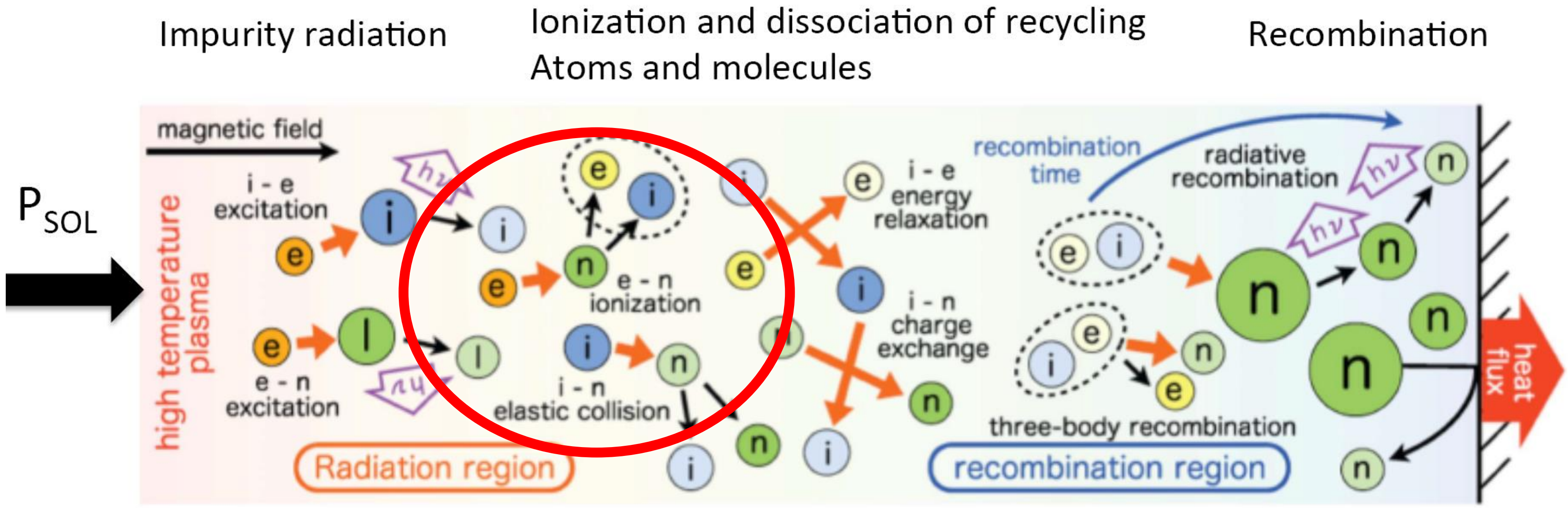
APPLICATION OF MONTE-CARLO METHODS FOR PHOTON TRANSPORT IN DIVERTORS

MARCH 29 2021 I SVEN WIESEN (FZJ)

CONTENT

- Introduction
- Radiative transport: transport, Boltzmann equation
- EIRENE Monte-Carlo for solving radiation transport
- Applications
  - Industrial: high pressure gas discharge lamps
  - Fusion: C-mod, JET, ITER (DEMO)

WHAT PROCESSES CONTROL POWER DISSIPATION?

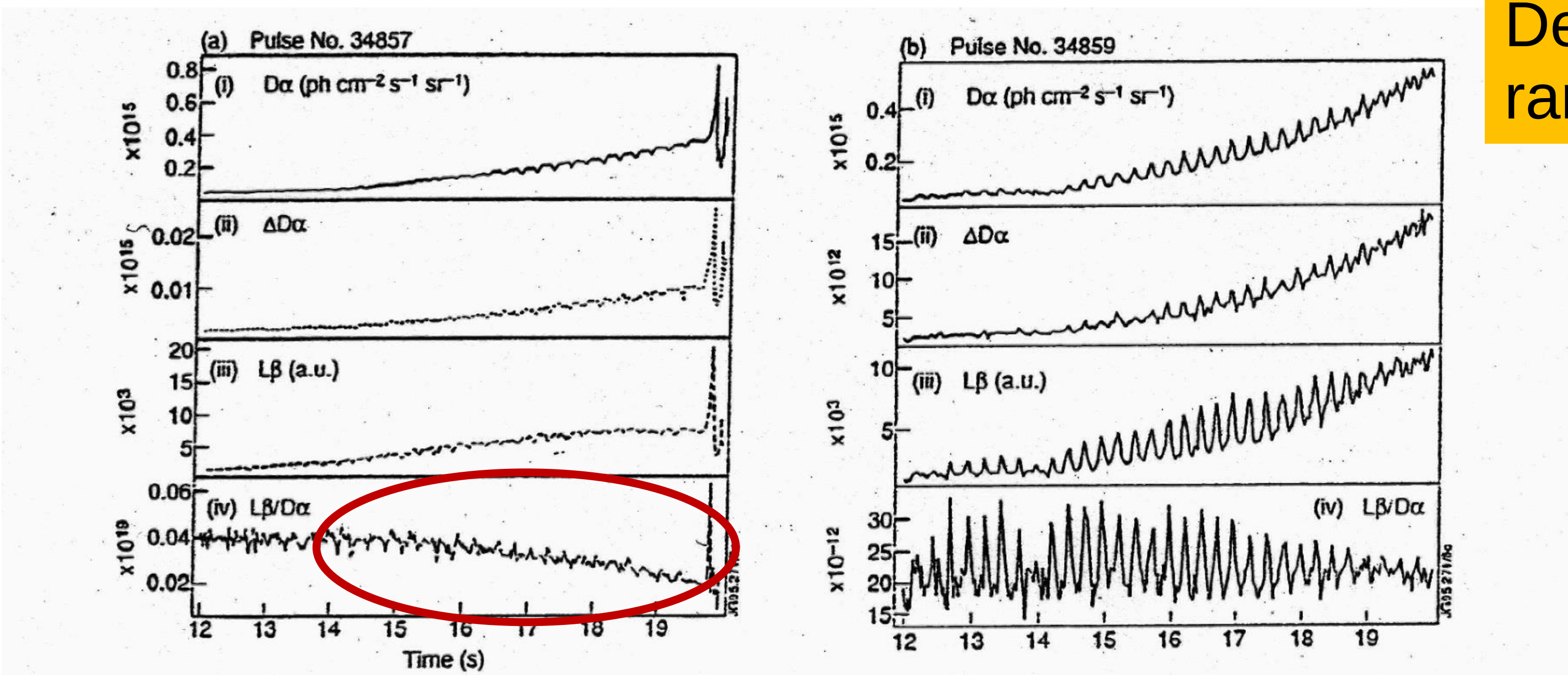


Change in ionisation-recombination balance due to photon opacity,re-absorption of strong Lyman lines

Complex physics → coupled fluid-kinetic 2D/3D edge plasma codes

1995: AT SOME JET SHOTS, "*OPACITY AT THE POINT OF BEING SIGNIFICANT*"

Density ramps

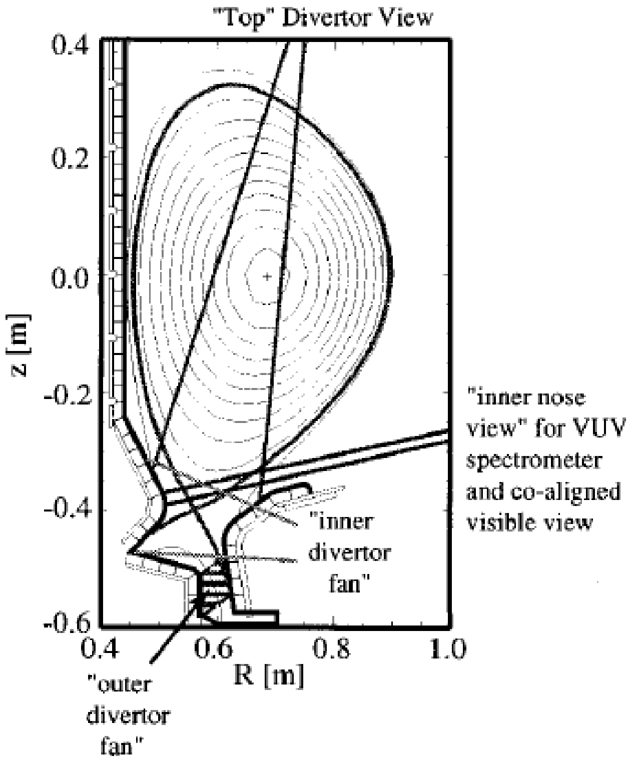


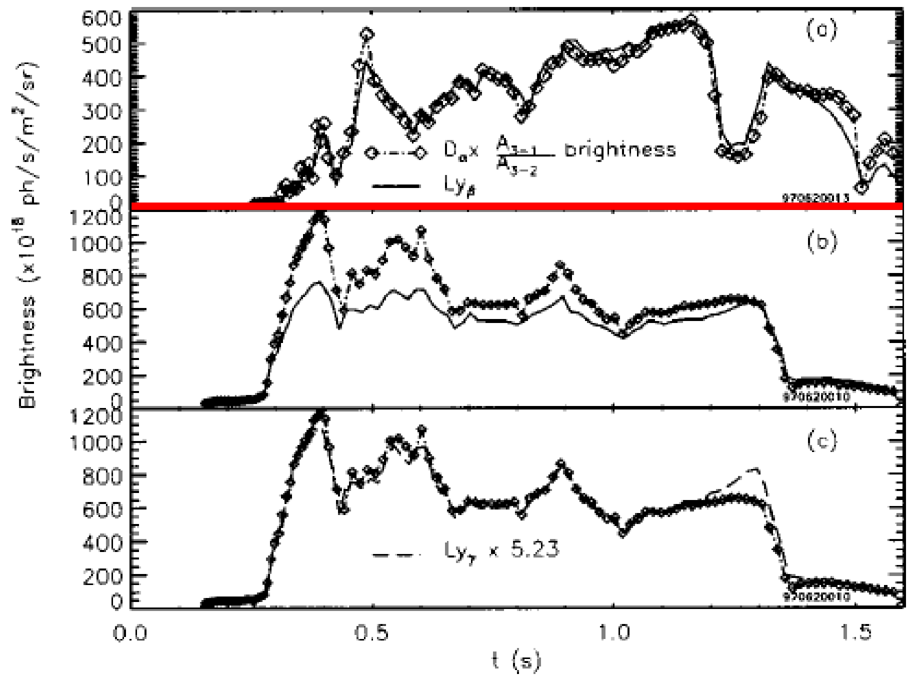
Higher neutral pressure in vertical target configurations

