



# Detailed atomic, molecular and radiation kinetics in current 2D and 3D edge plasma fluid codes



D. Reiter<sup>1</sup>, V. Kotov<sup>1</sup>, P. Börner<sup>1</sup>, H. Frerichs<sup>1</sup>, D. Harting<sup>1</sup>, R.K. Janev<sup>1</sup>, B. Küppers<sup>1</sup>, S. Wiesen<sup>1</sup>, M. Baeva<sup>2</sup>, S. Lisgo<sup>3</sup>

<sup>1</sup> Institut für Plasmaphysik, Forschungszentrum Jülich GmbH, EURATOM-Association, Trilateral Euregio Cluster, D-52425 Jülich, Germany

<sup>2</sup> FOM Institute for Plasma Physics Rijnhuizen, Edisonbaan 14, 3439 MN Nieuwegein, the Netherlands

<sup>3</sup> University of Toronto Institute for Aerospace Studies, Toronto, M3H 5T6, Canada

## OUTLINE: A&M Model in EIRENE, B2-EIRENE, EMC3-EIRENE, OSM-EIRENE, EDGE2D-EIRENE

[www.eirene.de](http://www.eirene.de)

- 1) A&M effects on ITER divertor predictions
- 2) A&M effects for divertor data interpretation

- 3) New databases: status
- 4) Radiation transport: status
- 5) Conclusions/Outlook

## Consistent Plasma-Gas-Radiation simulations (B2-EIRENE)

If the plasma is allowed to react self-consistently on modified gas-radiation properties, it does so (for ITER conditions) by an increased divertor plasma density, (up to factor 2), somewhat lowered plasma temperature, and a shift from a target recycling towards a volume recombination regime.

This is opposite to expectations for simple estimates that radiation trapping should reduce volume recombination [4,5].

Dominant recombination channels are threebody and radiative. MAR negligible in divertors [2]. Opposite finding, with same numerical model, for linear devices [3]

## Motivation

Atomic and molecular reactions in **B2-EIRENE 1996 (and SOLPS 5)**:

- ionisation of atoms, charge-exchange (*D*) and elastic (*He*) collisions
- 3-body and radiative recombination of *D*<sup>+</sup>
- electron-molecule collisions:  $D_2 \rightarrow 2D; D_2 \rightarrow D_2^+; D_2 \rightarrow D^+ + D$
- electron-molecular ion collisions:  $D_2^+ \rightarrow 2D; D_2^+ \rightarrow D^+ + D; D_2^+ \rightarrow 2D^+$

Update in **B2-EIRENE 2003-2004**:

- Neutral - Neutral collisions between *D*, *D*<sub>2</sub>, *He*
- Molecule - Ion elastic collisions (*D*<sub>2</sub> + *D*<sup>+</sup>)
- Effective rates for electron collisions with *D*<sub>2</sub> and *D*<sub>2</sub><sup>+</sup>
- Molecular Activated Recombination

} Viscosity

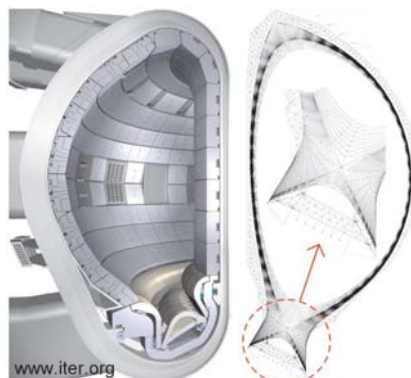
} Molecular Kinetics

Update in **B2-EIRENE 2005**

- Trapping (opacity) of Ly - series photons
- Ionisation of the photoexcited states

} Photon trapping

## B2-EIRENE



ITER design

Computational grid

Simulation of the steady state divertor (SOL) conditions for D-He-C plasma.

