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ATOMIC, MOLECULAR AND PMI DATABASE IN THE B2-EIRENE FAMILY OF 2D EDGE PLASMA TRANSPORT CODES

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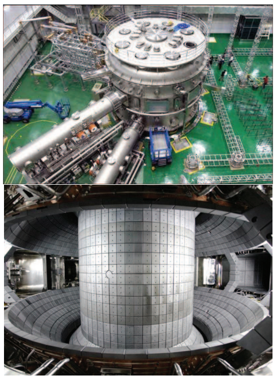
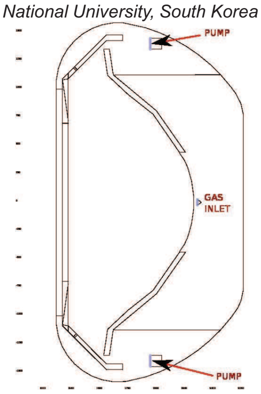
Online available since Oct. 2014:
3.5 hours DETAILED interview with **Richard Pitts (ITER-IO)**:
"ITER and Fusion: explained in context"

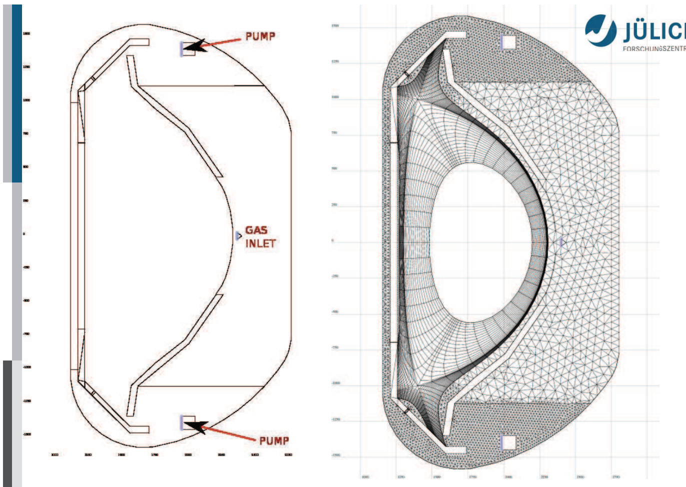
http://omegataupodcast.net/2014/10/157-fusion-at-iter/

B2-EIRENE (version SOLPS4.3-ITER) applied to KSTAR, 2012….
by: **Seung Bo Shim, Hae June Lee,** *Pusan National University, South Korea*

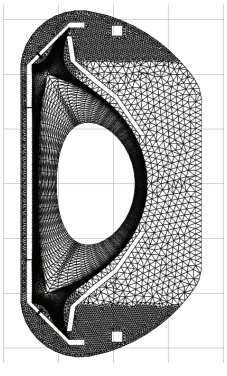




thanks also to: Vlad Kotov, Petra Börner from FZJ

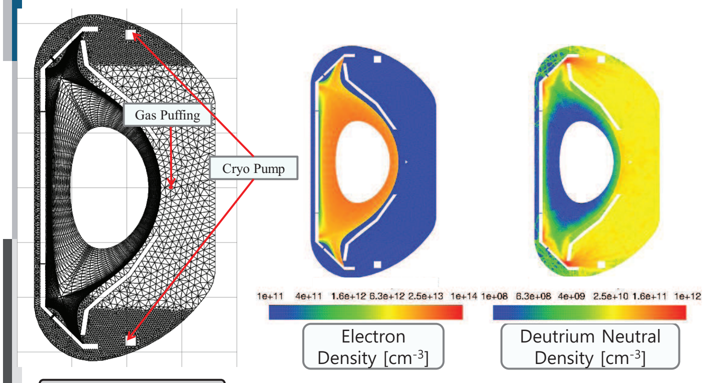


Input parameters	Value	Unit
Total heating power (P_{NBI})	8	MW
Radiation loss ratio in the core plasma	40	%
Out/in power split	3/1	
Plasma density at the core boundary	$3x10^{19}$	m^{-3}
Plasma flux at the core boundary	10^{21}	s^{-1}
Electron thermal diffusivity	1.0	m^2/s
Radial diffusion coefficient	0.5	m^2/s
Recycling ratio	1.0	
Decay Length	0.03	m
Sheath energy transmission coefficient	El : 2.0 Ion : 2.5	
Pumping speed	$5x10^4$	l/s
Initial Density	D:$1x10^{18}$ C:$1x10^{15}$	m^{-3}
Initial Temperature	10	eV



Computational Grid

- 2D (and also 3D) edge transport code models: realistic geometries including pump ducts and leaks to the main vessel, incorporate AM-PMI physics into plasma flow simulations ("plasma transport").



Computational Grid

Electron Density [cm^{-3}]

Deutrium Neutral Density [cm^{-3}]

1D core, 0D point reactor STRAHL, ETS

MACROSCOPIC

…d, bundled,…

B2: a …
(D+, H…
plasm…

Source ter…
(Particle,
Momentum…
Energy)

…ible

EDGE CODES

(B2-EIRENE)

processed data

Da…

… www.eirene.de

MICROSCOPIC

gyro-kinetic, N-body (ERO, PIC)

B2-EIRENE: D. Reiter, J. Nucl. Mat. (1992), 196, p80-89….
Since then: many versions, names, sets of physics,
→ incomprehensible jumble of Fortran code….

FZJ-F4E-ITER contractual work (2011-2013):
New ITER reference edge code B2-EIRENE,
version SOLPS_ITER (2014)

B2 FZJ-ITER	SOLPS4.3 ↔ 1995 → 2014	EIRENE (FZJ-ITER specific)
B2.5 St. Petersburg TU	SOLPS_ITER ↔	EIRENE (FZJ master version)

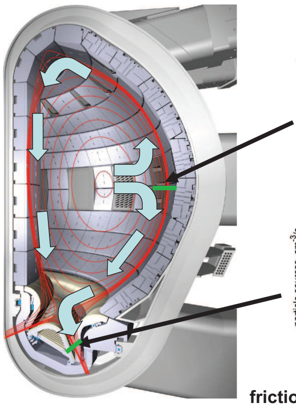
Now hosted by ITER-IO, Cadarache

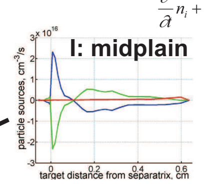
2014 → …???

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

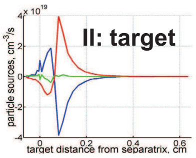
$\mathrm{div}(nv_{\parallel})+\mathrm{div}(nv_{\perp})=$ ionization/recombination/charge exchange

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





parallel vs. (turbulent) cross field flow



parallel vs. chemistry and PWI driven flow

dominant process:
friction: p + H_2, EIR → detachment

9

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

Continuity eq. for ions and electrons

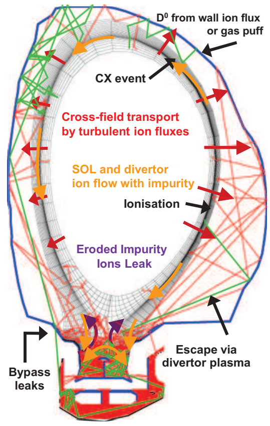
$$\frac{\partial}{\partial t}n_i+\vec{\nabla}\cdot\left(n_i\vec{V}_i\right)=\boxed{S_{n_i}}$$

Momentum balance for ions and electrons

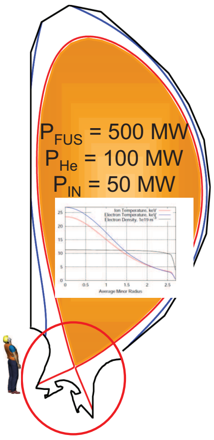
$$\frac{\partial}{\partial t}\left(m_i n_i\vec{V}_i\right)+\vec{\nabla}\cdot\left(m_i n_i\vec{V}_i\vec{V}_i\right)=$$
$$-\vec{\nabla}p_i-\vec{\nabla}\cdot\vec{\Pi}_i+Z_i e n_i\left(\vec{E}+\vec{V}_i\times\vec{B}\right)+\vec{R}_i+\boxed{\vec{S}_{m_i\vec{V}_i}}$$
$$-\vec{\nabla}p_e-en_e\left(\vec{E}+\vec{V}_e\times\vec{B}\right)+\vec{R}_e=0$$

energy balance for ions and electrons

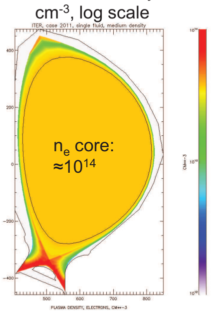
$$\frac{\partial}{\partial t}\left(\frac{3}{2}n_iT_i+\frac{m_in_i}{2}\vec{V}_i^2\right)+$$
$$\vec{\nabla}\cdot\left[\left(\frac{5}{2}n_iT_i+\frac{m_in_i}{2}\vec{V}_i^2\right)\vec{V}_i+\vec{\Pi}_i\cdot\vec{V}_i+\vec{q}_i\right]$$
$$=\left(en_iZ_i\vec{E}-\vec{R}\right)\cdot\vec{V}_i-Q_{ei}+\boxed{S_E^i}$$
$$\frac{\partial}{\partial t}\left(\frac{3}{2}n_eT_e\right)+\vec{\nabla}\cdot\left(\frac{5}{2}n_eT_e\vec{V}_e+\vec{q}_e\right)=-en_e\vec{E}\cdot\vec{V}_e+\vec{R}\cdot\vec{V}_i+Q_{ei}+\boxed{S_E^e}$$



