Introduction to edge plasma modelling

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Outline of course:

Introduction to edge plasma modelling

Like in any applied science: Three questions

I.) WHAT : …happens? \( \rightarrow \) A & M & plasma-wall interaction processes

II.) HOW : …can we make the application work? \( \rightarrow \) ITER

III.) WHY : understanding the edge plasma,

using A&M&S data in edge plasma modelling

See other lectures

Some unfinished business

www.eirene.de
www.hydkin.de
JET, MARK-I,
density ramp-up

-ohmic
-no imp. injection
-simply: D2-puff
Full detachment is a problem

Detachment which is too “strong” (particle flux reduced across the whole target) is often associated with zones of high radiation in the X-point region and confined plasma (MARFE)

MARFE formation can drive a transition from H to L-mode (H-mode density limit) or disruption

MARFE physics still not well understood

Limit detachment to regions of highest power flux (where it is needed most).
Maintain remainder of SOL in high recycling (attached)
A few ways to arrange that this happens more readily:

- Divertor closure
- Target orientation
- Impurity seeding

Courtesy: R. Pitts
Divertor closure

Increased closure significantly improves divertor neutral pressure $\rightarrow$ increased neutral density ($n_n$), promoting earlier detachment

Closing “bypass” leaks important for increasing $n_n$

Divertor closure also promotes helium compression and exhaust – very important for ITER and reactors

Courtesy: R. Pitts
Parallel heat fluxes significantly reduced for vertical cf. horizontal targets

Underlying effect is preferential reflection of recycled deuterium neutrals towards the separatrix

Neutrals into hotter plasma near separatrix

Neutrals into cooler, less dense plasma

Increased ionisation near sep.

Higher $n_t$, lower $T_t$

Higher CX losses

Pressure loss $\Rightarrow q_{||} \downarrow$

Courtesy: R. Pitts
Strong impurity seeding also reduces ELM size but high price can be paid in confinement.
ITER divertor designed to achieve partial detachment

Deep V-shaped divertor, vertical, inclined targets
Dome separating inner and outer targets – also helpful for diagnostics, neutron shielding and reducing neutral reflux to the core

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ITER Divertor DDD 17, Case 489 (SOLPS4.2 runs by A. Kukushkin)
Can we hope that magnetic confinement core plasma physics progress will mitigate plasma-surface problems?

**Candle, on earth**
- Convection, driven by buoyancy (i.e. gravity)
- Fresh air
- Used air

**Candle, under microgravity**
- Only Diffusion (no convection)
- e.g.: parabola flight, $g \approx 0$
- (only small, dim burn, at best)

**Can we hope that magnetic confinement core plasma physics progress will mitigate plasma-surface problems?**
Apart from power handling, primary function of divertor is to deal with He from fusion reactions \(\rightarrow\) compress D, T, and He exhaust as much as possible for efficient pumping (and therefore also good density control).

Critical criterion for an ITER burning plasma is that He is removed fast enough such that:

\[
\frac{\tau_{p,He}^*}{\tau_E} \leq 5 - 10
\]

is satisfied.

\(\tau_{p,He}^*\) is the global helium particle residence time – a function of \(\tau_p\), the He neutral density in the divertor and the pumping speed (conductance).

Helium enrichment:

\[
\eta_{He} = \frac{n_{He}^{pump} / 2n_{D2}^{pump}}{n_{He}^{plasma}/n_e} = \frac{C_{pump}}{C_{plasma}}
\]

is the ratio of He concentration in the divertor compared to the main plasma.

e.g. ITER: He prod. rate \(\sim 2 \times 10^{20}\) s\(^{-1}\)

Max. divertor pumping speed

\(\sim 200\) Pa m\(^3\) s\(^{-1}\) \(\sim 1 \times 10^{23}\) He atom s\(^{-1}\)

\(\rightarrow\) \(C_{pump} \sim 2 \times 10^{-3} = 0.2\%\)

Typical acceptable He conc. in the core: \(\sim 4\%\) \(\rightarrow\) \(\eta_{He} = 0.2/4 = 0.05\) is minimum required. The values of \(\tau_{p,He}^*\) and \(\eta_{He}\) required for ITER have been achieved experimentally.