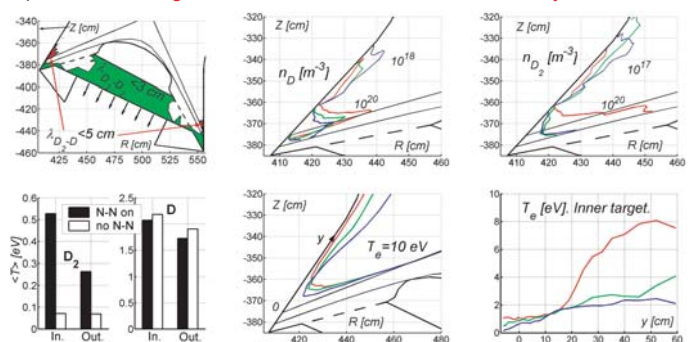
**B2.** 2D, time-dependent set of fluid (Braginskii) equations.

**EIRENE.** Monte-Carlo neutral transport. Calculates neutral related particle, momentum and energy sources for B2.

**The goal of the modelling for ITER:** quantitative assessment of the principal operational parameters (impurity concentration, loads) vs. control parameters (puffing/pumping, gas pressure)

## Effect of Viscosity

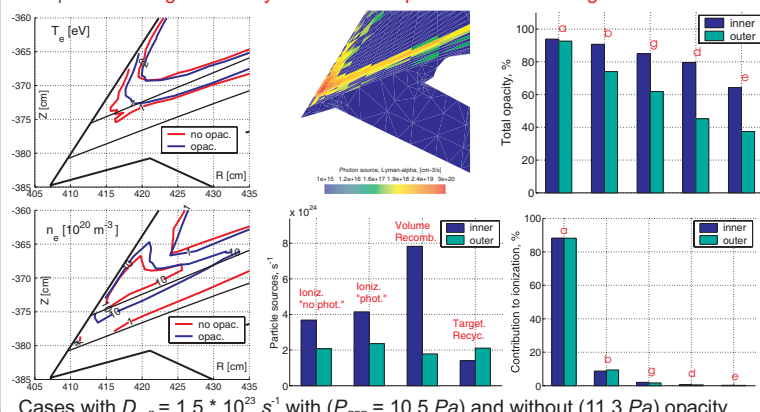
Principal effect: heating of molecules and reduction of their density



— EIRENE 1996 ( $q_{pk, in} = 2.7 \frac{MW}{m^2}$ ); — + NNC ( $2.9 \frac{MW}{m^2}$ ); — + *D*<sub>2</sub> viscosity & kinetics ( $3.3 \frac{MW}{m^2}$ )

## Effect of Photon Trapping

Principal effect: higher density and lower temperature near the targets

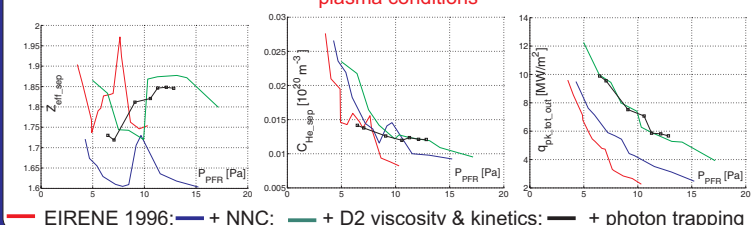


Cases with  $D_{puff} = 1.5 \times 10^{23} s^{-1}$  with ( $P_{PFR} = 10.5 Pa$ ) and without (11.3 Pa) opacity.

## ITER operational parameters

Principal effect of viscosity: shift of operational window towards higher pressure

Principal effect of photon trapping: none on operational parameters, but different plasma conditions



— EIRENE 1996; — + NNC; — + *D*<sub>2</sub> viscosity & kinetics; — + photon trapping

# Application on fixed (reconstructed) plasma background

Sensitivity at low temperature conditions to atomic and molecular physics details.  
Strong sensitivity to radiation opacity assumptions

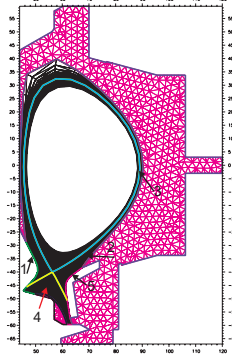
(same as observed in ITER case for frozen plasma conditions)

Inferred atoms density (and related line radiation) differs by factor 2 from opt. thin assumption. This confirms first predictions [6] and is not in conflict with the much lower sensitivity on neutral gas pressure found in self consistent B2-EIRENE ITER calculations.