Horizontal target configuration with less dense divertor

Lovegrove, Horton, et al, EPS Bournemouth, 1995

1998: C-MOD - DENSE DIVERTOR CLEARLY SHOWS LYMAN-BETA TRAPPING





Ly_β non-opaque

Ly_β opaque

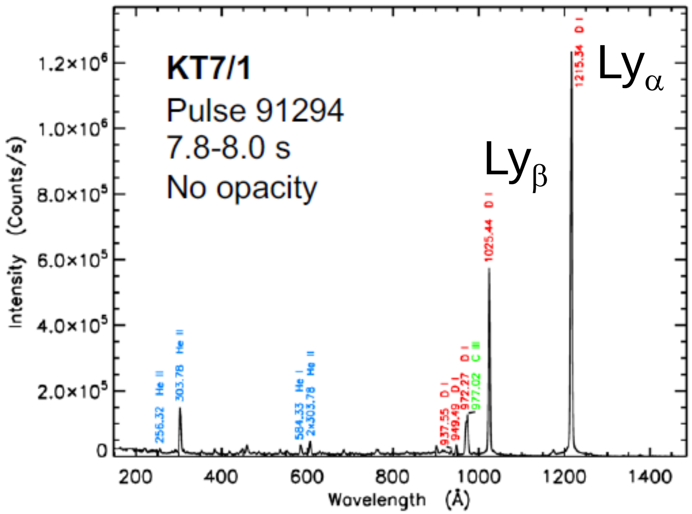
D_α & Ly_γ

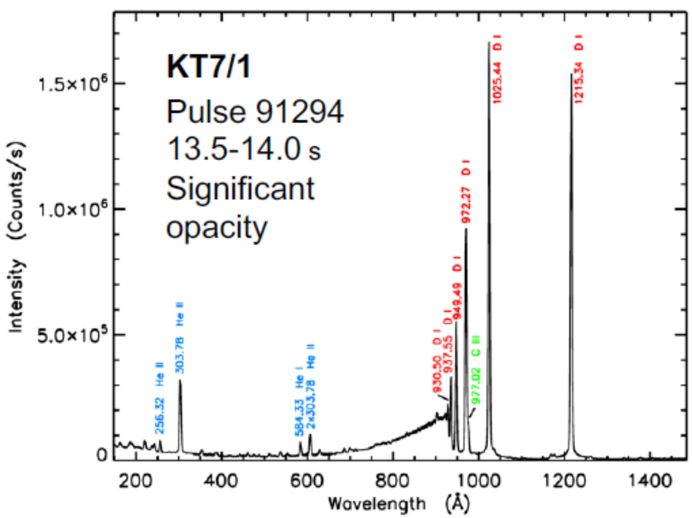
[G. 5. (a) Time histories of the Ly_β brightness compared to that predicted y the D_α brightness measured with essentially the same view for a discharge where there was no trapping of Ly_β. (b) The same as (a), but where some trapping is evident. (c) The time history of Ly_γ for the same discharge as (b), indicating that Ly_γ and D_α stay in a constant ratio, unlike Ly_β and D_α.

Terry et al 1998

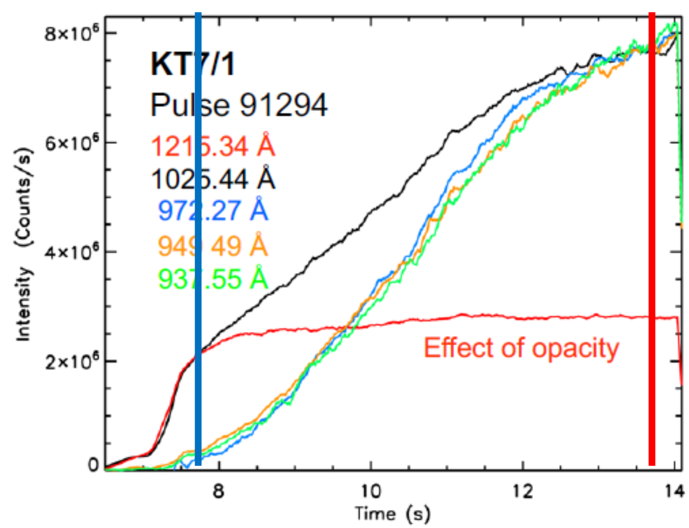
D I VUV SPECTRA AND MEASURED LINE INTENSITY RATIOS

JET-ILW





- Pulse 91294 is a H fuelled Ohmic density limit pulse at 2.5 T / 2.4MA.
- Opacity is seen to be important reducing Ly_α by ~55% and Ly_β by ~6%.
- The T_e dependence suggested by all the theoretical intensity ratios is not observed.
- Either the dominant emission in the line integration moves with a plasma region that has a constant T_e or there are questions regarding the population modelling.

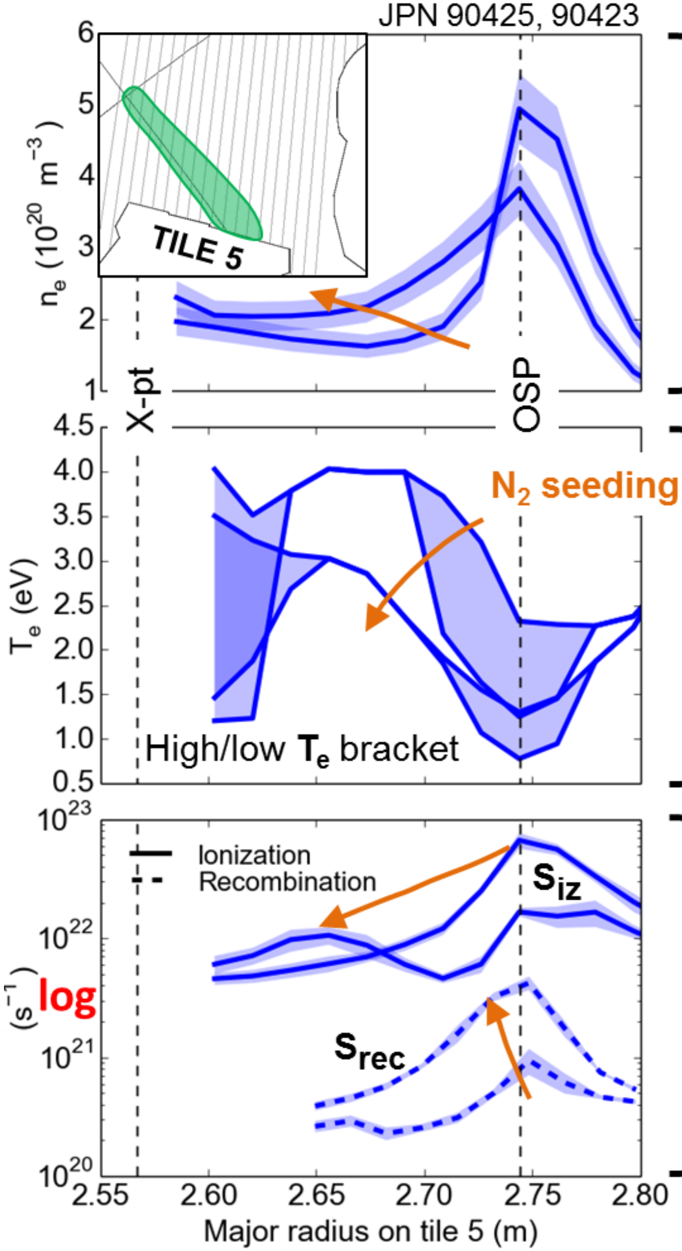


K. Lawson
A. Wynn
2017

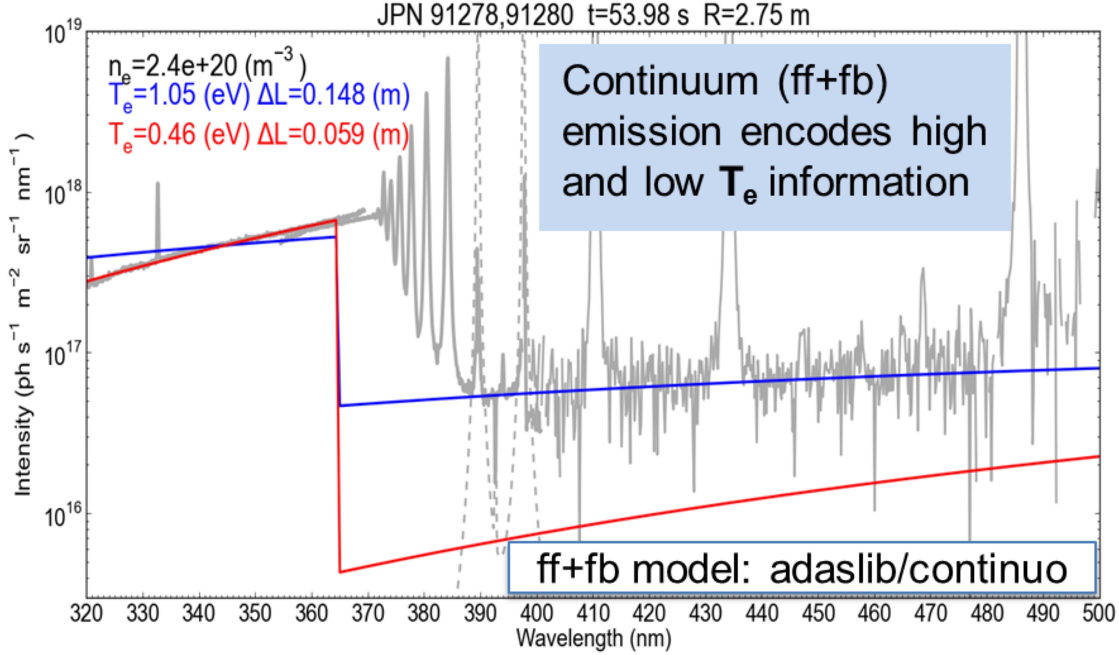
N_2 seeding (high $\langle n_e \rangle_{edge}$): D emission spectroscopy

JET-ILW

$\uparrow\Gamma_{N2}$ leads to outer leg cooling, inward shift in S_{iz} profile



n_e from Dδ Stark broadening – parameterized model [Lomanowski, NF, 2015]