Courtesy: R. Pitts
Opacity in Fusion edge plasmas?

Only for resonance lines: Lyman-series
The Photon mean free path

At line centre:

$$mfp_{\lambda_0} = \left(5.4 \cdot 10^{-9} \lambda_0 \left(\frac{\mu}{T}\right)^{1/2} \cdot n_a\right)^{-1} \approx 1.8 \cdot 10^{13} \cdot \frac{\sqrt{T}}{n_a} \text{ [cm]}$$

for Lyman lines

50 cm

30 cm

10 cm

Ly-α Doppler Profile (5 eV)

mfp for $n_a = 10^{13}$

Institut für Plasmaphysik
Assoziation EURATOM-Forschungszentrum Jülich
Experimental observations

Ratio: Lyman-\(\beta\) / Balmer-\(\alpha\): proof of opacity

Lyman-\(\alpha\) Voigt-Lineshapes \(\sim \frac{1}{mfp}\) (Photon mean-free-path)-¹
Escape factors: zero dimensional corrections to account for radiation trapping

Line escape factors:
for line of sight spectroscopy
(provided also by EIRENE, with zero statistical noise)

Population escape factors:
modify ionisation-recombination balance.
Important for dynamics in detached plasmas

\[
\Theta_P(\vec{r}) = 1 - \frac{\int_{4\pi} \int_{\text{line}} \alpha_v(\vec{r}) I_v(\vec{r}, \vec{\Omega}) \, d\nu \, d\Omega}{4\pi j_v(\vec{r})} = 1 - \frac{G}{E}
\]

\[A_{ik} \rightarrow \Theta_P(\vec{r}) A_{ik}\]
Comparison: **ADAS vs. EIRENE** escape factors
long cylinder case, homogeneous plasma
pure Doppler broadening (kT = 1 eV)

![EIRENE population escape factor evaluation](image-url)
Comparison of D atom profiles

before

after
Lyman-\(\alpha\) photon density (log scale), after iteration
population escape factor
Partial detachment, high $n_{\text{neut}}$ → Lyman series radiation MFP < 1 cm → strong increase of ionisation, change of ionisation/recombination balance

Radiation transport in Eirene: several Ly series, photons like neutrals

SOLPS calculations: no effect on $q_{pk}$ and $n_{\text{He}}$, although plasma parameters in divertor change strongly

Reason: stronger ionisation in cold region → increase of $n$ → increase of recombination ($S_{\text{ion}} \propto n^2$; $S_{\text{rec}} \propto n^3$)

Important for diagnostics, less for performance

→ don’t trust simple models!
Why do edge codes take forever to converge?
A simple model, to illustrate the numerical challenge

Major radius = 2-6 m (distance to torus center)

Plasma flow

Gas flow

target

plasma core

recycling

wall
The often hidden challenge: code convergence, iterating on noise ??,…..


Expected uncritical behavior, errors reduced exponentially to machine precision.
convergence behaviour of the coupled B2-EIRENE codesystem (1)

Numerical Convergence errors (residuals) during CFD run, vs. timestep

B2, $R=0.3$

B2 with analytic recycling model (without EIRENE), recycling coefficient $R=0.3$

B2-EIRENE, $R=0.3$

coupled B2-EIRENE calculation, recycling coefficient $R=0.3$

This is what we want
(Analytic recycling model= unrealistically simplified Boltzmann eq.)

And this is what we get
(full Boltzmann eq., Monte Carlo)
Code performance: serial, B2-EIRENE, ITER test case, Linux PC 3.4 GHz (typical for all “micro macro models” in computational science)

Convergence limited by statistical Monte Carlo noise. In order to reduce error by factor 10, runtime (or number of processors) has to be increased by factor 100

convergence behaviour of the coupled B2-EIRENE codesystem (2)

Convergence in given CPU-time depends on level of recycling (= vacuum pumping speed)
convergence behaviour of the coupled B2-EIRENE codesystem (3)

low recycling
R=0.3

high recycling
R=0.99

“Is is enough to see one lion to know you are in a desert”
Correlation sampling and convergence of B2-EIRENE

Here: correlation produced by simple manipulation of random number generator

Without correlation sampling cpu time has to be increased by a factor 100 to reach the same convergence level!