## Results

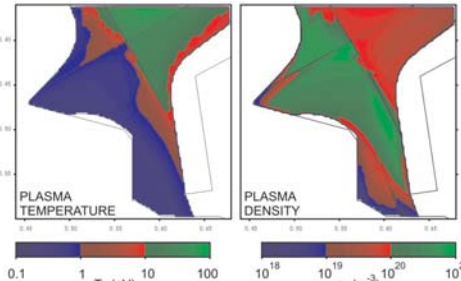
### Geometry and plasma background

The present study is carried out for operating conditions typical of the compact tokamak device Alcator-C-Mod [5,8].



The plasma parameters,  $T_e$ ,  $n_e$ , are set from comparisons with probe and spectroscopic measurements using the OSM Code [8].

The electron density in PFR is around  $10^{21} \text{ m}^{-3}$ . The electron temperature there is  $\sim 0.5 \text{ eV}$  and increases towards the outer divertor target.

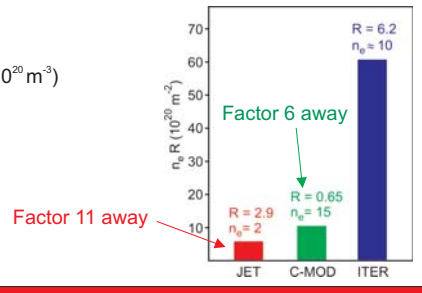


Divertor plasma solution from OSM-code.

## Current hypothesis: in the "detached state" the divertor dynamics and chemistry is controlled by "Collisionality" (inv. Knudsen number)

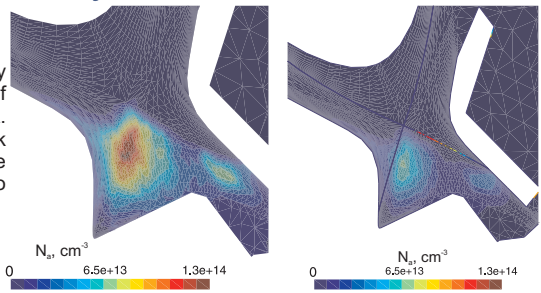
Estimate "Collisionality":  $n_e R$   
-  $n_e$ -Divertor Plasma density ( $\times 10^{20} \text{ m}^{-3}$ )  
- R- Major Radius (m)

**Alcator C-Mod (MIT)**  
10 times smaller than ITER  
similar shape  
Higher density



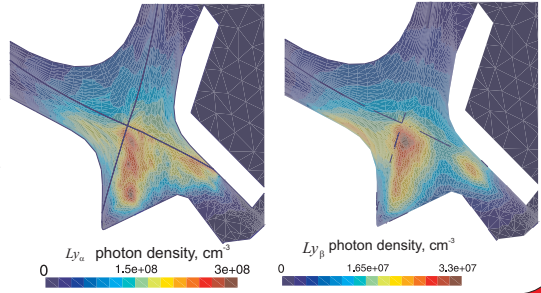
### Atomic and photon density

The atomic density reaches peak values of  $\sim 10^{14} \text{ cm}^{-3}$  in the PFR. Another smaller peak near the outer leg of the separatrix is also pronounced.

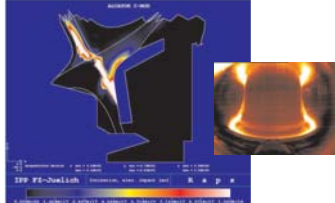


When accounting for absorption, the calculated atom density drops significantly

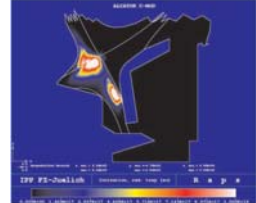
$L\gamma$ -photons generated by the five transitions  $L\gamma_\alpha$  to  $L\gamma_\epsilon$  are considered. The atoms, after absorption, can be ionized before re-emission of photons or suffer collisional decay.