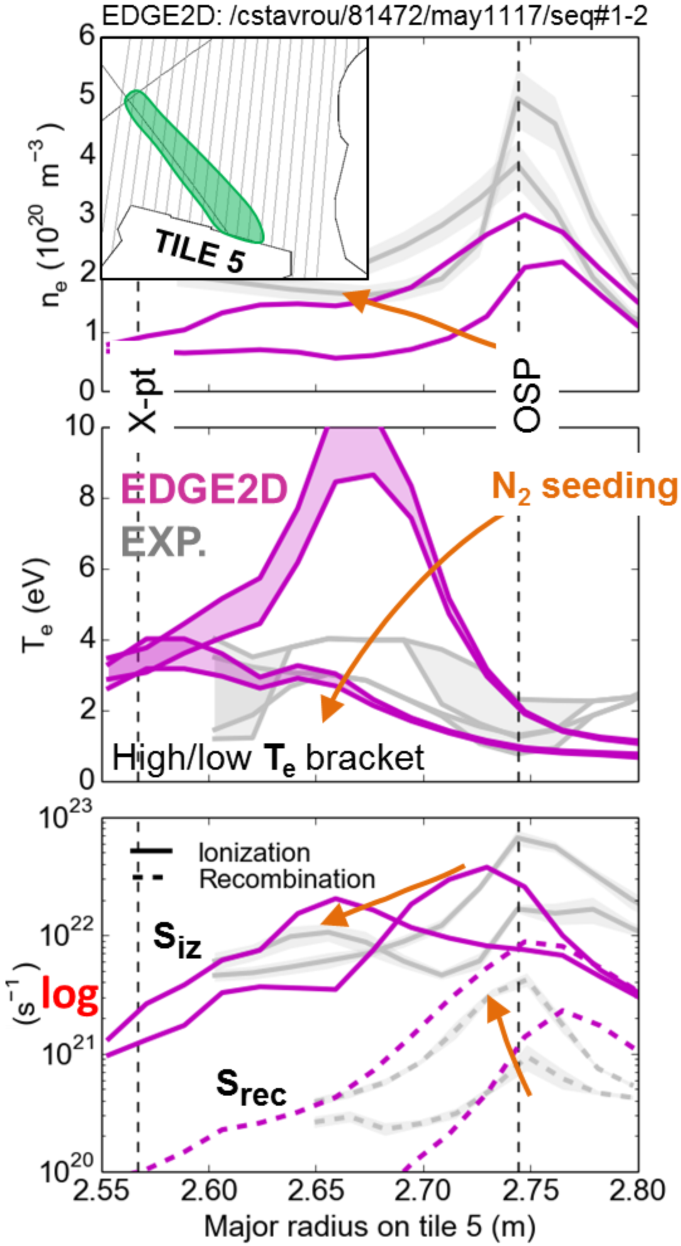


ADAS ADF11 ACD, SCD inverse photon efficiency:

⇒ **S_{iz}** from scanning VUV Ly-α (opacity corrected,

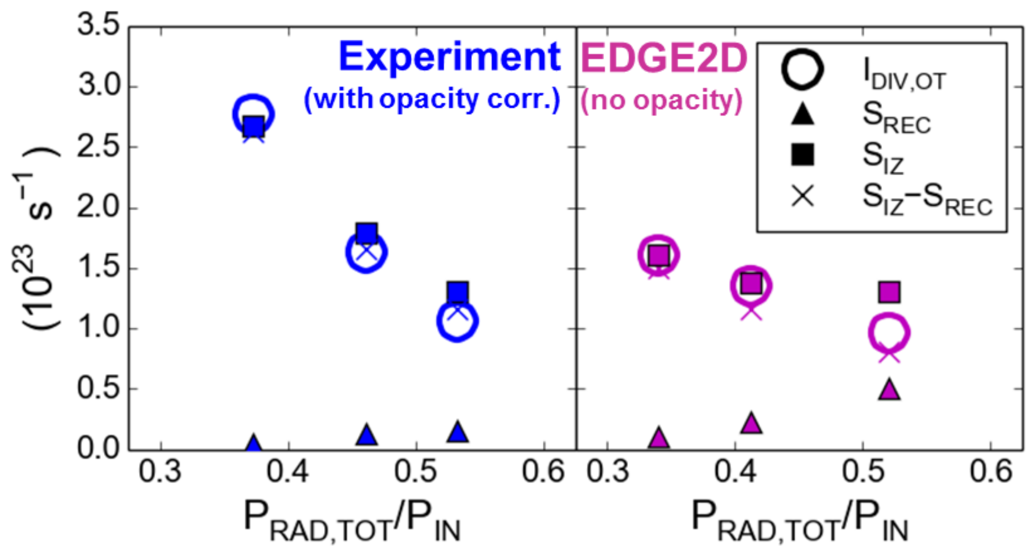
⇒ **S_{rec}** from Dε

Comparison with EDGE2D synthetic spectroscopy ⇒ qualitative agreement in profile evolution, best agreement at highest f_{RAD}



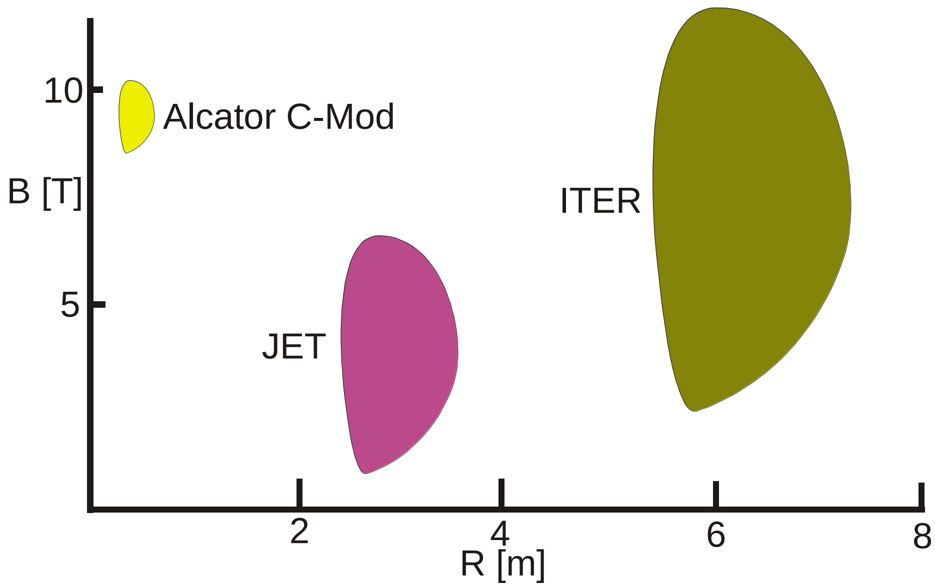
JET-ILW

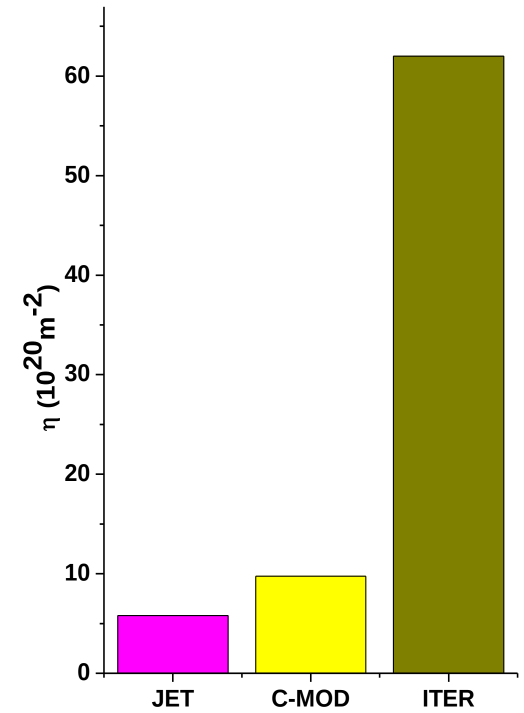
- EDGE2D n_e underestimated (~2x)
- Low N_2 seeding ⇒ EDGE2D hotter T_e
- High N_2 seeding ⇒ good match in T_e profiles
- Shift in ionization front reproduced ⇒ **what about particle balance?**



- **$I_{div,OT} \approx S_{iz}^{Ly-\alpha}$ - S_{rec}**
- **Exp. $S_{iz}^{Ly-\alpha}$ mediated by ↓T_e AND photoexcitation**
- **EDGE2D $S_{iz}^{Ly-\alpha}$ mediated only by ↓T_e**

SIZE-SCALING FOR OPACITY IN TOKAMAKS





$$\eta \approx \overline{n}_e^{div} R \approx \overline{n}_D^{div} R$$

- Similarity parameter for opacity importance: η
- From this: opacity relevant for ITER (DEMO)
- C-mod „closer“ to ITER

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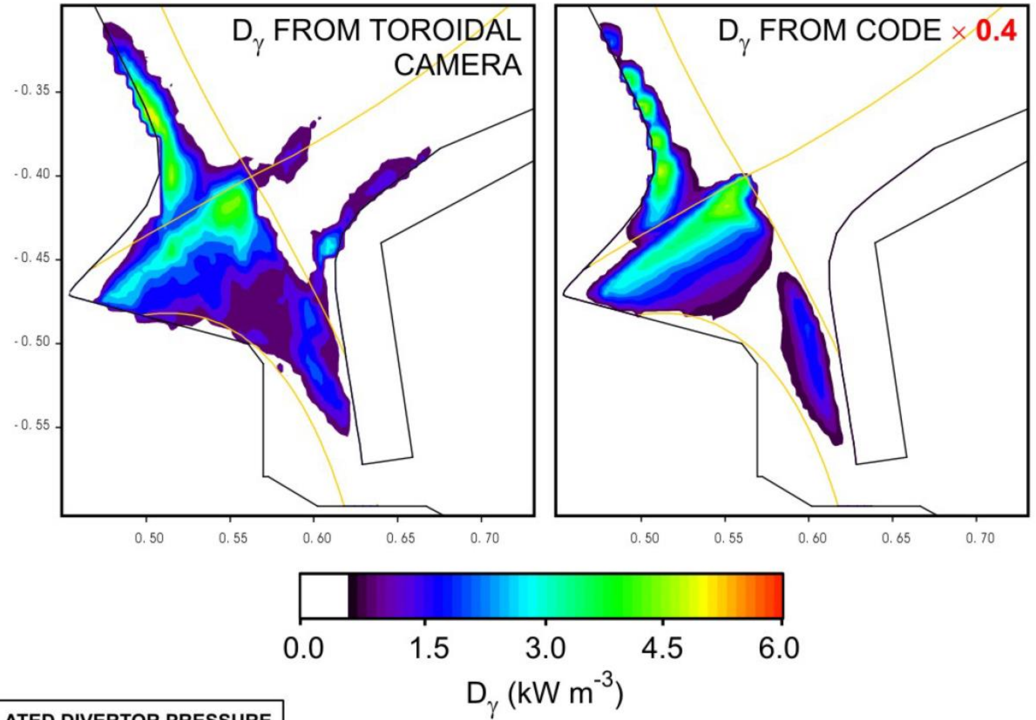
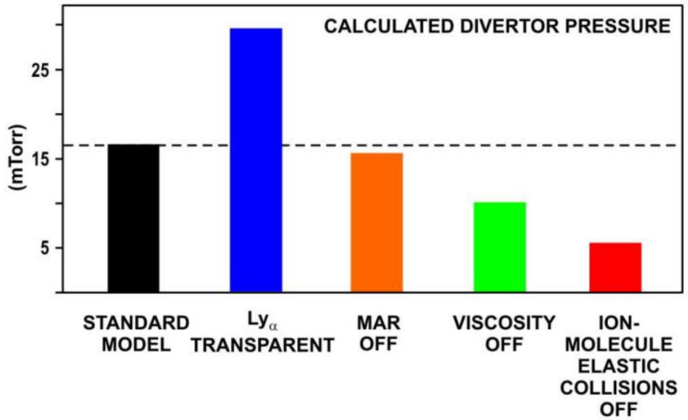
QUANTITATIVE ASSESSMENT OF DOMINANT PROCESSES GOVERNING NEUTRAL DYNAMICS