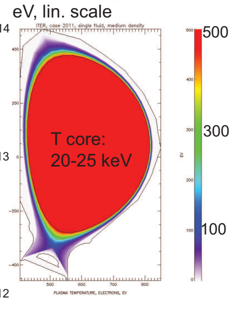
ITER, 500 MW fusion power, n_e, T_e



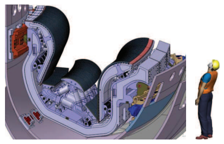
Plasma density
cm^{-3}, log scale



Electron temperature
eV, lin. scale



Narrowing down on the divertor plasma

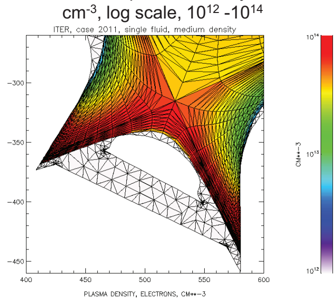


Electron thermalization time

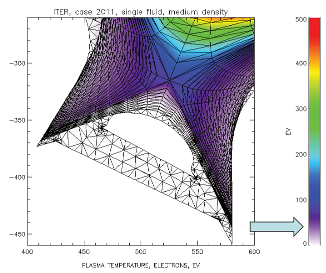
$$\tau_{ee}\approx 3.3\times10^{-13}\left(\frac{T_e}{100\ \mathrm{eV}}\right)^{3/2}\left(\frac{10^{21}\ \mathrm{cm}^{-3}}{n_i\ \log\Lambda}\right)\quad \mathrm{s}$$

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

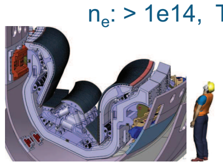
Divertor plasma density
cm^{-3}, log scale, 10^{12} - 10^{14}



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



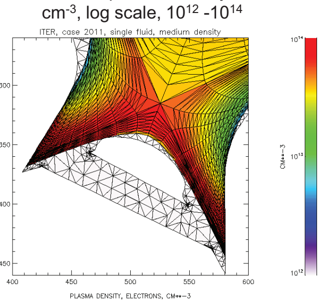
Plasma in weakly detached ITER divertor
n_e: > 1e14, T_e < 5 eV



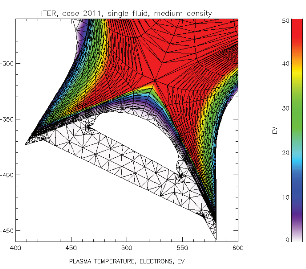
Tokamak Divertor Detachment:

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

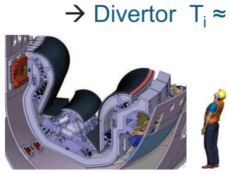
Divertor plasma density
cm^{-3}, log scale, 10^{12} - 10^{14}



Divertor electron temperature
eV, lin. scale, 0 – 50 eV



Electron – ion temperature equilibration:
→ Divertor $T_i \approx T_e$

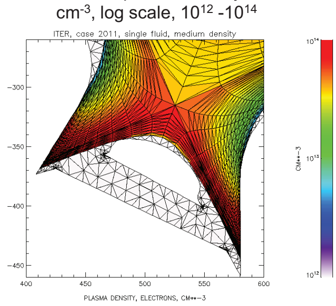


T_e – T_i equilibration time

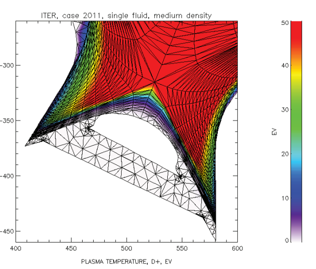
$$\tau_{eq}\approx 3.16\times10^{-10}\ \frac{A}{Z^2}\left(\frac{T_e}{100\ \mathrm{eV}}\right)^{3/2}\left(\frac{10^{21}\ \mathrm{cm}^{-3}}{n_i\ \log\Lambda}\right)\quad \mathrm{s}$$

≈ 1000 x τ_{ee} (for H plasma), but still fast.

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

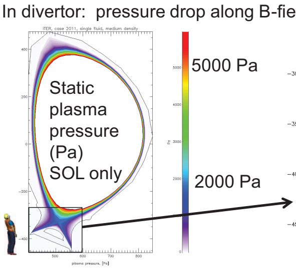


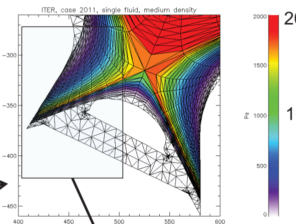
Divertor D^+ ion temperature
eV, lin. scale, 0 – 50 eV



(static) plasma pressure (Pa)

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



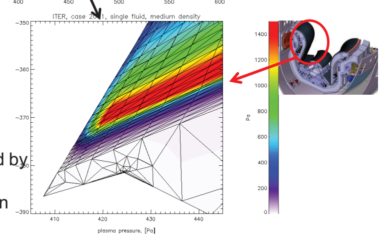


Momentum balance for H^+ ions

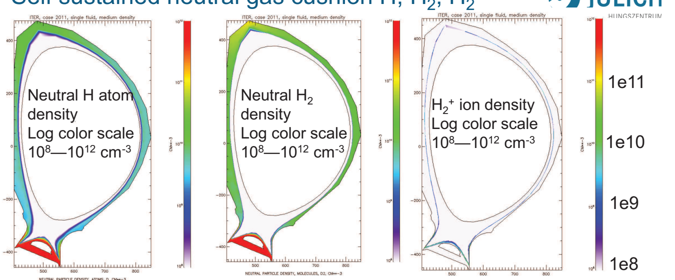
$$\frac{\partial}{\partial t}\left(m_i n_i\vec{V}_i\right)+\vec{\nabla}\cdot\left(m_i n_i\vec{V}_i\vec{V}_i\right)=$$
$$\boxed{-\vec{\nabla}p_i}-\vec{\nabla}\cdot\vec{\Pi}_i+Z_i e n_i\left(\vec{E}+\vec{V}_i\times\vec{B}\right)+\vec{R}_i+\boxed{\vec{S}_{m_i\vec{V}_i}}$$

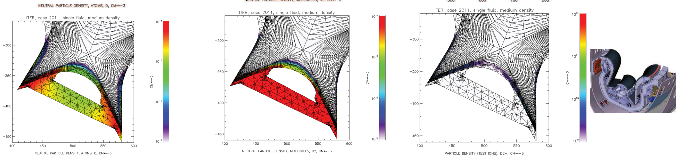
Near target pressure gradient balanced by momentum sinks:

- e + H^+ plasma volume recombination
- Neutral gas – plasma friction



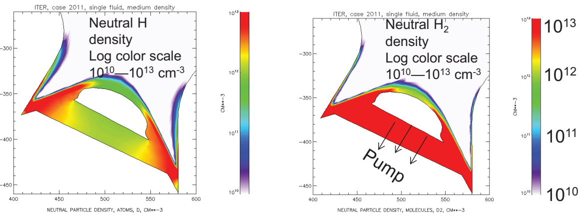
Self sustained neutral gas cushion H, H_2, H_2^+