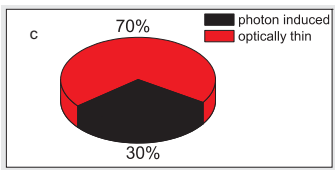
### Ionization sources



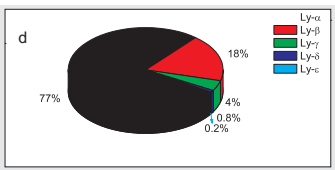
a) ordinary re-ionization source



b) extra re-ionization source due to photon absorption



c) contribution of photon trapping to the total ionization source.



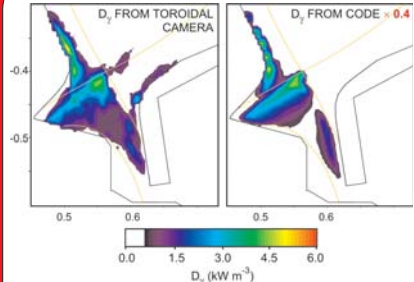
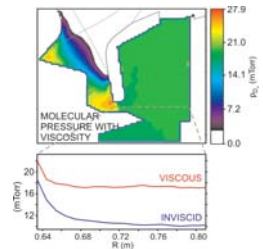
d) contribution of the individual lines to the photon-induced ionization.

Same figure for JET: 85-15  
Same figure for ITER: 30-70

### Neutral Pressure

Exp: 25 mTorr  
Calc 2D (2000) 3 mTorr  
Calc 2D (2003) 27 mTorr [8]  
(better A&M data, better Plasma data)

However  
 $L\gamma$ -opacity: 17 mTorr  
3D: 11 mTorr



$D_\gamma$  (from  $D, D_2, D^+, D_2^+$ ):  
Profile matched, but high by factor 2  
Calibration? Atomic Data? Plasma reconstruction?

Results very sensitive eg. to  $T_e$  profile

Model validation in the presence of many free parameters:

include ALL edge physics that we are sure must be operative even while our capability to confirm these directly remains limited

# New Hydride Collision Databases for Technical Plasmas and Fusion Plasmas

Databases used in (fusion) applications are sometimes either entirely obsolete, or, at best, incomplete and largely empirical

Reviewed cross section  $\sigma(E)$  Database Series 2002-2003, FZ-Jülich, NIFS (Japan), IAEA (R. Janev et al.)

Methane (CH<sub>4</sub>)      C<sub>2</sub>H<sub>2</sub>      C<sub>3</sub>H<sub>4</sub>      Silane (SiH<sub>4</sub>)



JUEL 3966, Feb 2002  
Phys. Plasmas,  
Vol 9, 9, (2002) 4071

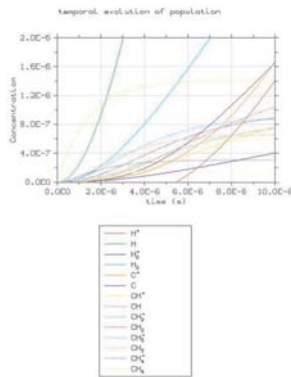
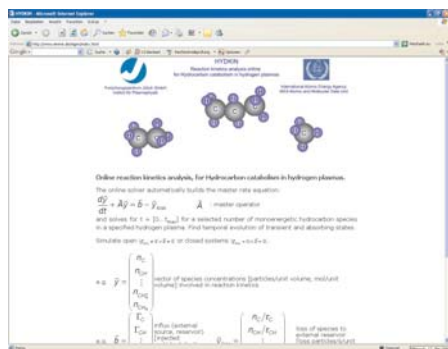
JUEL 4005, Oct. 2002  
Phys. Plasmas,  
Vol 11,2, (2004) 780

JUEL 4038, Mar. 2003  
Contr. Plas.Phys.,  
47, 7, (2003) 401-417

## Analysis tool for hydrocarbon catabolism in fusion edge plasmas

Online evaluation of cross sections  $\sigma(E)$ , rate coefficients K(T), rate equations and S/XB, based upon recent database (2004)