Alcator C-Mod

OSM-EIRENE interpretative modelling
S. Lisgo, Reiter, Kotov, Wiesen, et al.
PSI 2004



Modelling of “ITER-like” C-mod divertor (high density, vertical targets)

- Neutral pressure & D_γ (and D_α) emission within x2
- Calculated neutral pressure sensitive to volume recombination, Ly_α opacity, viscosity and ion-molecule elastic collisions

KINETIC (TRANSPORT) EQUATION

- linearized Boltzmann-Equation
- for particles travelling in straight lines between collisions
- with no forces acting on them between collisions

Solving for $f(\vec{r},\vec{v},t)$ or $f\left(\vec{r},E,\vec{\Omega},t\right)$:

$$\left[\frac{\partial}{\partial t}+v\vec{\Omega}\cdot\nabla\right]f\left(E,\vec{\Omega}\right)=S\left(E,\vec{\Omega}\right)-\mathrm{v}\sigma_a(E)f\left(E,\vec{\Omega}\right)$$

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

Monte-Carlo method:

- EIRENE: Solution of the kinetic transport equation by following test-particle histories
- Averaging over many particle-histories and collision types
  → approximate stochastical solution $f\left(\vec{r},E,\vec{\Omega},t\right)$

DICTIONARY OF QUANTITIES

Mathematically, the form of the linearised transport equation for photons and for kinetic particles is identical

Particles (fermions)		Photons (bosons)
Velocity v	⟷	const. lightspeed c
Energy $E_{kin} = \frac{m}{2} v^2$	⟷	$E_{ph} = h\nu$

Solution of transport equation results in:

$$\Phi_{kin} = v \frac{mv^2}{2} f_{kin}(\vec{r}, \vec{v}) \quad \longleftrightarrow \quad I = Ec \cdot f_{ph}\left(\vec{r}, E_{ph}, \vec{\Omega}\right)$$

kinetic particle (energy) flux ⟷ specific radiation intensity

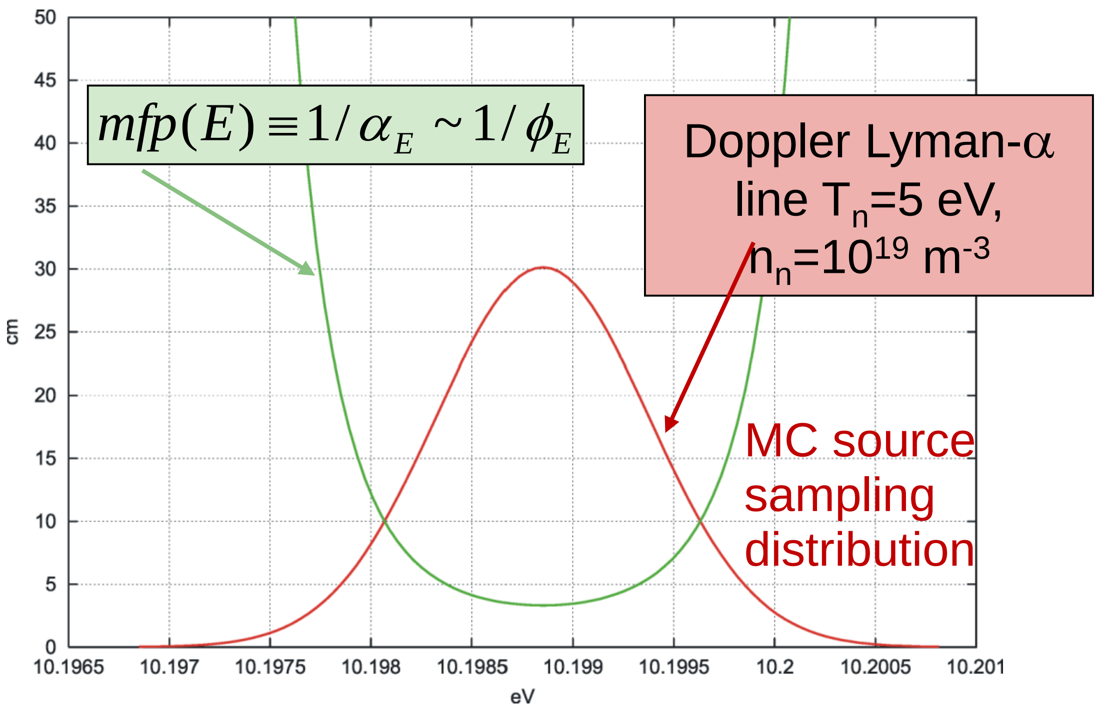
RADIATION TRANSPORT EQUATION
= BOLTZMANN-EQUATION FOR PHOTONS

$$\left[\frac{1}{c}\frac{\partial}{\partial t}+\vec{\Omega}\cdot\nabla\right]I(\vec{r},\vec{\Omega},E,t)=\mathrm{j}(\vec{r},\vec{\Omega},E,t)-\alpha(\vec{r},\vec{\Omega},E,t)I(\vec{r},\vec{\Omega},E,t)+\frac{\delta I(\vec{r},\vec{\Omega},E,t)}{\delta r}$$

Photons: sources & sinks

$$j_E^{spont}=n_2A_{21}\frac{E_{12}}{4\pi}\psi_E$$

$$\alpha_E^{abs}=n_1B_{12}\frac{E_{12}}{4\pi}\phi_E\left(1-\frac{n_2g_1\psi_E}{n_1g_2\phi_E}\right)$$



Optical thickness

$$\tau_E(z)=\int_{z_1}^{z_2}dz\,\alpha(z,E)\quad\begin{cases}<1 & \text{opt. thin}\\ >1 & \text{opt. thick}\end{cases}$$

$$\sim\eta=n^{div}\cdot L^{div}$$

ITERATIVE PROCEDURE #1

0. Setup initial conditions: e.g. $n_{n=1}(r)^0$=const, $n_{n=2}(r)^0$=const, $I_E(r)^0 = 0$

1. Follow photons with source $A_{21} n_{n=2}(r)^{i-1}$ on background $n_{n=1}(r)^{i-1} \rightarrow I_E(r)^i$

2. Follow neutrals on background $I_E(r)^{i-1} \rightarrow n_{n=1}(r)^i$ & $n_{n=2}(r)^i$

3. Calculate rate defect d, if d close to zero: stop, otherwise:

4. i=i+1; to save memory: copy all fields into background, i.e from i to i-1

5. Go to step 1

$$d = \left| \int d\nu^t \oint d\Omega_\nu^t \; R_{atom}^{abs} - \int dE^t \oint d\Omega^t \; R_{photon}^{abs} \right| \rightarrow 0$$

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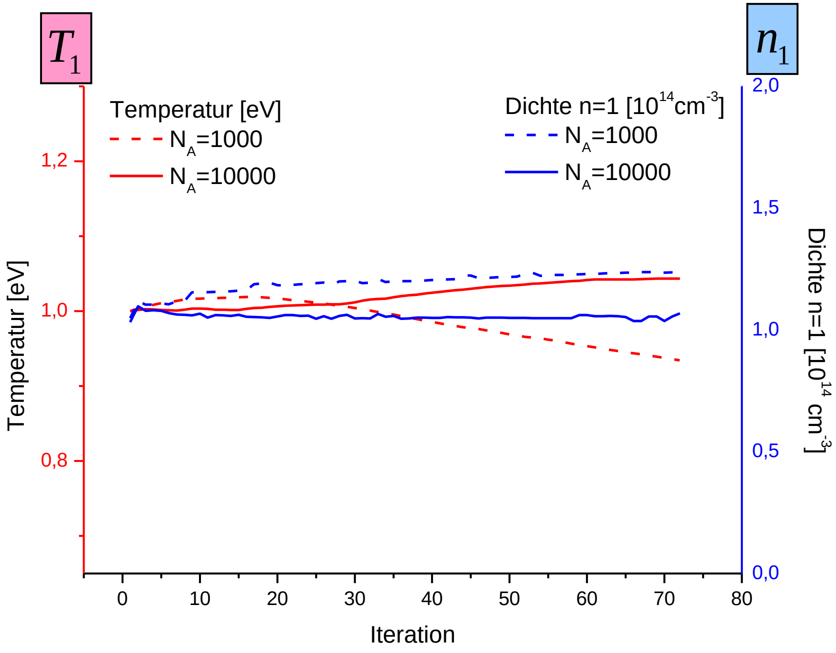
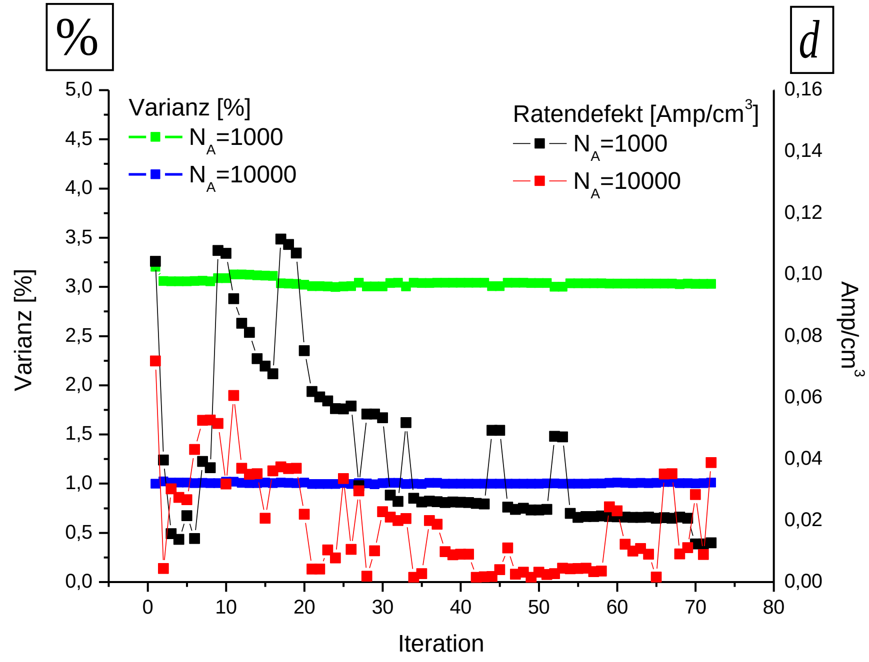
FIRST TEST: SLAB PLANCK-MODEL