How much correlation? Damping of noise, without freezing error from early iterations.
Recent Progress and Challenges

Going from 2D → 3D.....
The experimental experience: to stir a liquid
Creating turbulent (chaotic) flow can largely increase heat transfer (avoid local overheating)

The theory: “passive scalar transport in chaotic force fields”
Not yet understood on a quantitative level
very active modern research field of
• theoretical physics
• large scale numerical computing.
Avoid excessive heat loads by stirring (magnetically) the plasma?

TEXTOR-DED: Dynamic Ergodic Divertor
Dynamic Ergodic Divertor (DED) in TEXTOR
flexible tool to study the impact of resonant magnetic perturbations on transport, stability and structure formation (helical divertor)

16 coils mounted at the HFS:
- covered with graphite tiles
- helical set-up
- resonant on q=3 surface

resonant perturbation:
- m/n = 12/4, 6/2, 3/1 base mode
- different penetration depth
- $B_{\text{DED}}/B_\theta \sim 10\%$

different operation modes:
DC operation
AC operation [1-10kHz]
slow strike point sweeps
Field line tracing - 3D plasma fluid – neutral gas kinetic modeling

Partially ergodic 3D magnetic field topology
→ 3D edge codes → also Monte Carlo for plasma flow fields (EMC3)

TEXTOR-DED B-Field (R-Z)  TEXTOR-DED B-Field (r-θ)

D. Harting, D. Reiter, JUEL-4173, May 2005
“Particle” methods: also well established in fluid dynamics

- Lagrangian method ↔ Eulerian (grid based) method
- **Advantages:**
  - + concentrate “particle” in the interesting region
  - + Convective transport essentially without numerical dissipation in arbitrarily complex geometry
- **Disadvantages:**
  - - Non-convective terms (collisions, diffusion)
- **Solution:** Monte Carlo fluid (random walk model)
- in Fusion: this is the concept of E3D and EMC3-EIRENE codes (IPP Greifswald)
- - looses accuracy in region of interfacial boundaries
EMC3-EIRENE:
FZJ: mainly tokamak applications (RMPs)
Example: DIII-D ELM mitigation scenarios

Goal: quantify PSI, when RMPs are applied in ITER
Towards fully 3D CFD: The EMC3-EIRENE code (IPP Greifswald – FZ-Juelich)

(initially developed for stellarator applications W7AS, W7X, LHD) was advanced to a more flexible grid structure to allow divertor tokamak + RMP applications.

- first self-consistent 3D plasma and neutral gas transport simulations for poloidal divertor tokamak configurations with RMPs.

- Simulation results for ITER similar shape plasmas at DIII-D show a strong 3D spatial modulation of plasma parameter, e.g. in $T_e$.

- EMC3-EIRENE code verification (by benchmarks with 2D tokamak edge codes) and validation (TEXTOR, DIII-D, JET, LHD experiments) ongoing

- EMC3-EIRENE is currently being used for contractual ITER RMP design studies (jointly by FZJ and IPP, 2010-2012)
Atomic database, as currently used
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 resources

DataBase Processor → www hydkin.de

Reaction Mechanisms →

A "basic" global plasma model → B2-EIRENE

Visualizer and post-processor

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

*www.eirene.de/A+Mdata*

*www.hydkin.de*

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University of Illinois
Optical and Discharge Physics

GECA9907
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
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 catal
plasm

**Methane family:**

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

**Ethane/Propane family:**

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

**Silane family:**

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

**Hydro:**

Juel-F
Collision Processes of Hydrocarbon Species in Hydrogen Plasmas: F
(by R. Janev & D. Reiter)

All data, figs, and references: HERE
www.eirene.de: online (TRIM) reflection database

Data files with tables of reflection distributions, e.g. for particle simulation codes (conditional quantile format)
Monte Carlo simulation (BCA): C on C, $\alpha_{in} = 60^\circ$

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

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

Incident energy, eV

Hidden key parameter:
Surface binding energy ($\leftrightarrow$ from MD?)

Uncertain
MD ??