[www.eirene.de/eigen/index.html](http://www.eirene.de/eigen/index.html)



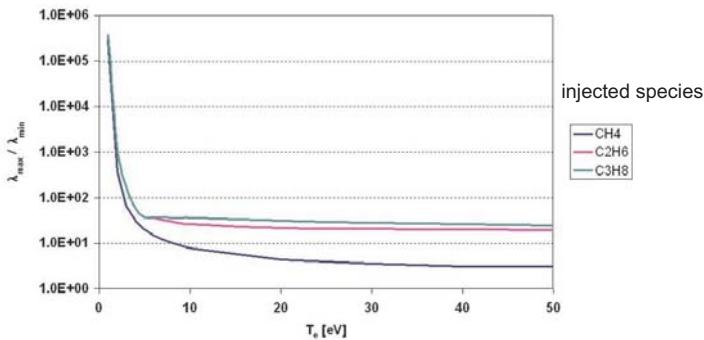
Online solution of time-dep. (1D) Hydrocarbon brake-up, for any prescribed divertor plasma conditions, up to C<sub>3</sub>H<sub>8</sub>

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":  $\lambda_{max} / \lambda_{min}$ , ratio of max. to min. eigenvalues

Fast slow

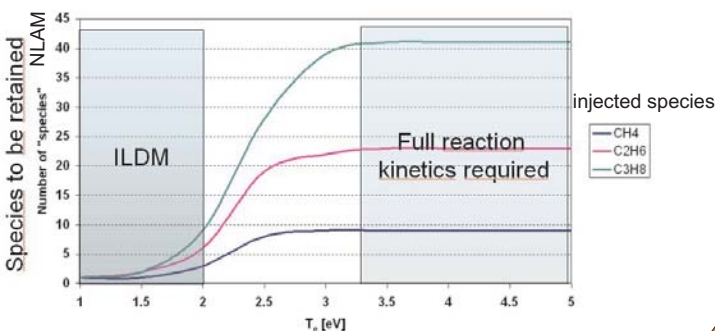
Stiffness Parameter for Hydrocarbon catabolism



Combustion and flame modelling is mathematically analog 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  $\lambda_{max} / \lambda_{min} < 100$ . (NLAM)



## IAEA-TCM 2005-2008: verification and new results (exp. + theor.)

Table 1

Branching ratios of the dissociative recombination of C<sub>3</sub>H<sub>4</sub><sup>+</sup>

Janev & Reiter

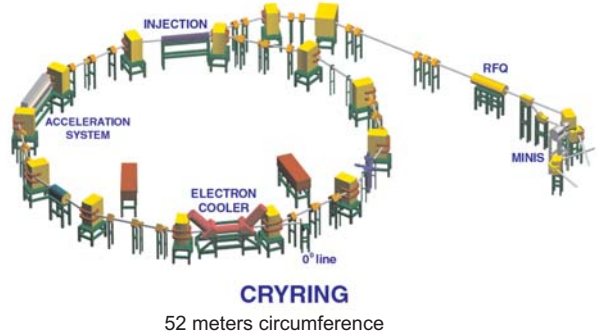
Reaction pathway	Products	Branching ratio
1a	C <sub>3</sub> H <sub>3</sub> + H	0.87 ± 0.04
1b	C <sub>3</sub> H <sub>2</sub> + H <sub>2</sub>	≤ 0.02
1c	C <sub>2</sub> H <sub>3</sub> + CH	0.01 ± 0.01
1d	C <sub>2</sub> H <sub>2</sub> + CH <sub>2</sub>	0.06 ± 0.02
1e	C <sub>2</sub> H + CH <sub>3</sub>	0.01 ± 0.01
1f	C <sub>3</sub> H <sub>2</sub> + 2H	≤ 0.05

0.30

0.55

Int. J. Mass Spectrom. 237, 25 (2004) (Mats Larsson)