- Lyman-α
- Periodic boundary Conditions
- T_1=1eV, n_1=10^{20}m^{-3}



variation of $N_{MC,A}$



variance & rate defect

Wiesen 2005

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FIRST TEST: SLAB PLANCK-MODEL

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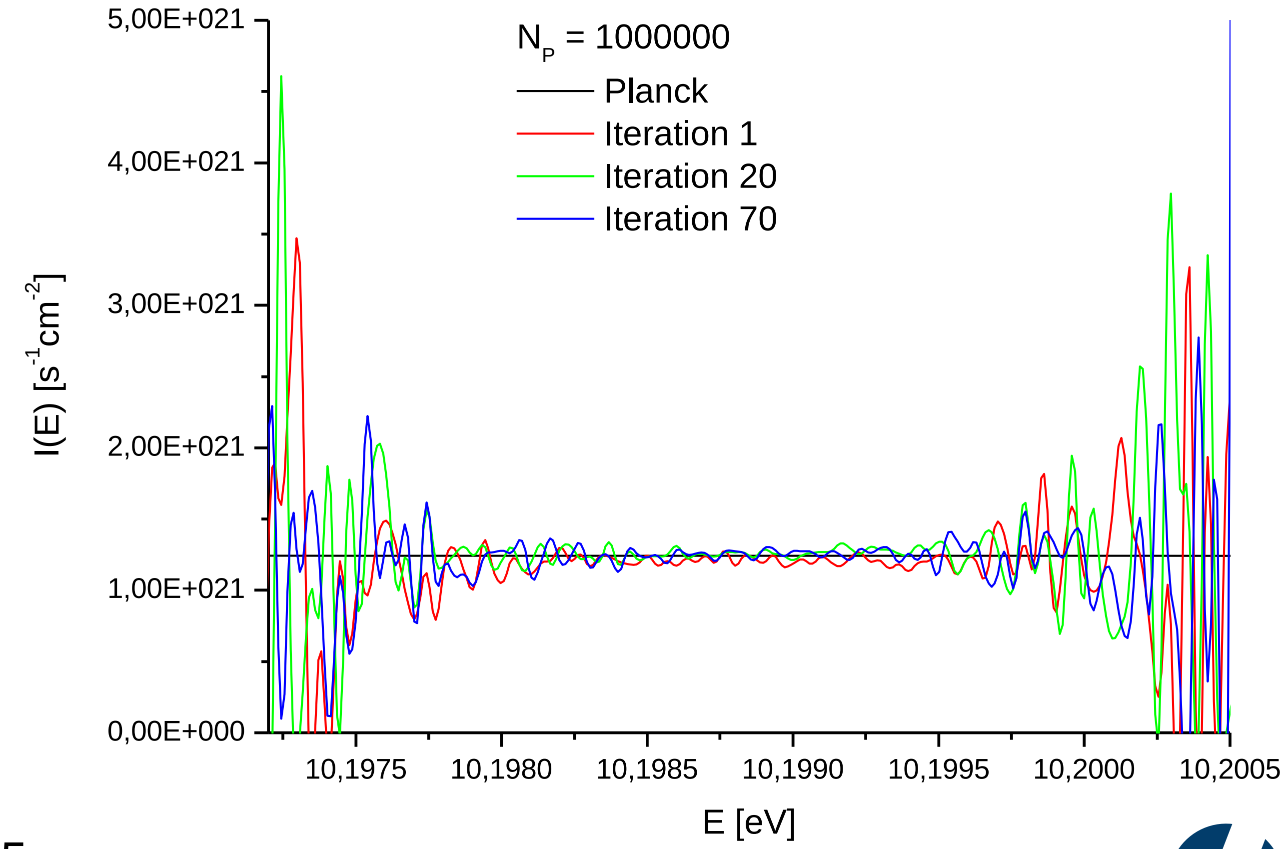
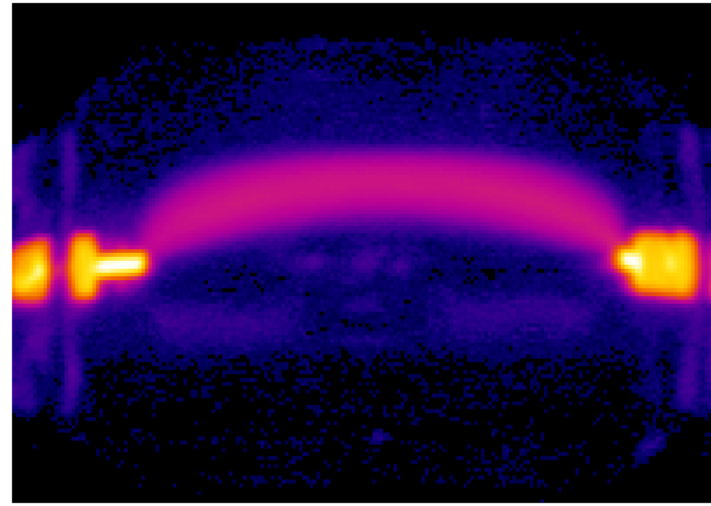
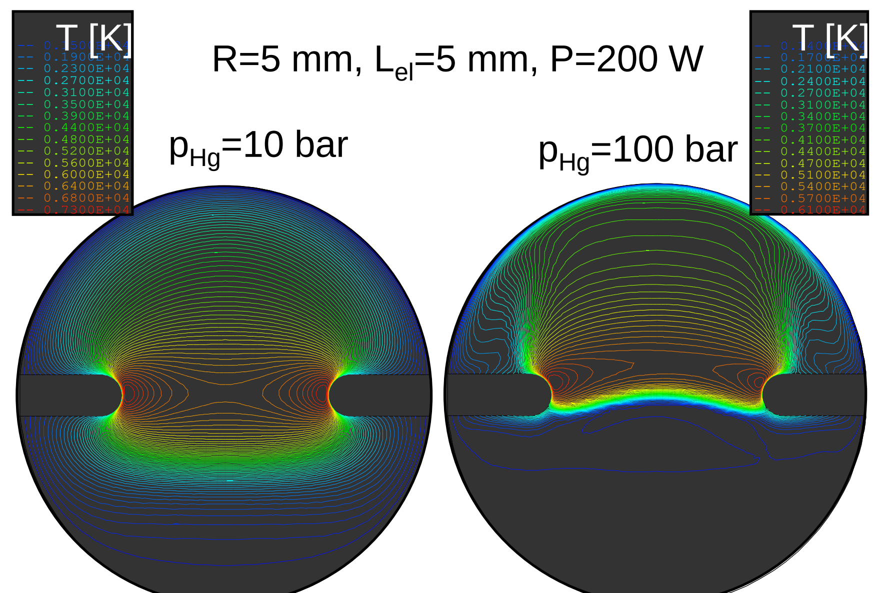


Wiesen 2005

V&V CONT‘D: HIGH-PRESSURE MERCURY-GAS DISCHARGES

Examples of High Intensity Discharge Lamps (HID)

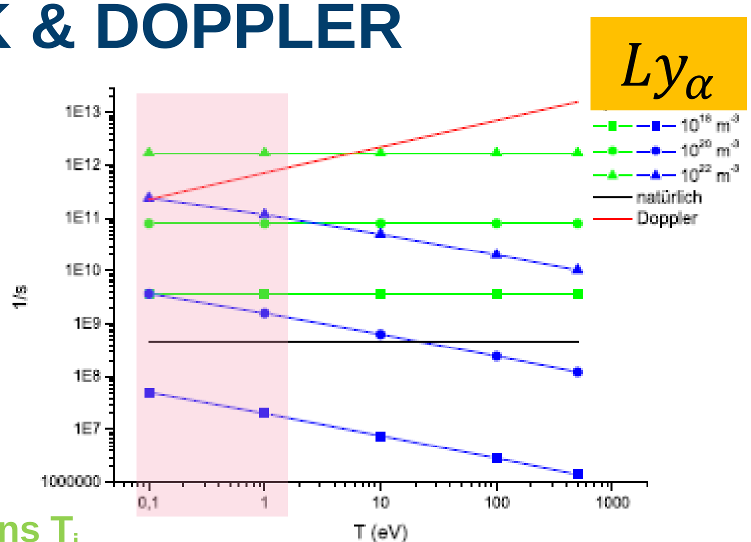


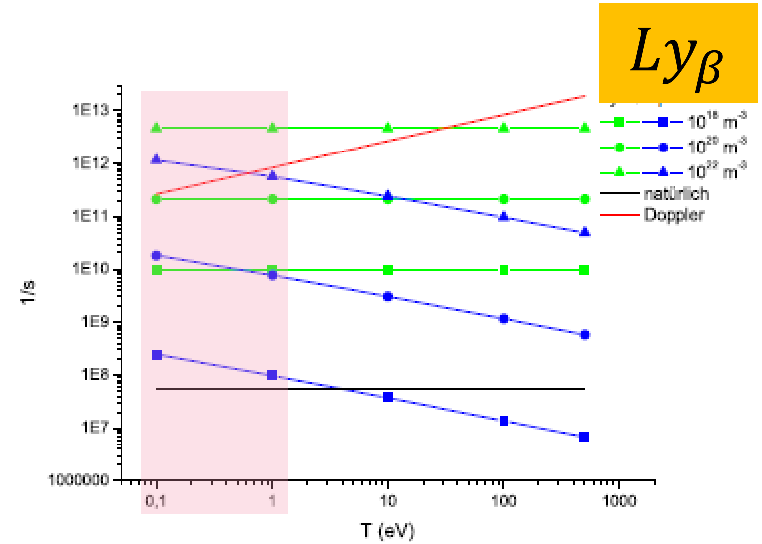


LINE BROADENING MECHANISMS & PROFILES

- Lorentz: natural (A_{ik}), Stark (n_e), Resonanz, Van-der-Waals, turbulence...
- Gaussian: Doppler (T)
- Voigt: convolution of Lorentz & Doppler
- Holtsmark (quasi-static)
- isotope-Mixing
- Zeeman splitting and broadening