Quite reliable,
BCA

Eckstein 1983
TRIM-1985
TRIM-2002
SDTrimSP 2007
TRIM.xxx: reflected energy spectra
red: 200,000 TRIM particles,
blue: reconstructed from 10 quantiles

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

Challenge: what is the minimal dataset that allows
to re-sample the full backscattering (and sputtering) \( E_{out}, \Theta_{out} \)-distribution?

See: www.eirene.de
Surface data
TRIM
TRIM-codes family, online database for fully kinetic reflection velocity space PDFs

Particle reflection coefficient, D → FE, 30 degree

Legend:
- Eirene Reflection Database (TRIM Code, section 1.1)
- W. Eckstein, "Calculated sputtering, reflection and range values", IPP-Report IPP 9/132, 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.
Goal: replace various scalings (e.g. Yamamura for incident angle dependence) by full database, same format as for EIRENE-reflection database.

Lost information, due to raw data processing at too early stage.

Sputter yield database
For normal incidence: probably ok.

80 degree incident angle
Still not decided: how to parameterize
a) Surface roughness,
b) Material mixing

Universal sputtering law: Janev, Ralchenko, et al. for normal incidence yield.
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

**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)

All data, figs, and references: [HERE](http://www.eirene.de)
History A&M Data, H and He, in EIRENE (=current status in ITER modelling)

1983 - 1999
Johnson-Hinnov CR model for H, H*, H+

1986 - ....
Polynomial fits
Automated Interface to EIRENE

1987 - ....
He, He*, He Metastable resolved.

Polyn. Fits produced, Elec. Cooling rates added

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Automated Interface to EIRENE

1987 - ....
He, He*, He Metastable resolved.

Polyn. Fits produced, Elec. Cooling rates added

2000 - ....
Rad. transfer Lyman opacity added

Effective ionization and dissociation rate coefficients of molecular hydrogen in plasma

Keiji Sawada
Department of Applied Science, Faculty of Engineering, Shinshu University, Nagano 380, Japan

Takashi Fujimoto
Department of Engineering Science, Faculty of Engineering, Kyoto University, Kyoto 606-01, Japan

(Received 5 December 1994; accepted for publication 22 May 1995)

A simplified collisional-radiative model has been constructed for the system of the ground state, electronically excited stable states, and the ionic state of molecular hydrogen in plasma. Effective rate coefficients have been calculated for production of electrons, molecular ions, protons, and hydrogen atoms from molecular hydrogen. The ratio of the effective ionization rate of molecular hydrogen to the Balmer α photon emission rate and the effective rate coefficients for radiation and energy losses are also presented. © 1995 American Institute of Physics.
Basic input for ITER divertor code: A&M data, ( & surface data)
Goal: publicly expose raw data used in any modelling

Online data base
and data analysis tool-box:

- CR model condensation
- Sensitivity analysis
- Fragmentation pathway analysis
- Reduced models

• Hydrocarbons
• Silanes
• H, H\textsubscript{2}, H\textsubscript{3}\textsuperscript{+}, ....
• W, W\textsuperscript{+}, ....W 74+
• N, N\textsubscript{2}

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:

$$\frac{d\vec{y}}{dt} + \vec{A}\vec{y} = \vec{b} - \vec{y}_{\text{loss}}$$  \(\vec{A}\) : master operator

\(\vec{A}\): 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”)

e.g. \(\vec{y} = \begin{pmatrix} n_C \\ n_{CH} \\ \vdots \\ n_{CH_4} \end{pmatrix}\) vector of species concentrations involved in reaction kinetics
[particles/unit volume, mol/unit volume]

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

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

Gas puff, chem. sputtering  Transport losses
NEW: surface reflection database

NEW: added after Juel-Reports and PoP papers
Choose plasma background
Integration time
Graphical presentation

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<td>1e+300</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Printout:

Reflect input as selected
(composition, initial condition, Influx, transport losses, per species)

Printout:

All individual rates used
Output for interface to EIRENE
Solution, vs. time (distance)

Here: $0 \rightarrow 1e^{-4} \text{ s}$

Species selected for printout and plotting

Same, integration time 0 → 1e-3

Runtime of online code is independent of chosen time interval for integration

(same for 1e-6 or 1e+6 s integration period),

time dependent solution is given fully explicitly in terms of A matrix elements (+ initial cond.)
If A matrix is upper triagonal, all eigenvalues and eigenvectors are explicitly given