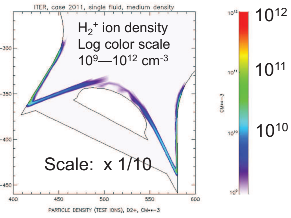


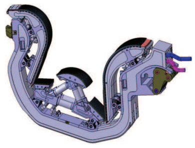


In ITER: neutral gas – plasma exchange is a narrow boundary layer effect

Self sustained neutral gas cushion H, H_2, H_2^+

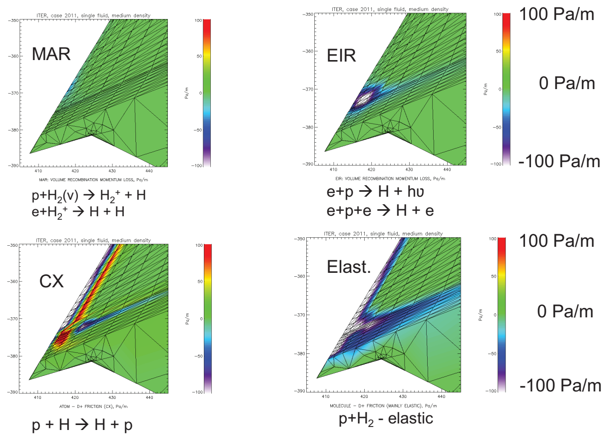






$n_{H_2^+} << n_{H_2}$ → **no significant H_3^+ formation**
(competing electron collisions on H_2^+ are too strong)
(Distinct from some linear plasma devices operated at low n_e/n_{H_2} ratios)

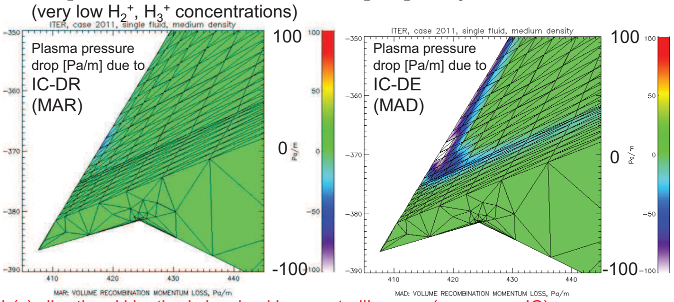
ITER divertor detachment:
Plasma pressure gradient [Pa/m] provided by:
MAR < EIR < p+H (CX) < p+H_2 (elastic) friction



Competition between processes:

(outcome in fusion divertors is sometimes quite distinct from that in linear plasma "divertor simulators")

- p+ H_2 → H_2^++…, e + H_2^+ → p + H + e "DE wins over DR": …..e+H_2^+ → H+H
- e+H_2^+ → …fragments "wins over PR": H_2 + H_2^+ → H_3^+ + H
  (very low H_2^+, H_3^+ concentrations)

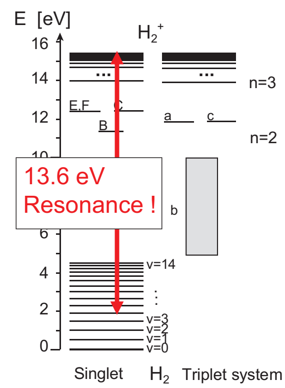


$H_2(v)$ vibrational kinetics is involved in a controlling way (resonance IC)
Isotopomeres? D^+ + HD(v) → … vs. H^+ + D_2(v)→ … , and DT, T_2 ?

unknown territory (in fusion edge plasma science) ?
Isotopomeres: Currently only simple scalings of cross sections with transition energies

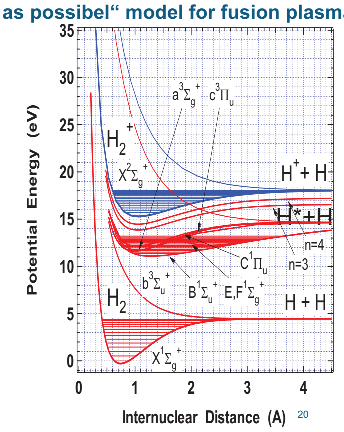
H_2 molecule, status in present SOLPS-ITER code

initially compiled 1997



Courtesy: K. Sawada, Shinshu Univ. Jp.

More complete models are available → identify „as simple as possibel" model for fusion plasma

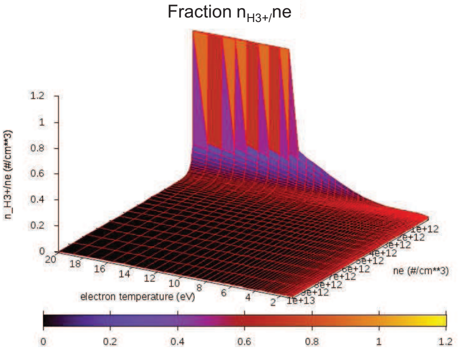


What is the positive charge carrier in a hydrogen plasma ?

$n_e = n_{H+} + n_{H2+} + n_{H3+}$

n_{H2} = 1E12 cm^{-3}
T_{H2+} = 0.5 eV

Fraction n_{H3+}/ne



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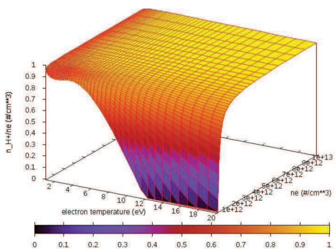
Ratio n_{H+}/n_e



Significant n_{H3+} fraction requires:

1. High n_{H2}/n_e
2. Low n_e
3. High T_e, T_i

not in fusion plasmas, typically also not in linear PMI plasma devices (exceptions may exist…)

"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:
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H^++H_2 is the most fundamental ion-molecule system
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“Battle field” of hydrogen molecule: Two-electronic, strongly coupled potential-surfaces of H_3^+

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$H^+ + H_2$ is the most fundamental ion-molecule system

We should know all about it

P. Krstic, ORNL, US, talk @ IAEA, DCN, 2013

Proton impact of molecule

$p+H_2(v)\to p+H_2(v')$ Also large σ

$p+H_2(v)\to H+H_2^+(v')$ Charge transfer

$p+H_2(v)\to H+H^+ +H$

$p+H_2(v)\to H+H^+ +H^+ +e$ Dissoc Double ion

$p+H_2(v)\to p+H_2(n,v')$ Exc. elec. vib.

Processes with molecular ion

$H + H_2^+(v) \to H + H_2^+(v')$

$H + H_2^+(v) \to p + H_2(v')$

$H + H_2^+(v) \to p + H + H$

Numerous other processes with molecules

$H^- + H_2(v)\to H+H_2(v')+e$

$H+H_2(v)\to H+H_2(v')$

$H+H_2(v)\to H+H+H$

$H_2(v')+H_2(v'')\to H_2(v''')+H_2(v'''')$

$H_2+H_2(v)\to H_2+H+H$

Creation of H_3^+

$H_2^+(v')+H_2(v)\to H_3^+(v'')+H$

H_3^+ Series of interesting reactions: DE, DR, branching ratios with electrons

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- Rotational analysis is missing
- Isotopic constitution: D_2, T_2, HD, HT and DT, sensitive on vib. energy levels

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raw data

2004 -- ……(ongoing)

HYDKIN database toolbox

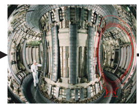
→ Spectral (time scale) analysis

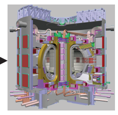
→ Public exposure of data

→ Sensitivity analysis

Interface

EIRENE 3D Monte Carlo kinetic transport





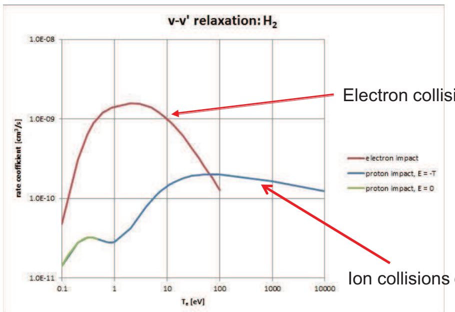
KSTAR, TEXTOR, JET, ASDEX, DIII-D, LHD, W7X,… JT-60, LHD, …..

ITER

JÜLICH FORSCHUNGSZENTRUM

Build v-v’ transition rate matrix, for e and p collisions on H_2 → HYDKIN

→ slowest timescale (smallest eigenvalue): relaxation of T_{vib} to T_e or T_i



Electron collisions on H2(v)

Ion collisions on H2(v)

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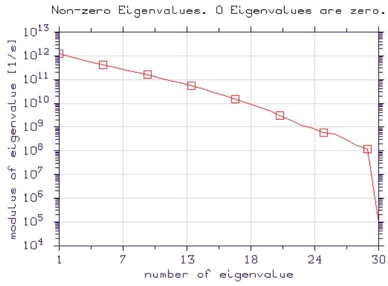
HYDKIN: spectral analysis for reaction kinetics