COMPARISON FOR LYMAN LINES: NATURAL, LINEAR STARK & DOPPLER



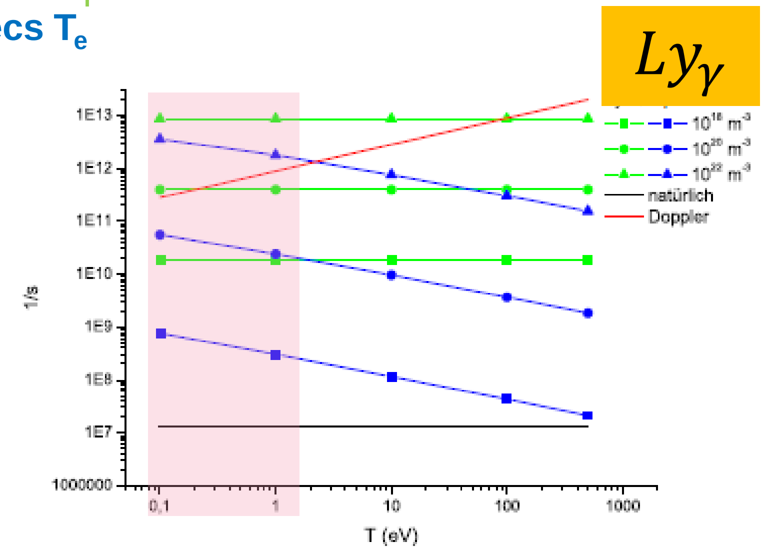


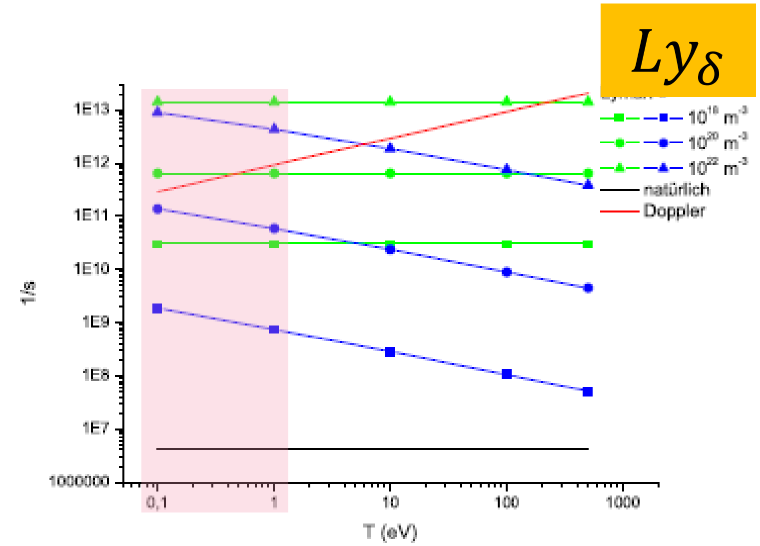
Quasi-static ions T_i

Collisional elecs T_e

Doppler T_n

natural





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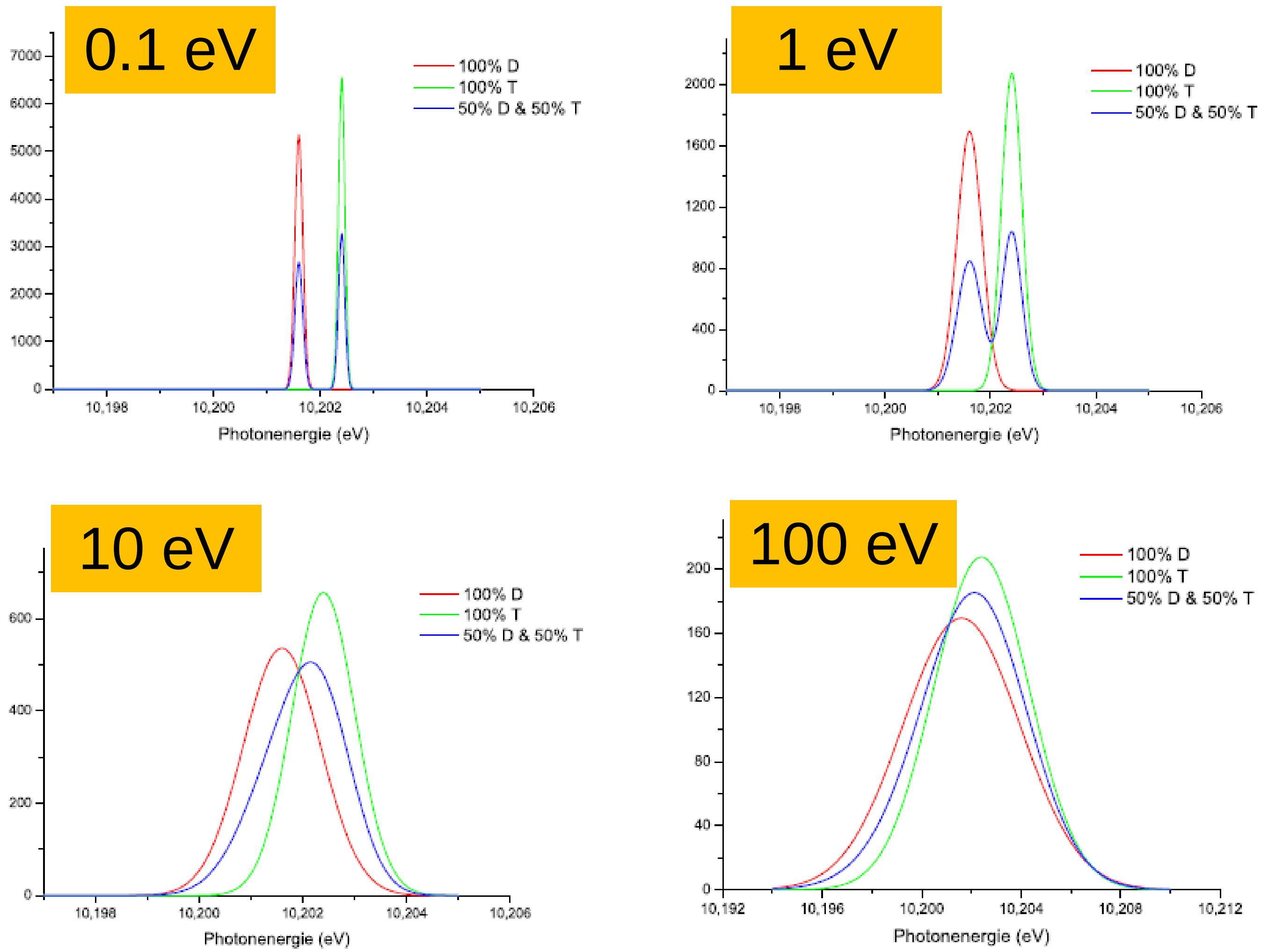
ISOTOPE EFFECT & EFFECTIVE BROADENING

Ly_α



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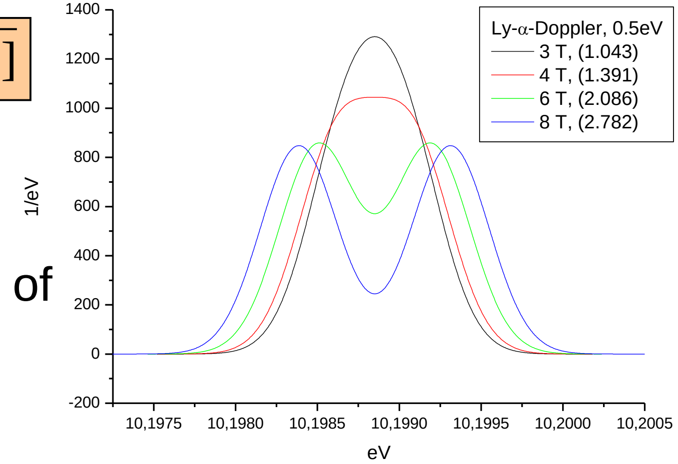
(NORMAL) ZEEMAN EFFECT

$$\phi_{DZ}(\Delta E,\theta)=\frac{1}{2}\phi_D(\Delta E,T)\sin^2\theta+\frac{1}{4}\left[\phi_D(\Delta E-\mu_B B,T)+\phi_D(\Delta E+\mu_B B,T)\right]\left(1+\cos^2\theta\right)$$

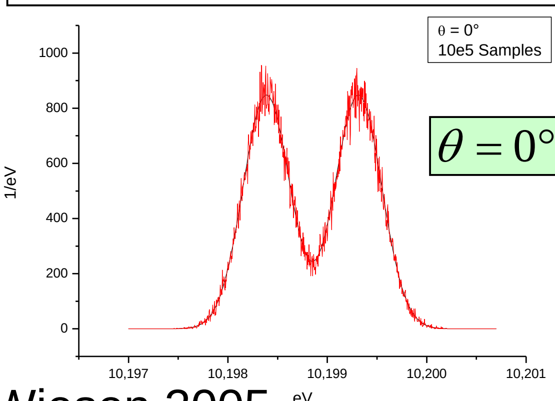
Relevanz: Zeeman vs Doppler

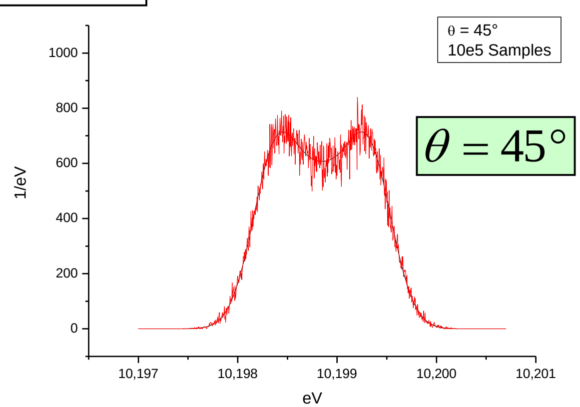
$$B[T] > E_0[eV]\sqrt{T[eV]}$$

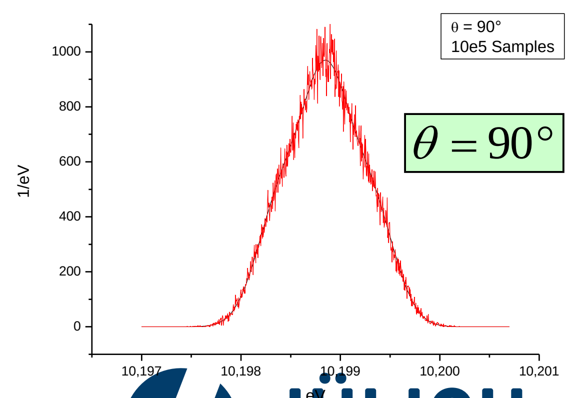


- normal Zeeman effect leads to additional broadening of line shape → reduction of effective optical thickness τ
- anisotropisation of radiation field