## Manne Siegbahn Laboratory

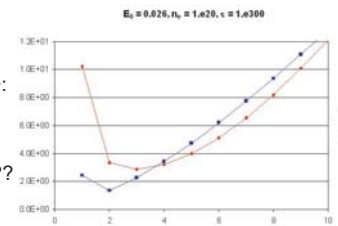


## S/XB, compare: Ehrhardt-Langer (EL) - Janev-Reiter (JR)

- S/XB values (photon-efficiencies) for interpretation of CH, C<sub>2</sub> band emission

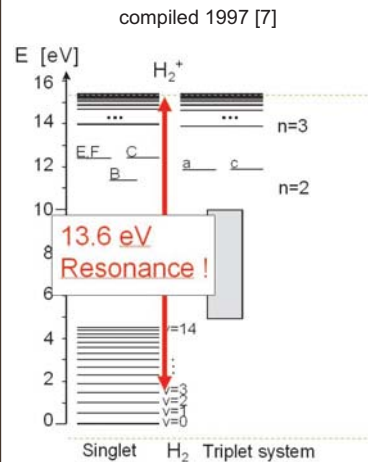
$$S/XB = [\text{Influx}_{C_xH_y} / n_{CH}] / \langle \text{ex} \rangle$$

- First factor from HYDKIN online tool  $\langle \text{ex} \rangle$ : excitation rate coefficient
- **3 major remaining uncertainties:**
- Born-Bethe approximation for  $\langle \text{ex} \rangle$ ??
- other processes populating upper state??
- spectral range and v-v Band contributions??



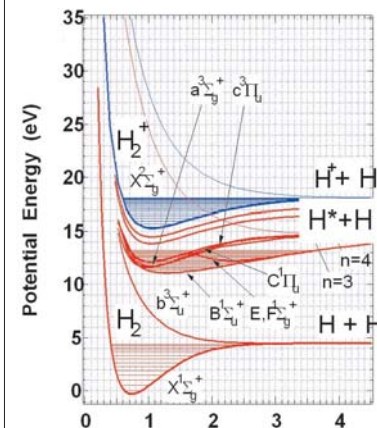
## New Hydrogen Collision Database for Technical Plasmas and Fusion Plasmas

H<sub>2</sub> molecule, status in present divertor code



More complete models available, still need to be integrated

compiled 2005 [K. Sawada, priv. comm.]



2006-2007 ? New compilation: Janev/Reiter/Samm

p, H, H<sup>+</sup>, H<sub>2</sub>, H<sub>2</sub><sup>+</sup>, H<sub>3</sub>



JUEL 4105, Dec. 2003  
Encycl. Low Temp. Pl.  
2006, in printing, (in Russian)

## Transport of photons

### Monte-Carlo transport of photons in EIRENE [6].

- 1) Sampling of direction of emission
- 2) Sampling of Zeemann component
- 3) Sampling of Natural broadening of component plus Doppler shift:

$$E_m = E_0 + m \cdot \mu_B B, \quad P(m) = \frac{1}{4} \begin{cases} 1 + \cos^2 \Theta, m = \pm 1 \\ 2 \sin^2 \Theta, m = 0 \end{cases}, \quad \cos \Theta = \frac{v_{ph} B}{cB}$$

$$E = E' \left( 1 + \frac{v_{ph} \cdot v_n}{c^2} \right), \quad f(E') = \frac{1}{\pi} \frac{\gamma}{(E' - E_m)^2 + \gamma^2}, \quad \gamma = \frac{A_{n1} h}{4\pi}$$

Absorption cross section (Convolution Integral for Doppler broadening):

$$\sigma_a(E) = \frac{B_{ln} E_0}{\sqrt{\pi} c \Delta_D} \sum_{m=-1,0,1} \left( \text{Re} \left[ W \left( \frac{E - E_m}{\Delta_D}; \frac{\gamma}{\Delta_D} \right) \right] P(m) \right) \quad E_m = E_0 \left( 1 + \frac{v_{ph} \cdot U}{c^2} \right) + m \cdot \mu_B B,$$

$$\Delta_D = \frac{E_0}{c} \sqrt{\frac{2T}{m_a}} \quad W(x, y) = W(z = ix - y) = e^{-z^2} \cdot \left[ 1 - \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt \right] \quad (\text{Faddeeva function})$$