Warm up: H-atom, CR model: H(1),H*(2),….,H*(30),H⁺

(I,k-excitation, i-ionization A_ik, and k,i de-excitation



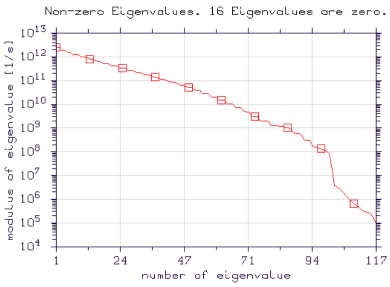
@ Te = 10 eV, ne = 1e13

HYDKIN: spectral analysis for reaction kinetics

JÜLICH FORSCHUNGSZENTRUM

Coupled H-H⁺-H_2-H_2^+ CR model, @ 10 eV, 1e13 cm-3

134 species/states, 16 final states, 117 non-zero eigenvalues

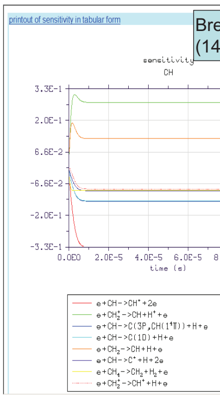


HYDKIN.de: online sensitivity analysis

JÜLICH FORSCHUNGSZENTRUM

D. Reiter, Phys. Scr. **T138** (2009) 014014

Breakup of CH4 @ 40 eV (143 parameters)



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)=d(ln[n_Y])/d(ln<rate>)

Identify, print and plot the most sensitive parameters:

If <rate> changes by x %
Then n_Y changes by x * Z %

ITER, D-He-C, non-linear neutral, no radiation transport
(full report: Kotov,Reiter, Juel, 2007, at www.eirene.de)

JÜLICH FORSCHUNGSZENTRUM

```
SURFMOD_2_CARBON_SPT_580K
*** 4. Data for species and atomic physics module
**  Reactions
   26
  1 AMJUEL H.4 2.1.5     EI   0  1 0.00000E+00 0.00000E+00 0.00000E+00
  2 AMJUEL H.102.1.5     EI   0  1 0.00000E+00 0.00000E+00 0.00000E+00
  3 HYDHEL H.1 3.1.8     CX   1  1 0.00000E+00 0.00000E+00 0.00000E+00
  3 HYDHEL H.3 3.1.8     CX   1  1 0.00000E+00 0.00000E+00 0.00000E+00
  4 HYDHEL H.2 2.3.9     EI   0  4 0.00000E+00 0.00000E+00 0.00000E+00
  5 METHAN H.2 2.23      EI   0 12 0.00000E+00 0.00000E+00 0.00000E+00
  6 AMJUEL H.4 2.2.9     EI   0  2 0.00000E+00 0.00000E+00 0.00000E+00
  7 AMJUEL H.4 2.2.5g    DS   0  2 0.00000E+00 0.00000E+00 0.00000E+00
  8 AMJUEL H.4 2.2.10    DS   0  2 0.00000E+00 0.00000E+00 0.00000E+00
  9 AMJUEL H.4 2.1.8     RC   0  1 0.00000E+00 0.00000E+00 0.00000E+00
 10 AMJUEL H.102.1.8     RC   0  1 1.36000E+01 0.00000E+00 0.00000E+00
 11 AMJUEL H.1 0.2T      EL   1  4 0.00000E+00 0.00000E+00 0.00000E+00
 11 AMJUEL H.3 0.2T      EL   1  4 0.00000E+00 0.00000E+00 0.00000E+00
 11 AMJUEL H.0 0.2T      EL   1  4 0.00000E+00 0.00000E+00 0.00000E+00
 12 CONST  H.2           EL   1  1
-2.1091E+01  0.2500E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 13 CONST  H.2           EL   2  2
-2.0589E+01  0.2500E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 14 CONST  H.2           EL   1  2
-2.0357E+01  0.2500E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 15 CONST  H.2           EL   1  2
-2.0357E+01  0.2500E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 16 CONST  H.2           EL   1  4
-2.1014E+01  0.2500E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
 0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00  0.0000E 00
```

Starts with a list of “reactions”, collected from various databases linked to EIRENE

All raw (unprocessed) data from databases are publicly exposed: www.hydkin.de

Simple Krook Collision rates for Neutral-Neutral Collisions.

JÜLICH

```
 25 AMJUEL H.4 2.2.14    DS   0  2 0.00000E+00 0.00000E+00 0.00000E+00
 26 AMJUEL H.8 2.2.14    DS   0  2 0.00000E+00 0.00000E+00 0.00000E+00
**4a.   Neutral atom species
    3
 1 D          2  1  1  0  1 -1  0  6  0  0 99
    1   115   114      0 30000
 2.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
    3   114   111   114  1001
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   12  1014   111  1014  1001      0   111
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   14  1214   111  1214  1001      0   112
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   16  1414   111  1414  1001      0   211
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   16  2114   111  2114  1001      0   311
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 2 He         4  2  1  0  2  2  0  6  0  0 99
    4   115   214      0      0
-2.45500E+01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   11   114   211   114  1001
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   17  1514   211  1514  1001      0   111
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   19  1714   211  1714  1001      0   112
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   20  1814   211  1814  1001      0   211
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   16  2514   211  2514  1001      0   311
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
 3 C         12  6  1  0  0  0  0  5
    5   115   414      0      0
-1.13000E+01 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   17  2014   311  2014  1001      0   111
 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00
   17  2414   311  2414  1001      0   211
```

List of (chemical) elements (atoms, molecules ions)

and

a mapping between these elements and the included set of reactions

Molecular Processes considered in fusion:

e,p + $H_2(v_i)$ → …, e+$H_2^+(v_i)$ → H + H*

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

www.amdis.iaea.org, database & data center network, Wuenderlich, Fantz, IPP Garching,….
H. Takagi, Phys. Scr. (2002) 52, and: Conference series: DR 1-9

e,p + C_xH_y →…., e+$C_xH_y^+$ → …. C erosion and migration, tritium retention in remote areas,…. Excited states of products (CH(A→X)) ?

R. Janev et al., Phys. Plasma (2004) 11, www.hydkin.de, IAEA: www.amdis.iaea.org

e+$H_3^+(v_3)$ → …., DR, DE,….

- H_3^+ probably irrelevant in fusion plasmas

M. Larsson et al., PRL (1993) 70, S. Datz et al., PRL (1995) 74, and: Conference series: DR 1-9

e+ BeH/BeH$^+$ → …. possible role on spectroscopy and on material migration: Formation rates ?? 10% of Be sputtering?

J.B. Roos et al. Phys. Rev A (2009) 80, IAEA Atomic Molec. data unit CRP 2012-2015
Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre,J. Tennyson et al. (Univ. College London), R. Celiberto et al. (Bari)

e+ N_2, N_2^+ → …. NN

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

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

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 + H_2, e + H_2^+, isotopomeres,
- inelastic vs. transport

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

N_2 plasma cooling:
- molecular database used in fusion: obsolete, perhaps not critical (?)

Focus in (magnetic) fusion modeling will likely be on

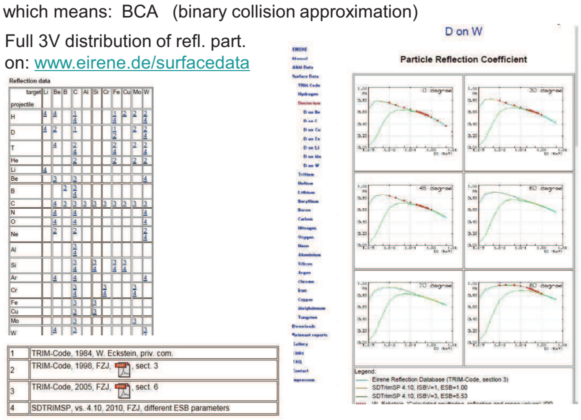
Understand radial transport: synthetic turbulence in edge codes, turbulence averaged CR models, momolitic or heterogeneous coupling of edge transport and turbulence codes

Uncertainty propagation in edge/divertor models (as by-product from “adjoint based automated optimization” in fusion power plant design)

→ New AMS data have to come in pretty “bite-sized” ,
→ “as unprocessed as possible”
→ publicly exposed

Surface processes in B2-EIRENE:
Jargon in edge modelling talks/papers: “we use TRIM code data….”
(wrt. “physical sputtering and reflection”)
which means: BCA (binary collision approximation)

Full 3V distribution of refl. part.
on: www.eirene.de/surfacedata



TRIM code (reflection) results currently in use in EIRENE are fully reproducible, until back 1986 (all raw data kept, and online: www.eirene.de/surfacedata)

Sometime during past 3-5 years, somebody changed the default setting for: “projectile surface binding energy” in AB_TRIM_xy.

D on W: ESB=1 eV (Eckstein), until ???, then 5.53 eV

with significant effects on modelling the incremental effects when replacing C by W targets (as in all, 15 years, ITER divertor modelling)

Can we narrow down on ESB in TRIM ?? (MD to find ESB ??)

This would remove a major uncertainty from all present edge models.