Sampling: e.g. T=0.5 eV, B=8T:







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(NORMAL) ZEEMAN EFFECT

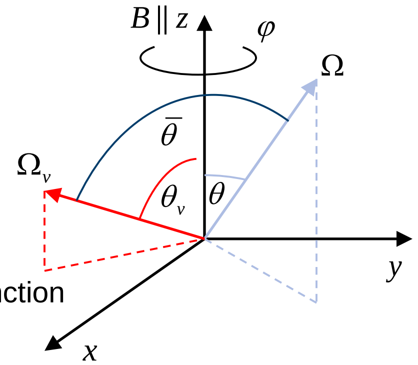
Epansion of radiation field into cubic splines $I^S(E)$ and orthonormal $Y_{lm}(\Omega)$

$$R_{atom}^{abs} = B_{12}\bar{J} = B_{12}\int dE \sum_{lm} I_{lm}^{S}(E) \oint d\Omega Y_{lm}(\Omega)\phi_{DZ}(E,\nu,\Omega\cdot\Omega_\nu)$$

Zeeman component q

$$\phi_{DZ}(E,\nu,\Omega\cdot\Omega_\nu) = \sum_{q=\pm1,0}\sum_{k=0,2} a_{qk} Y_{k0}(\Omega)\phi^{q}(E,\nu,\Omega\cdot\Omega_\nu)$$

$$R_{atom}^{abs} = B_{12}\int dE \sum_{lm} I_{lm}^{S}(E) \sum_{q=\pm1,0}\sum_{k=0,2} a_{qk} \oint d\Omega Y_{lm}(\Omega) Y_{k0}(\Omega)\phi^{q}(E,\nu,\cos\bar{\theta})$$



Rotation: $\Omega_\nu \parallel B \longrightarrow Y_{lm}(\Omega) = \sum_{m'} Y_{lm'}(\Omega_\nu) D_{m'm}^{l}(\varphi_\nu,\theta_\nu,0)$

Wigner rotation function

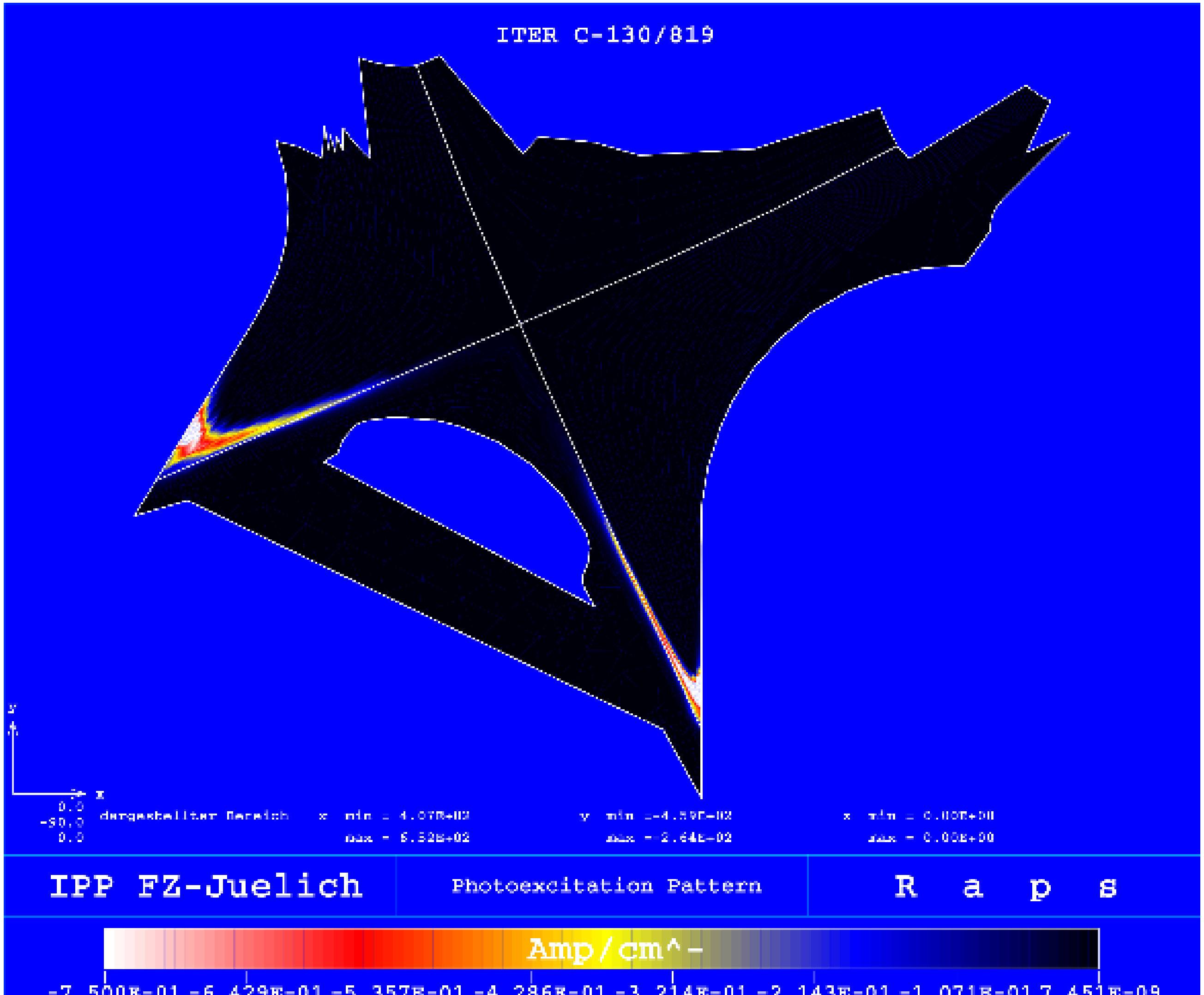
$$R_{atom}^{abs} = B_{12}\int dE \sum_{lm} I_{lm}^{S}(E) \sum_{qk} a_{qk} \sum_{m'm''} D_{m'm}^{l}(\varphi_\nu,\theta_\nu,0) D_{m''0}^{k}(\varphi_\nu,\theta_\nu,0)\cdot \bar{\phi}_{l,qk}^{m'm''}(E,\nu)$$

$$\bar{\phi}_{l,qk}^{m'm''}(E,\nu) = \oint d\Omega_\nu Y_{lm'}(\Omega_\nu) Y_{km''}(\Omega_\nu)\phi^{q}(E,\nu,\cos\theta_\nu)$$

Assuming azimuthal symmetry, i.e. only terms w/ $m' = m'' = 0$

Analog: $R_{photon}^{abs} = B_{12}\bar{F}$ Here: assume isotropic Maxwell atoms

PHOTOEXCITATION IN ITER TOKAMAK



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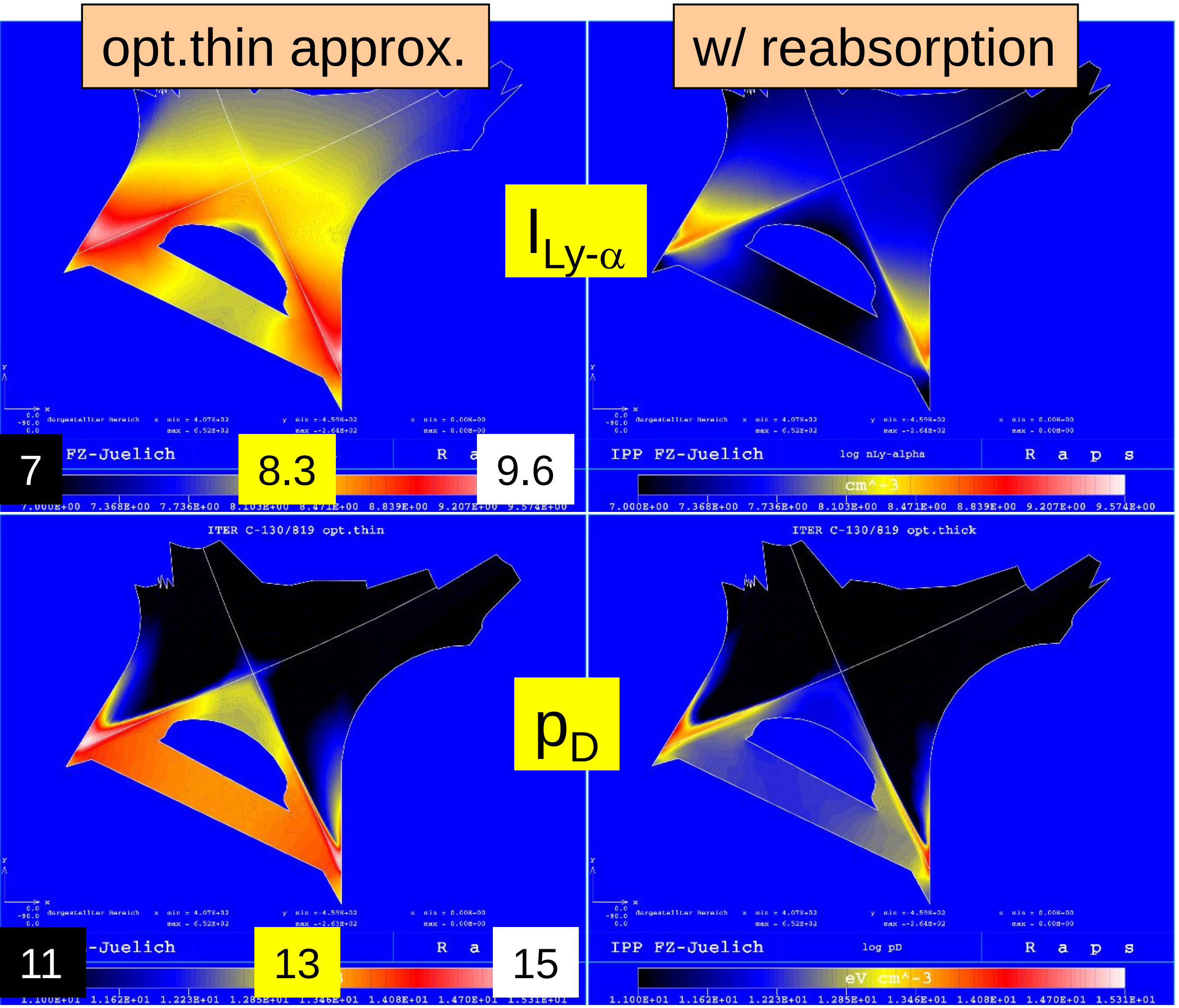
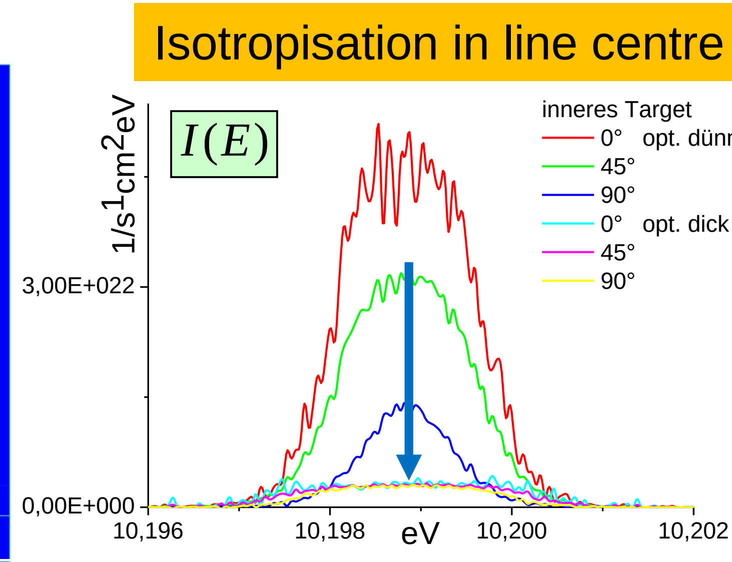
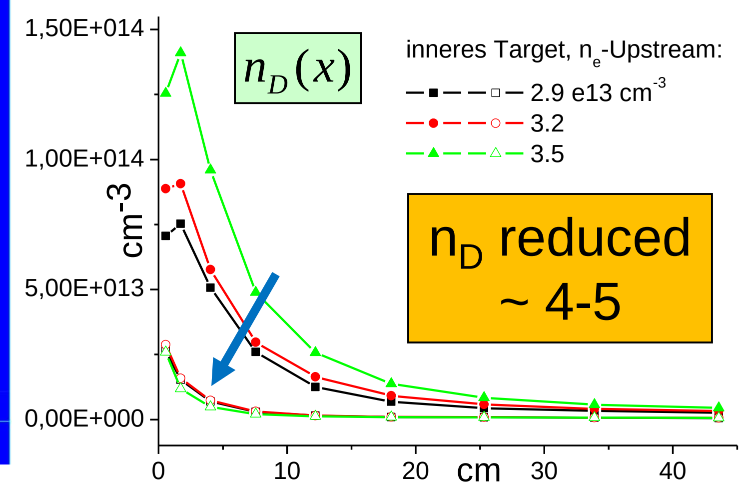
ITER: LYMAN-ALPHA REABSORPTION IN DIVERTOR