## Collision-radiative model

Sawada-Fujimoto model [7] supplemented with photo-excitation sources:

$$\left( \sum_{q>p} C_{p \rightarrow q} + \sum_{q<p} F_{p \rightarrow q} + S_p \right) \cdot n_e + \sum_{q<p} A_{p \rightarrow q} \cdot n_p - \sum_{q>p} C_{q \rightarrow p} n_e n_q - \sum_{q>p} F_{q \rightarrow p} n_e n_q - \sum_{q>p} A_{q \rightarrow p} n_q = \\ = R_p n_e n_i + \underbrace{\left( C_{1 \rightarrow p} n_e + B_{1 \rightarrow p} n_{ph}^{1p} \right)}_{\text{Population } n_p^e} \cdot n_1$$

Where C: electronic excitation; F: electronic de-excitation; A: spontaneous transition; S: ionization; R: recombination; B: photo-excitation.

Effective ionization rate ( $r_p = n_p^1/n_1 \approx n_p^1/n_0$ ):

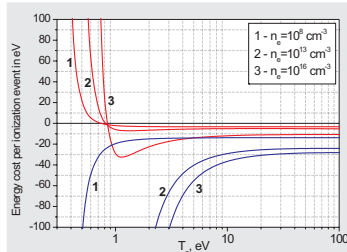
$$S^{ph} = \sum_p S_p r_p = S_1 + \sum_{p>1} \left[ (B_{1p} r_p n_{ph}^{1p} + C_{1p}) - (F_{p1} + A_{p1}/n_e) r_p \right]$$

Effective electron cooling rate:

$$S_E^{ph} = S_1 E_0 + \sum_{p>1} S_p \Delta E'_p r_p + \sum_{p>1} C_{1p} \Delta E_{1p} + \sum_{p>1} \sum_{q>p} C_{pq} \Delta E_{pq} r_p - \sum_{p>1} \sum_{q<p} F_{pq} \Delta E_{pq} r_p = \\ = S_1 E_0 + \sum_{p>1} \sum_{q<p} A_{pq} \Delta E_{pq} r_p - \sum_{p>1} B_{1q} n_{ph}^{1p} \Delta E_{1p}; \quad \Delta E'_p = E_0 - E_p, \quad \Delta E_{pq} = |E_p - E_q|$$

## Radiative heat transfer into PFZ

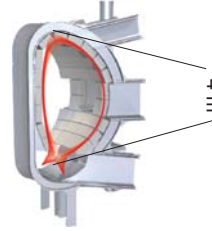
In the case of Ly-alpha absorption stimulated ionization the values of the energy cost per one ionization event are positive for  $T_e$  below 1 eV, i.e. electrons re-gain energy through this ionization channel, via the radiation field. This effect can result in radiative heat transfer from hotter to colder regions even in divertor plasmas.



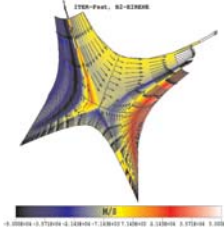
Effective energy source per one ionization event: in blue: ordinary ionization, in red: photon absorption stimulated ionization

## Radiation transfer module: verification and validation using HID lamps

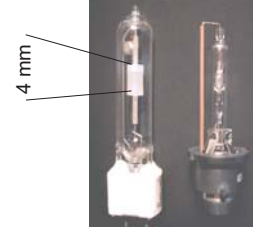
ITER



B2-EIRENE



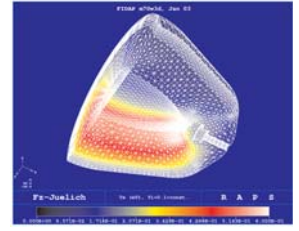
High Intensity Discharge Lamps



D2-36 W  
Automotive  
Material: Quartz

CDM-75 W  
Shop-Lighting  
Material: PCA

FIDAP-EIRENE



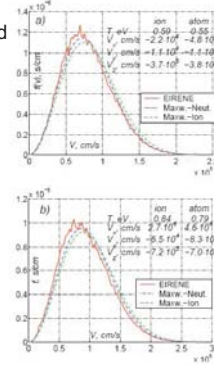
## Velocity-space effects (differences to Cretin-Beline modelling [9])

