues: 11
- Re-evaluate solution with 11 non-zero eigenmodes.

Derived Quantities

1. D/XB

The D/XB values depend upon experimental details (spectral range, ro-vibrational distribution of emitter molecule, etc.). Only certain "reference light emission rates" are utilized in HYDKIN, see memo D/XB.

<table>
<thead>
<tr>
<th>Band</th>
<th>Transition</th>
<th>Ref</th>
<th>Density [#/unit volume]</th>
<th>(&lt;\text{ex}) [cm(^3)A]</th>
<th>D/XB</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH(_4)X, Gerd-band (430nm)</td>
<td>CH: 4.710934e-07</td>
<td>CH4L: 5.455710e-07</td>
<td>(&lt;\text{emis}&gt; = 5.182375e-09)</td>
<td>4.096040e+01</td>
<td>direct excitation of CH</td>
</tr>
<tr>
<td>CH(_4)X, Gerd-band (430nm)</td>
<td>CH4: 5.455710e-07</td>
<td>CH4L: 5.455710e-07</td>
<td>(&lt;\text{emis}&gt; = 4.650862e-10)</td>
<td>3.941267e+02</td>
<td>dissociative excitation of CH4</td>
</tr>
<tr>
<td>CH(_3)X (390nm)</td>
<td>CH: 4.710934e-07</td>
<td>CH4L: 5.455710e-07</td>
<td>(&lt;\text{emis}&gt; = 1.417931e-06)</td>
<td>1.497056e+02</td>
<td>direct excitation of CH</td>
</tr>
<tr>
<td>S(^+)</td>
<td>513.9 A</td>
<td>ADAS</td>
<td>C(^-): 1.018439e-05</td>
<td>(&lt;\text{emis}&gt; = 8.242522e-11)</td>
<td>0.000000e+00</td>
</tr>
<tr>
<td>C(^{2+})</td>
<td>4159.9 A</td>
<td>ADAS</td>
<td>C(^{2+}): 9.471070e-05</td>
<td>(&lt;\text{emis}&gt; = 2.683128e-16)</td>
<td>0.000000e+00</td>
</tr>
</tbody>
</table>

D/XB, Examples

\(<\text{emis}>\), Examples
Very complex reaction chains (approx. 500 individual processes) in fusion plasmas: catabolic sequence dominant, little: anabolism → Eigenmode analysis of reaction rate equations very simple: → Define “Stiffness parameter”: $\lambda_{\text{max}} / \lambda_{\text{min}}$, ratio of max. to min. eigenvalues

**Fast**  **Slow**

---

**Stiffness Parameter for Hydrocarbon catabolism**

![Diagram showing the stiffness parameter for hydrocarbon catabolism](image-url)
Combustion and flame modelling is mathematically analogous to diffusion-reaction modelling of ITER divertor detachment.

Unfortunately: reduced models ("intrinsic low dimensional manifolds, ILDM") only applicable at very low plasma temperatures.

**Number of remaining eigenmodes for \( \lambda_{\text{max}} / \lambda_{\text{min}} < 100 \).**

Species to be retained

Full reaction kinetics required

- CH4
- C2H6
- C3H8