Online solution of time-dep. (1D) Hydrocarbon breakup, for any prescribed divertor plasma conditions, up to C₃H₈
2004 -- ……(ongoing)

HYDKIN database toolbox

Spectral (time scale) analysis
fragmentation pathways
Sensitivity analysis

Interface

EIRENE 3D Monte Carlo kinetic transport

ITER

raw data

TEXTOR, JET, ASDEX, DIII-D, JT-60, LHD, …..
Verify Interface: HYDKIN --- EIRENE
(check for correct transfer of chemisty, correct integration of cross sections)

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

Mostly H from CH4 fragmentation
→ focus stat. weights on C containing fragments
Choose in HYDKIN and in EIRENE:
same Influx: \( \text{CH}_4 \), density: \( 5\times10^{12} \text{ cm}^{-3} \), \( T_e=T_i=1 \text{ eV} \), same \([0,t_{\text{max}}]\) time period

Density of \( \text{CH}_x \) vs. time
1 eV, 1000000 Eirene particles (~23 sec cpu)
Diagnostics from this run at t = t_{max} = 1.0 \times 10^{-3} \text{ s}

T_{e} [\text{eV}] = 25
T_{p} [\text{eV}] = 25
T_{H} [\text{eV}] = 10
n_{0} [\text{#cm}^{-3}] = 1.0 \times 10^{13}
n_{p} [\text{#cm}^{-3}] = 1.0 \times 10^{13}
n_{H} [\text{#cm}^{-3}] = 1.0 \times 10^{13}

E_{0} [\text{eV}] = 1
\text{total influx [#/unit volume]} = 1.00 \times 10^{00}

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

<table>
<thead>
<tr>
<th>Species</th>
<th>external source [#/unit volume]</th>
<th>production rate [#/unit volume]</th>
<th>loss rate [#/unit volume]</th>
<th>\text{dy/dt} [#/unit volume]</th>
<th>abs. error at t = t_{max}</th>
</tr>
</thead>
<tbody>
<tr>
<td>reservoir p</td>
<td>0.0000000e+00</td>
<td>0.0000000e+00</td>
<td>-2.695983e-01</td>
<td>5.260287e-13</td>
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<td>reservoir e</td>
<td>0.0000000e+00</td>
<td>1.082178e+01</td>
<td>-6.726742e+00</td>
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<tr>
<td>reservoir H</td>
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<td>0.0000000e+00</td>
<td>-4.737731e+02</td>
<td>-4.328673e-17</td>
<td></td>
</tr>
<tr>
<td>H^{+}</td>
<td>0.0000000e+00</td>
<td>1.314818e+00</td>
<td>0.0000000e+00</td>
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<tr>
<td>H</td>
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<td>1.990817e+00</td>
<td>0.0000000e+00</td>
<td>7.251043e-14</td>
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<tr>
<td>H_{2}^{+}</td>
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<td>6.366019e-13</td>
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<tr>
<td>H_{2}</td>
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<td>4.558201e-01</td>
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<td>6.852297e-13</td>
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<tr>
<td>C^{+}</td>
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<td>-1.052959e+00</td>
<td>1.370015e-13</td>
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<tr>
<td>C</td>
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<td>7.099571e-01</td>
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<td>1.370015e-13</td>
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</tr>
<tr>
<td>CH^{+}</td>
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<td>5.585668e-01</td>
<td>-5.585668e-01</td>
<td>6.064949e-13</td>
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<tr>
<td>CH</td>
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<td>4.723670e-01</td>
<td>-4.723670e-01</td>
<td>6.064949e-13</td>
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<tr>
<td>CH_{2}^{+}</td>
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<td>5.203546e-01</td>
<td>-5.203546e-01</td>
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<tr>
<td>CH_{2}</td>
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<td>3.835393e-01</td>
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<tr>
<td>CH_{3}^{+}</td>
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<tr>
<td>CH_{3}</td>
<td>0.0000000e+00</td>
<td>3.612934e-01</td>
<td>-3.612934e-01</td>
<td>6.064949e-13</td>
<td></td>
</tr>
</tbody>
</table>
**Spectral analysis of reaction kinetics**

- Non-zero eigenvalues: 11, $\lambda_{min} = 1.049495\times10^4$, $\lambda_{max} = 2.231726\times10^6$
- Stiffness parameter, $\lambda_{max}/\lambda_{min} = 2.126476\times10^2$
- Number of non-zero eigenmodes with $|\lambda| < 1000$: 11
- Used non-zero eigenvalues: 11
- Re-evaluate solution with 11 non-zero eigenmodes.