Lessons learned from 18 years ITER divertor design modeling

- B2-EIRENE code as main “working horse”, for ITER divertor,
- “4.3-code version” jointly maintained at IO and FZJ

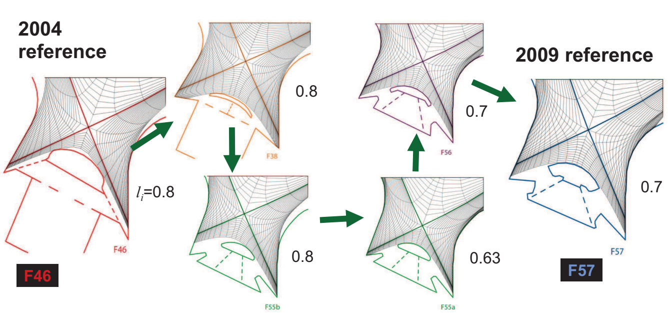
- Successful compensation of all gains in CPU speed, by adding more physics into model (Moore’s law: 10 times doubling of computing – speed):
- But: code run time remained constant over 18 years.
- → Impractical for an “ITER – analogue” DEMO divertor code analysis.

- Edge code speed for large machines (ITER → DEMO) is an issue (actually: not the speed, but assessment of the numerical accuracy for given run-time)

- **B2-EIRENE may be right or wrong: the ITER divertor is designed, …… “some time to breathe”.**

The geneology of ITER divertors 2007-2009: New reference design

B2-EIRENE: main ITER edge plasma design tool



Calculations slow → so use the previously studied variants to see the progression
Extend parallelization of EIRENE to B2-EIRENE (2008), + HPC-FF, ….

This was quite a hassle. It would have been Impossible for DEMO-size configurations.

Given: Design goal : (I, target heat load, plasma purity,…)
Design variable: (ϕ, target shape, divertor coils, pumps, …)
Equations : (partial diff. eqs., “pde”, AMS data, to find I from ϕ)

What was done: “design by analysis”: I(ϕ) many (expensive) forward B2-EIRENE runs, scanning ϕ-space.

What was needed: “design by optimization”: dI/dϕ Search for optimum, gradient based.

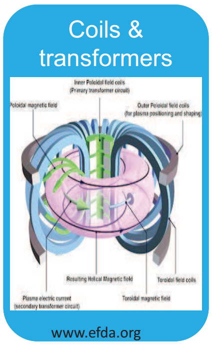
I and ϕ are connected by B2-EIRENE model ((“pde”) and AMS data).

Goal: gradient computation, gradient based search for optimum

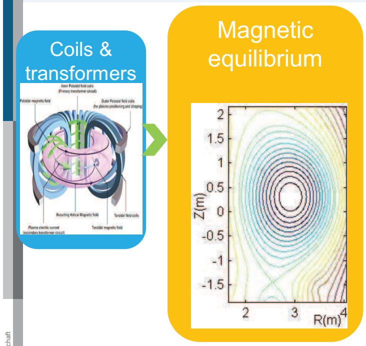
“pde- constrained optimization”

Divertor design: an “optimal control problem”?

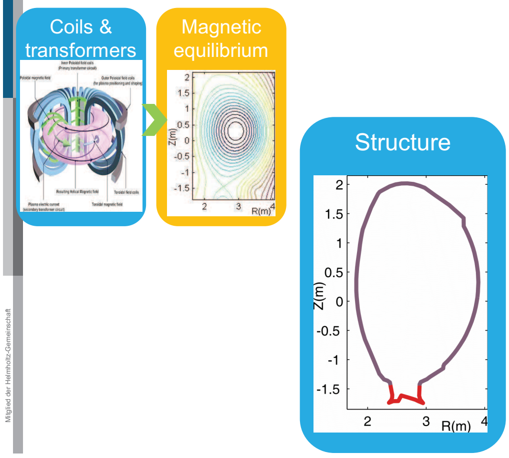
actuators: puff, pump, seeding ,sweeping….



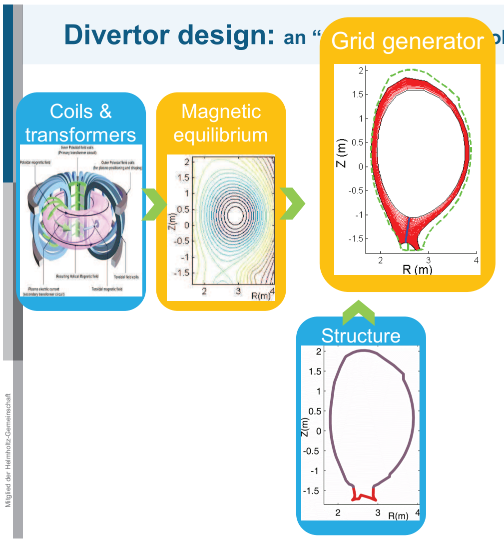
Divertor design: an “optimal control problem”?



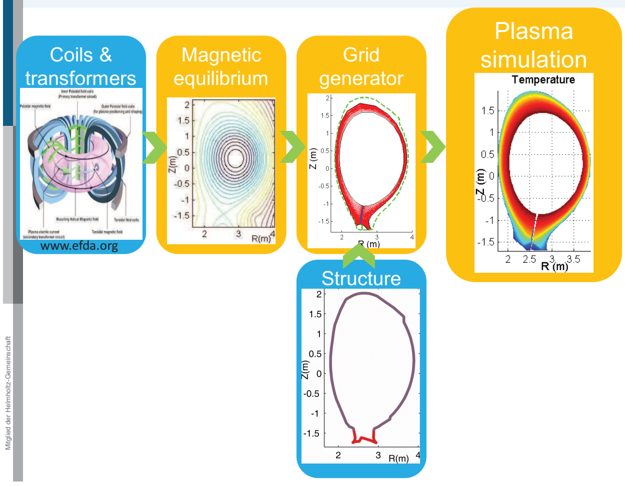
Divertor design: an “optimal control problem”?



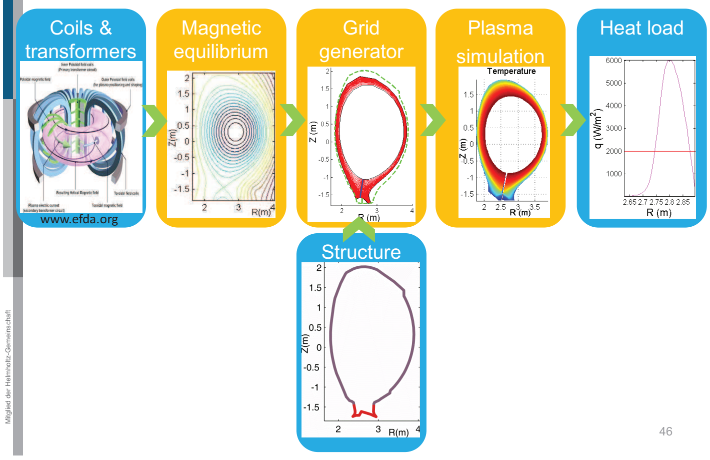
Divertor design: an “optimal control problem”?



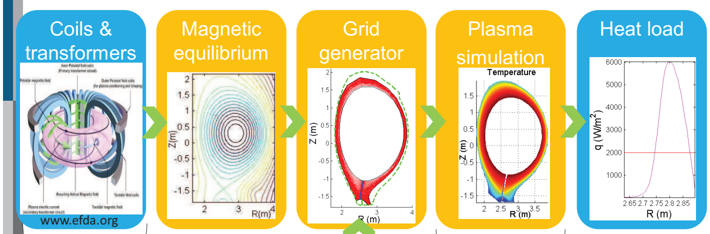
Divertor design: an “optimal control problem”?

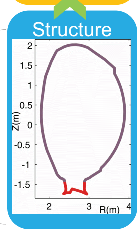


Divertor design: an “optimal control problem”?



Divertor design: an “optimal control problem”?