Instead of photo-induced ionization one can use ionization and recombination rates with suppressed spontaneous transitions. Both approaches are equivalent in terms of particle balance, but not equivalent in terms of kinetic equation:

$$\text{Continuity equation} \quad \frac{1}{n_e} \left( \frac{dn_e}{dt} \right)_{ifr} = Rn_i - Sn_0 \quad \left| \quad \text{Boltzmann equation} \quad \frac{1}{n_e} \left( \frac{df_0}{dt} \right)_{ifr} = Rn_i \hat{f}_+ - Sn_0 \hat{f}_0$$

S and R are effective ionization and recombination rates.

How much is the difference between  $\hat{f}_+$  and  $\hat{f}_0$ ? An example of Velocity Distribution function for D atoms on separatrix in front of the inner (a) and outer (b) target →



## Emission and absorption line shape profiles in EIRENE (2006)

- 0) monoenergetic (delta-function, ohne emission)
- 1) 0 + Doppler (Gaussian profile)
- 2) Natural broadening, electr. Stark effect (Lorentz-profile)
- 3) 2 + Doppler (Voigt-profile)
- 4) **Pressure broadening: v.d. Waals, resonance broadening, quadr. Stark (complex Faddeeva function)**
- 5) Not in use
- 6) Normal Zeeman triplet, (3 monoenergetic components, anisotropic)
- 7) 6 + Doppler (3 gaussian components, anisotropic)
- 8) Normal Zeeman triplet, (3 Lorentzian components, anisotropic)
- 9) 8 + Doppler (weighted sum of 3 Voigt profiles, anisotropic)
- 10) Full Zeeman-Stark quantum line shape calculation (Rosato et al., Univ. Marseille) (weighted sum of 10 Lorentzian profiles, anisotropic)
- 11) 10 + Doppler (weighted sum of 10 Voigt profiles, anisotropic)

4): for code verification using HID lamp spectroscopy, LTE, industrial applications (FIDAP-EIRENE)

9): current EIRENE default in B2-EIRENE, OSM-EIRENE, EMC3-EIRENE  
10,11): new options (2006), under evaluation

## Conclusions/Outlook

- Radiation transfer included also in self consistent 2D plasma-gas-radiation code (B2-EIRENE\_ITER)
- Complementary results in interpretative and predictive mode
- Hydrocarbons: online analysis tool HYDKIN: ([www.eirene.de/eigen/index.html](http://www.eirene.de/eigen/index.html))
- spectral analysis indicates: no reduced models above 3-5 eV ??

## References

See also:

- [1] A. Kukushkin et al., this conf.
- [2] V. Kotov et al., Contrib. Plasmas Physics 2006, in printing
- [3] M. Baeva et al., this conf.
- [4] D. Reiter, S. Wiesen, M. Born, Plasma Phys. Control. Fusion 44 (2002), 1723.

- [5] J. L. Terry, B. Lipschultz, A. Yu. Pigarov et al., Phys. Plasmas 5 (1998), 1759.
- [6] D. Reiter, S. Wiesen, M. Born, J. Nuclear Materials, vol. 313-316 (2003), p. 845
- [7] K. Sawada, T. Fujimoto, J. Appl. Phys. 78 (1995) 2913.
- [8] S. Lisgo, P. Börner, C. Boswell et al., J. Nucl. Mat. 337-339 (2005), 139.
- [9] H.A. Scott, M.L. Adams, Contrib. Plasma Phys, 44, 51(2004) and M.L. Adams, H.A. Scott, Contrib. Plasma Phys, 44, 262 (2004)