**Spectral analysis:**
**Identification of reduced models:**
**ILDM**

**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>$&lt;\text{emis}&gt; [\text{cm}^3/\text{s}]$</th>
<th>D/XB</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$\alpha$</td>
<td></td>
<td>CH$_4$, $4599$ (430nm)</td>
<td>4.710934e-07</td>
<td>$&lt;\text{emis}&gt; = 6.1245678\times10^{-6}$</td>
<td>$4.096040\times10^1$ direct excitation of CH</td>
</tr>
<tr>
<td>CH$\alpha$</td>
<td></td>
<td>CH$_4$, $545910$ (430nm)</td>
<td>5.455710e-07</td>
<td>$&lt;\text{emis}&gt; = 6.058421\times10^{-6}$</td>
<td>$3.941267\times10^2$ dissociative excitation of CH</td>
</tr>
<tr>
<td>CH$_3$</td>
<td></td>
<td>CH$_4$, $471034$ (390nm)</td>
<td>4.710934e-07</td>
<td>$&lt;\text{emis}&gt; = 1.417931\times10^{-6}$</td>
<td>$1.497056\times10^2$ direct excitation of CH</td>
</tr>
<tr>
<td>S$^+$</td>
<td></td>
<td>ADAS</td>
<td>$513.9$</td>
<td>$&lt;\text{emis}&gt; = 8.228522\times10^{-6}$</td>
<td>$0.000000\times10^0$ direct excitation of S$^+$</td>
</tr>
<tr>
<td>C$^{2+}$</td>
<td></td>
<td>ADAS</td>
<td>$4159.9$</td>
<td>$&lt;\text{emis}&gt; = 2.631282\times10^{-6}$</td>
<td>$0.000000\times10^0$ direct excitation of C$^{2+}$</td>
</tr>
</tbody>
</table>
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

text only

![Stiffness Parameter for Hydrocarbon catabolism](image_url)

- CH4
- C2H6
- C3H8

**$T_e$ [eV]**

$\lambda_{\text{max}} / \lambda_{\text{min}}$
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.
importance of CX-DR over DE-DI channels:
put one $C_xH_y$ into plasma. How many e,p pairs are neutralized?

\[ p + C_xH_y \rightarrow H + C_xH_y^+ \quad \text{or} \quad C_xH_y^+ \rightarrow \text{DR} \]
### Molecular Data analysis (www.HYDKIN.de):

**ITM, IAEA**

<table>
<thead>
<tr>
<th></th>
<th>CH$_4$</th>
<th>C$_2$H$_6$</th>
<th>C$_3$H$_8$</th>
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</thead>
<tbody>
<tr>
<td><strong>DE</strong></td>
<td>RKJ 2009</td>
<td>JR 2004</td>
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<tr>
<td><strong>DE</strong></td>
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<td><strong>I-DI</strong></td>
<td>RKJ 2009</td>
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<td>JR 2004 ##</td>
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<td>RKJ 2009</td>
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<tr>
<td><strong>CX-PR</strong></td>
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</tr>
<tr>
<td><strong>R-DR</strong></td>
<td>RKJ 2009</td>
<td>RKJ 2009</td>
<td></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

#### New Experiments
- New experiments planned in 2010, Univ. Louvian la Neuve, P. Defrance et al.
- Revision planned in 2010, Univ. Innsbruck, T. Märk et al.