Many **design variables**:

- Coil locations and current magnitude
- Target shape
- …

Many **design requirements**:

- Core stability
- Shielding
- Peak heat flux low
- Efficient helium-removal
- …

- Computationally expensive

Divertor design: Optimization-based

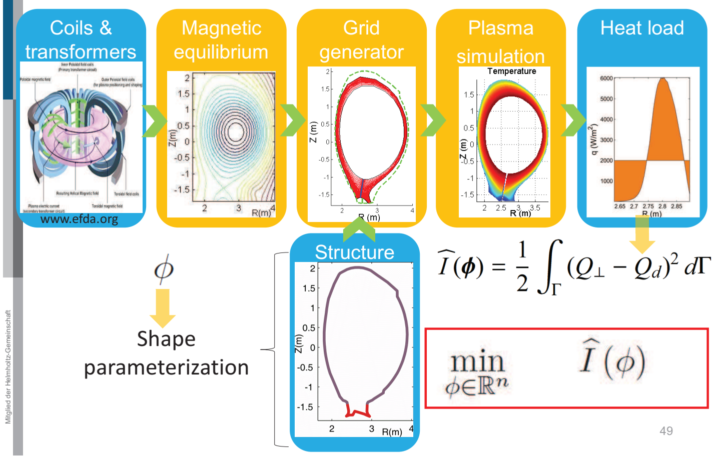
Propose:

1. Re-phrase “fusion heat exhaust problem” as “optimal control problem” or as “optimization problem”. Then: connect to comp. engineering science community
2. Decide: “continuous adjoint” or “discrete adjoint” for gradient computation

Advantages

- Automated design process (vs. human design by changing one parameter at a time: Mostly with one objective in their mind)
- Very efficient methods possible (perhaps ? Our flow is orders of magnitude more complex than that in sub-sonic aeronautics. Strong exchange between three states of matter: solid – gas – plasma !)
- Complicated trade-offs including various design requirements are quantified and optimized

Divertor design: Shape Optimization



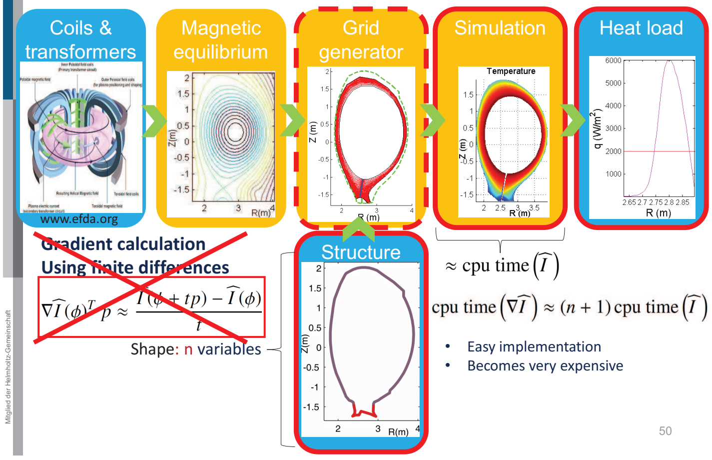
ϕ

Shape parameterization

$$\widehat{I}(\boldsymbol{\phi}) = \frac{1}{2}\int_{\Gamma} (Q_{\perp} - Q_d)^2 \, d\Gamma$$

$$\boxed{\min_{\phi \in \mathbb{R}^n} \quad \widehat{I}(\phi)}$$

Divertor design: Gradient calculation



~~Gradient calculation~~

~~Using finite differences~~

$$\cancel{\nabla \widehat{I}(\phi)^T p \approx \frac{\widehat{I}(\phi + tp) - \widehat{I}(\phi)}{t}}$$

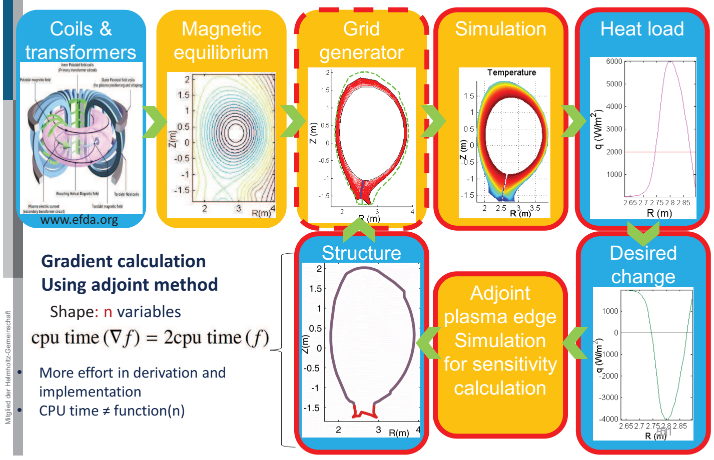
Shape: n variables

$\approx$ cpu time $(\widehat{I})$

cpu time $(\nabla \widehat{I}) \approx (n+1)$ cpu time $(\widehat{I})$

- Easy implementation
- Becomes very expensive

Divertor design: Gradient calculation



Gradient calculation

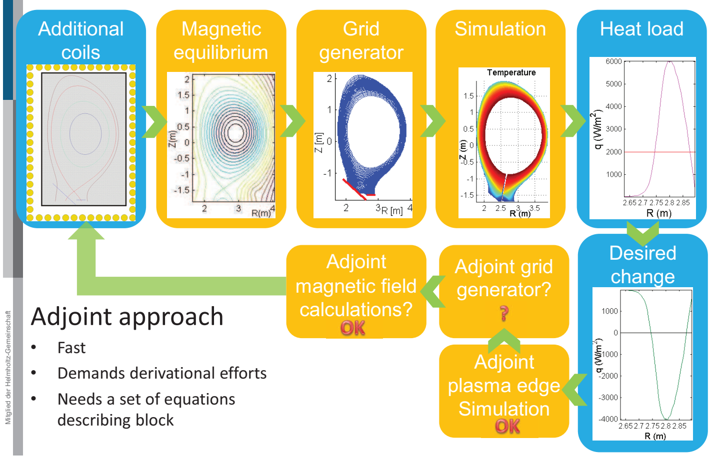
Using adjoint method

Shape: n variables

cpu time $(\nabla f) = 2$cpu time (f)

- More effort in derivation and implementation
- CPU time ≠ function(n)

Optimization: Gradient computation



Adjoint approach

- Fast
- Demands derivational efforts
- Needs a set of equations describing block

Status:

- Small team of experts is being formed
- Connection to computational **engineering** community established (rather than computational science)
- Design Code "B2-EIRENE_light" under development, somewhat reduced physics, but additional equations for gradient computation
- First promising case studies:

  Dekeyser, Reiter, Baelmans,

  Int. J. of Computational Science and Engineering, 2013,

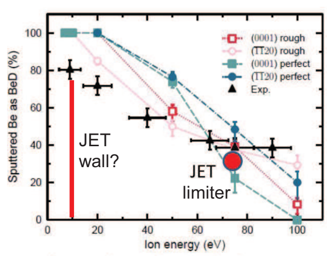
  J. Nucl. Fus (2014), Journal Computational Physics (2014)

Thank you for your attention!

Reserve slides

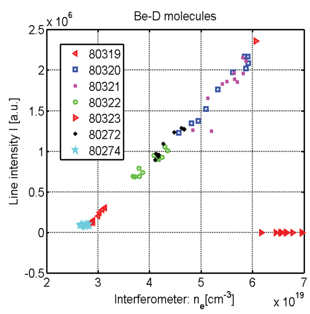
EFDA JET Variation of BeD with plasma conditions

BeD contribution to total Be yield in PISCES and MD simulations



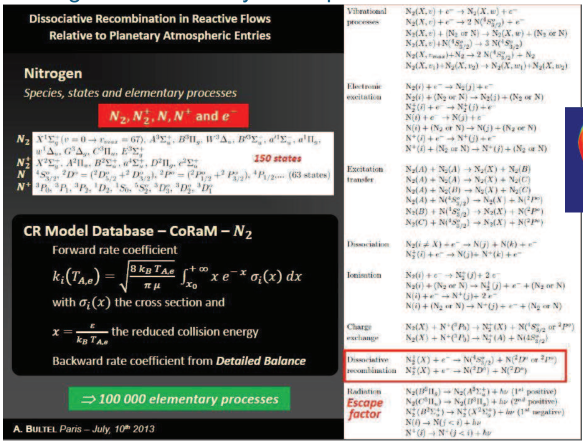
Exp. from D. Nishijima et al, PPCF 50(2008)125007.
Sim. from C. Bjorkas et al., New J. Physics 11(2009)123017.