#### References
- R. K. Janev and D. Reiter, Phys. Plasmas 9, 4071 (2002);
2010: more (DR) channels for Geroe Band emission added

### 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;emis&gt; [cm³/s]</th>
<th>D/XB</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHₐ-X, Gerö-band (430nm)</td>
<td>CH: 9.711607e-07</td>
<td>&lt;emis&gt; = 5.531311e-09</td>
<td>1.861576e+01</td>
<td>direct excitation of CH</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHₐ-X, Gerö-band (430nm)</td>
<td>CH₄: 1.698022e-06</td>
<td>&lt;emis&gt; = 1.141715e-10</td>
<td>5.158207e+02</td>
<td>dissociative excitation of CH₄</td>
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<td></td>
</tr>
<tr>
<td>CHₐ-X, Gerö-band (430nm)</td>
<td>CH₄⁺: 3.303721e-07</td>
<td>&lt;emis&gt; = 7.216877e-10</td>
<td>4.194182e+02</td>
<td>dissociative recombination of CH₄⁺</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHₐ-X, Gerö-band (430nm)</td>
<td>CH₃⁺: 1.025480e-06</td>
<td>&lt;emis&gt; = 5.582491e-10</td>
<td>1.746806e+02</td>
<td>dissociative recombination of CH₃⁺</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CHₐ-X, Gerö-band (430nm)</td>
<td>CH₂⁺: 9.258322e-07</td>
<td>&lt;emis&gt; = 1.162343e-09</td>
<td>9.292515e+01</td>
<td>dissociative recombination of CH₂⁺</td>
<td></td>
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</tr>
<tr>
<td>CHₐ-X, Gerö-band (430nm)</td>
<td>CH: 9.711607e-07</td>
<td>&lt;emis&gt; = 1.475368e-09</td>
<td>1.341797e+01</td>
<td>all contributions</td>
<td></td>
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</tr>
<tr>
<td>CHₐ-X (390nm)</td>
<td>5143.3 A</td>
<td>ADAS C⁺: 8.756071e-05</td>
<td>6.979248e+01</td>
<td>direct excitation of C⁺</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C⁺</td>
<td>5143.3 A</td>
<td>ADAS C⁺: 8.756071e-05</td>
<td>0.0000000e+00</td>
<td>direct excitation of C⁺</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C²⁺</td>
<td>4159.9 A</td>
<td>ADAS C²⁺: 1.556560e-07</td>
<td>0.0000000e+00</td>
<td>direct excitation of C²⁺</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

D/XB Examples
<emis>, Examples

Detlev Reiter | Institute of Energy and Climate Research – Plasma Physics | Association EURATOM – FZJ No 71
New class of processes in thermal region
May 2011
New class of processes (2011), thermal region, data from Astrophysics

previous database

- $H_b^+ + CH_4 \rightarrow H + CH_4^+$
- $H_b^+ + CH_5 \rightarrow H_2 + CH_4^+$
- $CH_2^+ + H \rightarrow CH_3^+ + H_2 (CH_4 + H_2)$
- $CH_2^+ + H \rightarrow CH_3^+ + H_2 (CH_4 + H_2)$
- $H_2^b + CH_4 \rightarrow CH_3^+ + H (CH_4 + H_3)$
- $H_2^b + CH_4 \rightarrow CH_3^+ + H_2 (CH_4 + H_2)$
- $H_3^b + CH_4 \rightarrow CH_3^+ + H_2 (CH_4 + H_3)$
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 $n_i$ 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.
Breakup of CH$_4$ @ 40 eV (143 parameters)

Analytic solution for sensitivity, online

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

Identify, print and plot the most sensitive parameters:

If \(<\text{rate}_{k}>\) 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)

Analytic solution for sensitivity, online

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

Identify, print and plot the most sensitive parameters:

If \text{<rate}_k \text{> changes by x %}

Then \text{n}_j \text{ changes by x * Z}_{jk} \text{ %}

---

At 2 eV (detached divertor, PSI-2)

Only CX, DR processes are relevant, strong dependence on transport details
Similar to previous steps: progress to ITER is based mainly on experimental and empirical extrapolation guided by theory and aided by modelling.

Present goal:
include all of edge physics that we are sure must be operative (opacity, A&M physics, surface processes, drifts..., even while our capability to confirm these directly remains limited.

Codes = bookkeeping tools

Present upgrading:
- low temperature plasma chemistry
- consistent wall models
- drifts and electrical currents in the edge
- \(2D \rightarrow 3D\)
- coupling to first principle edge turbulence codes
- code integration: Core- ETB – Edge (ELM modelling)