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

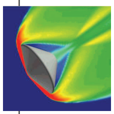


JET BeD limiter data in good agreement with yields deduced from PISCES exp. and MD simulations

Current Nucl. Fusion N_2 database: obsolete !
see e.g.: Planetary Atmospheric Entries



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 I

Line emission

$$\varepsilon = \frac{1}{4\pi} n_A^* A_{ij}$$

$$n_A^* \sum_{k \le i} A_{ik} = n_A n_e < \sigma_{Exg} \upsilon_e >$$

with B as branching ratio:

$$B = A_{ik} / \sum_{k\le i} A_{ik}$$

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

Particle flux <=> number of ionisation events

$$\frac{d\Gamma_A}{dr} = \frac{d(n_A \upsilon_A)}{dr} = -n_A(r) n_e(r) < \sigma_I \upsilon_e >$$

$$\Gamma_A = \int_{r_1}^{r_2} n_A(r) n_e(r) < \sigma_I \upsilon_e > dr$$

$$\Gamma_A = 4\pi \frac{I_{tot}}{B h\nu} \frac{\int_{r_1}^{r_2} n_A(r) n_e(r) < \sigma_I \upsilon_e >_{(r)} dr}{\int_{r_1}^{r_2} n_A(r) n_e(r) < \sigma_{Exg} \upsilon_e >_{(r)} dr}$$

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

$$\Gamma_A = 4\pi \frac{I_{tot}}{B h\nu} \frac{< \sigma_I \upsilon_e >}{< \sigma_{Exg} \upsilon_e >} = \frac{4\pi I_{tot}}{h\nu} \frac{S}{BX}$$

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 $f(\vec{r}, \vec{v}, t)$

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

Free flight — External source — Absorption

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

microscopic collision kinetics, microscopic boundary conditions

Altogether, just a balance in phase space

Kinetic (transport) equation, one for each species

$$\frac{\partial f(E,\vec{\Omega})}{\partial t} + v\vec{\Omega}\cdot\nabla f(E,\vec{\Omega}) + \frac{f}{\tau} + Forces = S(E,\vec{\Omega}) - v\sigma_a(E) f(E,\vec{\Omega})$$

Transport — External source — Absorption

EIRENE (3D3V,t)

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

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, → multiparametric CR model)

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

Kinetic (transport) equation, one for each species

$$\frac{\partial f(E,\vec{\Omega})}{\partial t} + v\vec{\Omega}\cdot\nabla f(\cancel{E,\vec{\Omega}}) + \frac{f}{\tau} + Forces = S(\cancel{E,\vec{\Omega}}) - v\sigma_a(E) f(\cancel{E,\vec{\Omega}})$$

Transport — External source — Absorption

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

Collisions, Boundary Conditions

System then becomes analogous to:

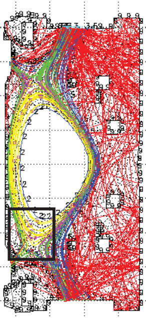
$$\frac{\partial f}{\partial t} = \vec{S} + \overleftrightarrow{M}\vec{f}, \overleftrightarrow{M} = \vec{C} + \frac{1}{\tau}$$

Ordinary (0D0V) CR model, "Plasma chemistry Model"

for those f_i, for which the transport has been removed from kinetic equation

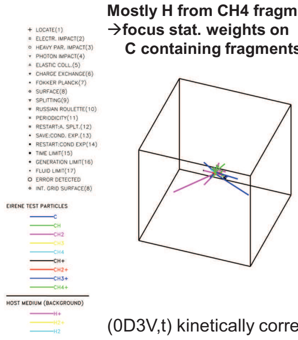
Verify Interface: HYDKIN --- EIRENE (check for correct transfer of chemistry, correct integration of cross sections)

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



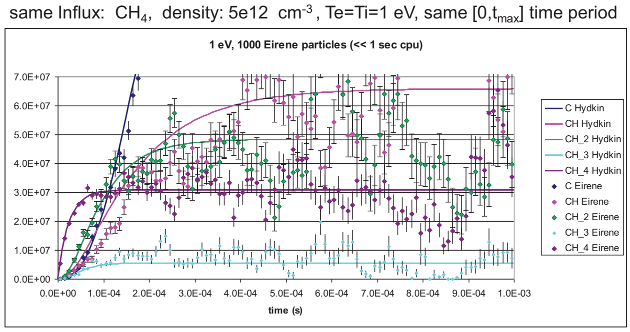
(3D3V,t) kinetic transport

Mostly H from CH4 fragmentation →focus stat. weights on C containing fragments



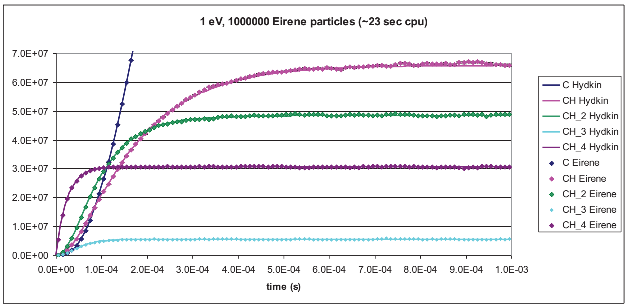
(0D3V,t) kinetically correct CR model

Choose in HYDKIN and in EIRENE:
same Influx: CH_4, density: 5e12 cm^{-3}, Te=Ti=1 eV, same [0,t_{max}] time period



Density of CH_x vs. time

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



EIRENE: 3D3V,t → 0D3V,t → 0D0V,t exact CR model, by Monte Carlo transport

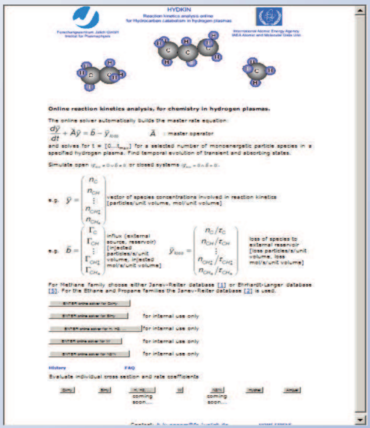
The data evaluation (e.g. for an ITER reference AM&S data set) should be on an as microscopic as possible level
plus: asymptotics (near threshold, high energy)
plus: rules for forming reverse processes (unless trivial)
(plus, perhaps, provide simple toolbox to process/condense).

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

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, H_2, H_3^+,….
- W, W^+, ….W^{74+}
- N, N_2

Next GOAL: BeH,…

HYDKIN: select a number of species, and a set of reactions. Then:

The online solver automatically builds the master rate equation:

$$\frac{d\bar{y}}{dt} + \bar{A}\bar{y} = \bar{b} - \bar{y}_{loss} \qquad \bar{A} \text{ : master operator}$$

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")

e.g. $\bar{y} = \begin{pmatrix} n_C \\ n_{CH} \\ \vdots \\ n_{CH_3} \\ n_{CH_4} \end{pmatrix}$ vector of species concentrations involved in reaction kinetics [particles/unit volume, mol/unit volume]

e.g. $\bar{b} = \begin{pmatrix} \Gamma_C \\ \Gamma_{CH} \\ \vdots \\ \Gamma_{CH_3} \\ \Gamma_{CH_4} \end{pmatrix}$ influx (external source, reservoir) [injected particles/s/unit volume, injected mol/s/unit volume] $\bar{y}_{loss} = \begin{pmatrix} n_C/\tau_C \\ n_{CH}/\tau_{CH} \\ \vdots \\ n_{CH_3}/\tau_{CH_3} \\ n_{CH_4}/\tau_{CH_4} \end{pmatrix}$ loss of species to external reservoir [loss particles/s/unit volume, loss mol/s/unit volume]

Gas puff, chem. sputtering **Transport losses**

Error propagation and sensitivity analysis

Atomic structure
collision codes
experimental data
fundamental data
Velocity distribution: Boltzmann solver, Maxwellian →
Processed data (rate coef.)
CR transition matrix A =
A_excit+
A_radiative+
A_ionis+
A_cx+
A_recomb+….
Linear algebra, ODE solvers →
effective rates,
population coefficients
cooling rates,
beam stopping rates,….

Error propagation and sensitivity analysis

A&M experts
Atomic structure
collision codes
experimental data
Evaluation, … Data centers
fundamental data → PMI, and kinetic models
Data centers and/or user community
Processed data (rate coef.)
CR transition matrix A =
A_excit+
A_radiative+
A_ionis+
A_cx+
A_recomb+….
effective rates,
population coefficients
cooling rates,
beam stopping rates,….
near
edge plasma
far
core plasma

Error propagation and sensitivity analysis

Monte Carlo, C. Ballance
Atomic structure
collision codes
experimental data
fundamental data
Processed data (rate coef.)
Lin. Algebr. D. Reiter
CR transition matrix A =
A_excit+
A_radiative+
A_ionis+
A_cx+
A_recomb+….
effective rates,
population coefficients
cooling rates,
beam stopping rates,….
reduced chemistry models

Error propagation and sensitivity analysis

Monte Carlo, C. Ballance
Atomic structure
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Processed data (rate coef.)
ODEq. Lin. Algebr. D. Reiter
CR transition matrix A =
A_excit+
A_radiative+
A_ionis+
A_cx+
A_recomb+….
effective rates,
population coefficients
cooling rates,
beam stopping rates,….
reduced chemistry models
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)

Uncertainty propagation…

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:

$$Z = d(\ln n_j) / d(\ln R_k)$$

For n species in the system, and m different processes active, there are n x m such sensitivity functions.

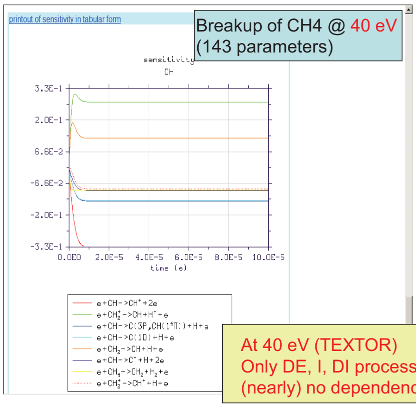
Fortunately: the system of DGL for these Z has the same form as that for the densities n, and can also be solved in closed form using the known eigenvalues and eigenvectors.

If this option is activated, HYDKIN prints and plots the s (input) largest (at $t=t_{max}$) such sensitivity functions

Phys. Scr. **T138** (2009) 014014

HYDKIN.de: online sensitivity analysis

D.Reiter et al., Phys. Scr. **T138** (2009) 014014



Breakup of CH4 @ 40 eV (143 parameters)

Analytic solution for sensitivity, online

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

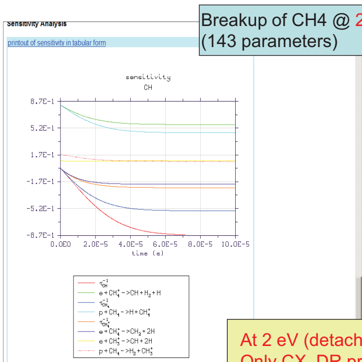
Identify, print and plot the most sensitive parameters:

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

D.Reiter et al., Phys. Scr. **T138** (2009) 014014



Breakup of CH4 @ 2 eV (143 parameters)

Analytic solution for sensitivity, online

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

Identify, print and plot the most sensitive parameters:

If $<rate_k>$ changes by x %
Then n_j changes by x * Z_{jk} %

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

SENSITIVY, uncertainty propagation

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

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

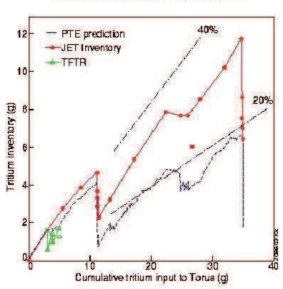
Adjoint B2-fluid (2D, -t) ←→ AM&S kinetic (3D3V, -t)

Available since 30 years	
Recent development	for "adjoint" automated divertor design
Missing link	Start with simpler 2D fluid neutral formulation

The tritium retention issue:

On JET, operated with tritium (1997), the tritium inventory built up without saturation limit.

JET: Retained Tritium

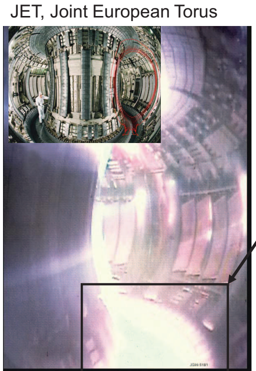


The rate of T retention in JET during DTE1 was 40% of input, reducible to 17% after cleanup in D, without sign of saturation.
P. Andrew, et al, FED 47 (1999) 233.

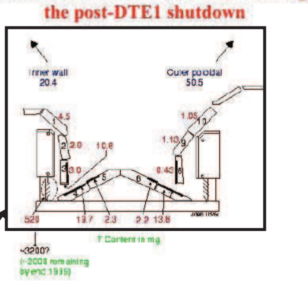
Extrapolation to ITER: the permitted in-vessel T inventory, 0.7 kg, could be reached in 100 shots

Carbon re-deposition, tritium co-deposition in JET

JET, Joint European Torus



Location of tritium in JET vessel during the post-DTE1 shutdown



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.
J.P. Coad, et al, J Nucl Mater 290-293 (2001) 224.

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

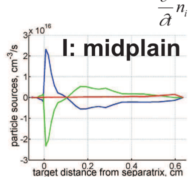
$\mathrm{div}(nv_{\parallel})+\mathrm{div}(nv_{\perp})=$ ionization/recombination/charge exchange

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

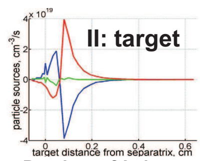
In tokamak edge, all three phenomena are active everywhere

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

"edge transport codes" do the **"bookkeeping"** between these three processes.



parallel vs. (turbulent) cross field flow



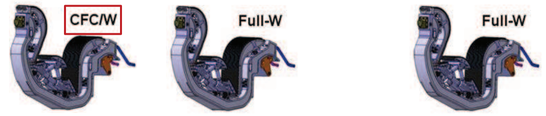
parallel vs. chemistry and PWI driven flow

Dominant friction: p + H_2, detachment

Proposed ITER divertor strategy: decision at the end of 2013

BASELINE

H/He — D/DT



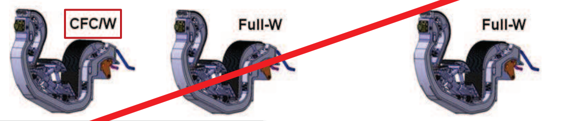
CFC monoblocks at 10 MW m^{-2},
W monoblocks at 5 MW m^{-2}

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

BASELINE

H/He — D/DT



CFC monoblocks at 10 MW m^{-2},
W monoblocks at 5 MW m^{-2}

FULL-W START

H/He — D/DT

W monoblocks at 10 MW m^{-2}

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

Database Series 2002-…., (several IAEA coord. research projects "CRP's")
FZ-Jülich www.eirene.de & www.amdis.iaea.org

Methane (CH_y) C_2H_y C_3H_y Silane (SiH_y) p,H,H^-,H_2,H_2^+,H_3^+

JUEL 3966, Feb 2002	JUEL 4005, Oct. 2002	JUEL 4038, Mar. 2003	JUEL 4105, Dec. 2003
Phys. Plasmas, Vol 9, 9, (2002) 4071	**Phys. Plasmas, Vol 11,2, (2004) 780**	**Contr. Plas.Phys, 47, 7, (2003) 401-417**	**Encycl. Low. Temp. Pl. 2007 (in russian)**

Before we go any further….:

most applications of A&M&N data in plasmas:

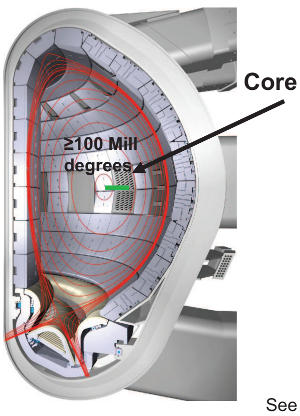
$$\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i\right) = S_{n_i}$$

In magnetically confined fusion plasmas:

$$\frac{\partial}{\partial t} n_i + \underbrace{\vec{\nabla}_\perp \cdot \left(n_i V_\perp\right)}_{\text{unknown}} + \underbrace{\vec{\nabla} \cdot \left(n_i V_\perp\right)}_{\text{known}} = S_{n_i}$$

Relative importance of plasma flow forces over chemistry and PWI

div(nv$_\parallel$)+div(nv$_\perp$)= 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* → nZ
Transport Model : nZ → D⊥, V⊥

See talk bei R.Barnley

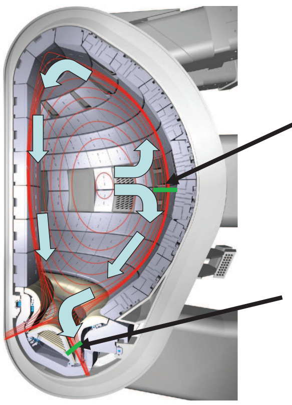
```
 2.00000E+00 1.00000E+00 1.00000E+00 1.00000E-05
     1     2     0     0     0     1     0     0     0     3
 4.91389E+02-3.94193E+02-1.00000E+20 4.81061E+02-3.90124E+02 1.00000E+20
SURFMOD_2_CARBON_SPT_580K
*** 4. Data for species and atomic physics module
include KOTOV-2008-nonlin
*** 6a. General data for reflection model
TF
PATH:
He_on_C
D_on_C
 1.00000E+00 1.00000E+00 1.00000E+00
 1.00000E+00
 1.00000E+00
 1.00000E+00 5.00000E-01 5.00000E-01 1.66667E-01 1.66667E-01 1.66667E-01
 1.66667E-01 1.66667E-01 1.66667E-01 0.00000E+00 0.00000E+00 0.00000E+00
 0.00000E+00
 0.00000E+00
 0.00000E+00
```

- Replace 4&5 by a (small) library of well documented A&M physics modules. (warning: hidden links with other input blocks….)
- Verify the validity of dataset over relevant range via HYDKIN tool online.
- Option 2: numerical and graphical diagnostic of rate coefficients (additional input tally (block 14)

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

div(nv$_\parallel$)+div(nv$_\perp$)= 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!

H_2 molecule, status in present SOLPS-ITER code

Several dedicated CR models have been constructed.
see: IAEA, AMD-unit (CRPs)
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 possibel" model for fusion plasma