Fixed plasma, only iterate D_0(n=1,2) & Ly_α photons

Wiesen 2005

ITERATIVE PROCEDURE #2

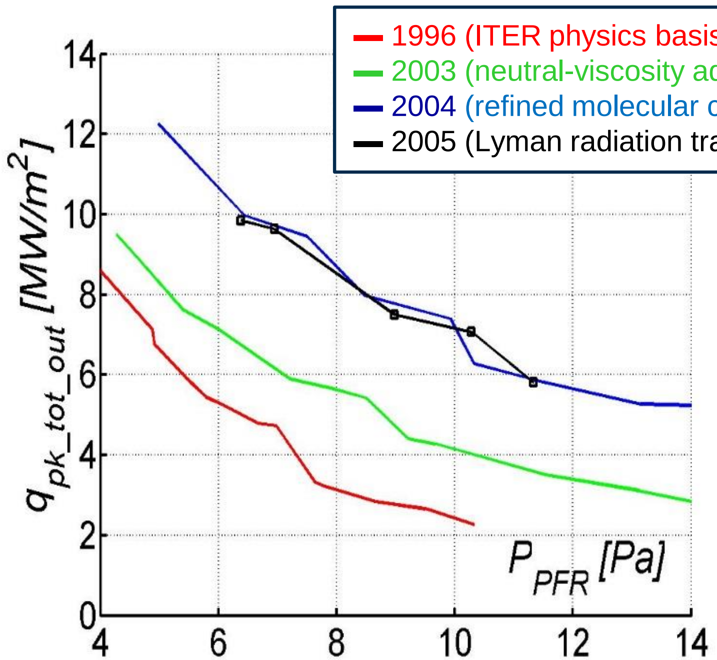
- Include iteration of neutrals with plasma:
  coupling of EIRENE (neutrals & photons) with SOLPS-ITER or EDGE2D or equivalent → fully coupling numerically expensive

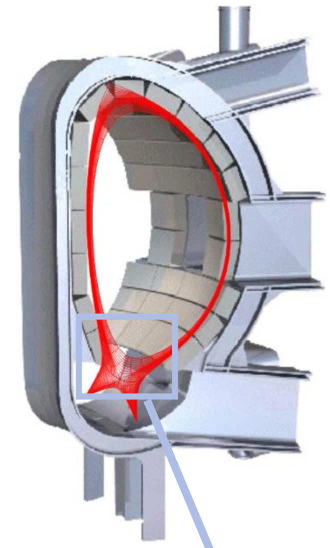
- We do not iterate photons/neutrals on themselves
  (as we can take into account the non-linear interaction of photons with neutrals when iterating with plasma)

- **Calculate upper state of a neutral by using a collisional radiative model taking into the reabsorption rates of photons into account from iteration step before**

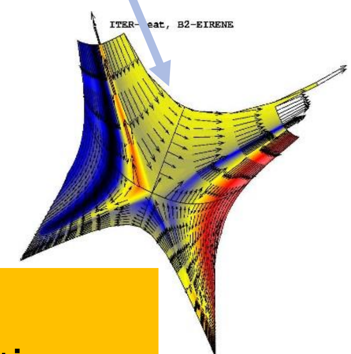
→ That assumes that the upper stages have very short (meta-stable) lifetimes (~A_{ik}), i.e no transport for the upper state included
(usually for fusion applications this seems to be a good approximation)
also: neglect Zeeman-effect and only Doppler broadening

ITER DIVERTOR ENGINEERING PARAMETER: *PEAK TARGET HEAT FLUX VS. DIVERTOR GAS PRESSURE*





SOLPS4.3 modelling
V.Kotov, D.Reiter, S. Wiesen, A. Kukushkin et al



Lyman opacity not an issue for ITER divertor operational space (shift in required throughput), but change in ionisation-recombination balance and density further upstream (factor 2)

ITER CASE

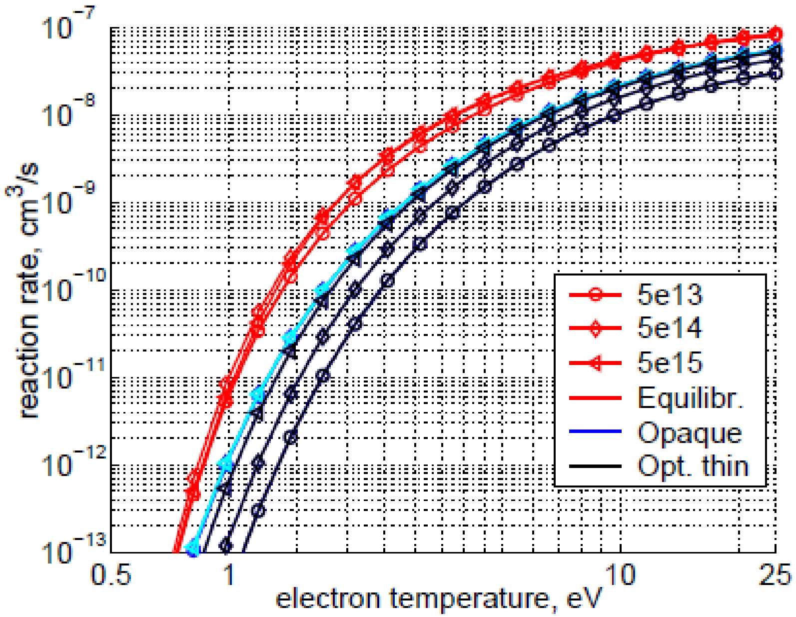


Figure 4.3: The "equilibrium" effective ionization rate, Formula (4.27), the "opaque" ionization rate and the optically thin ionization rate

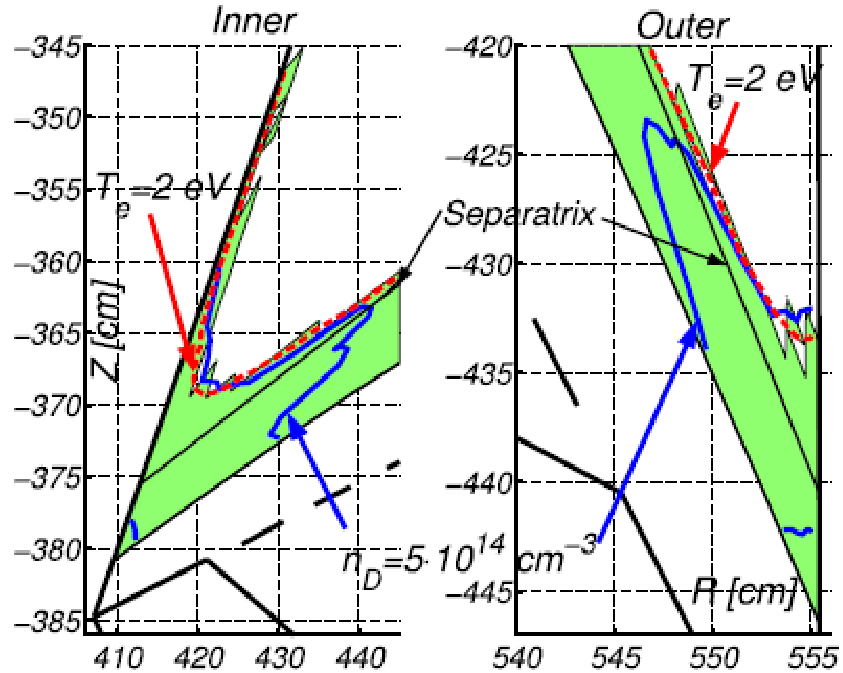


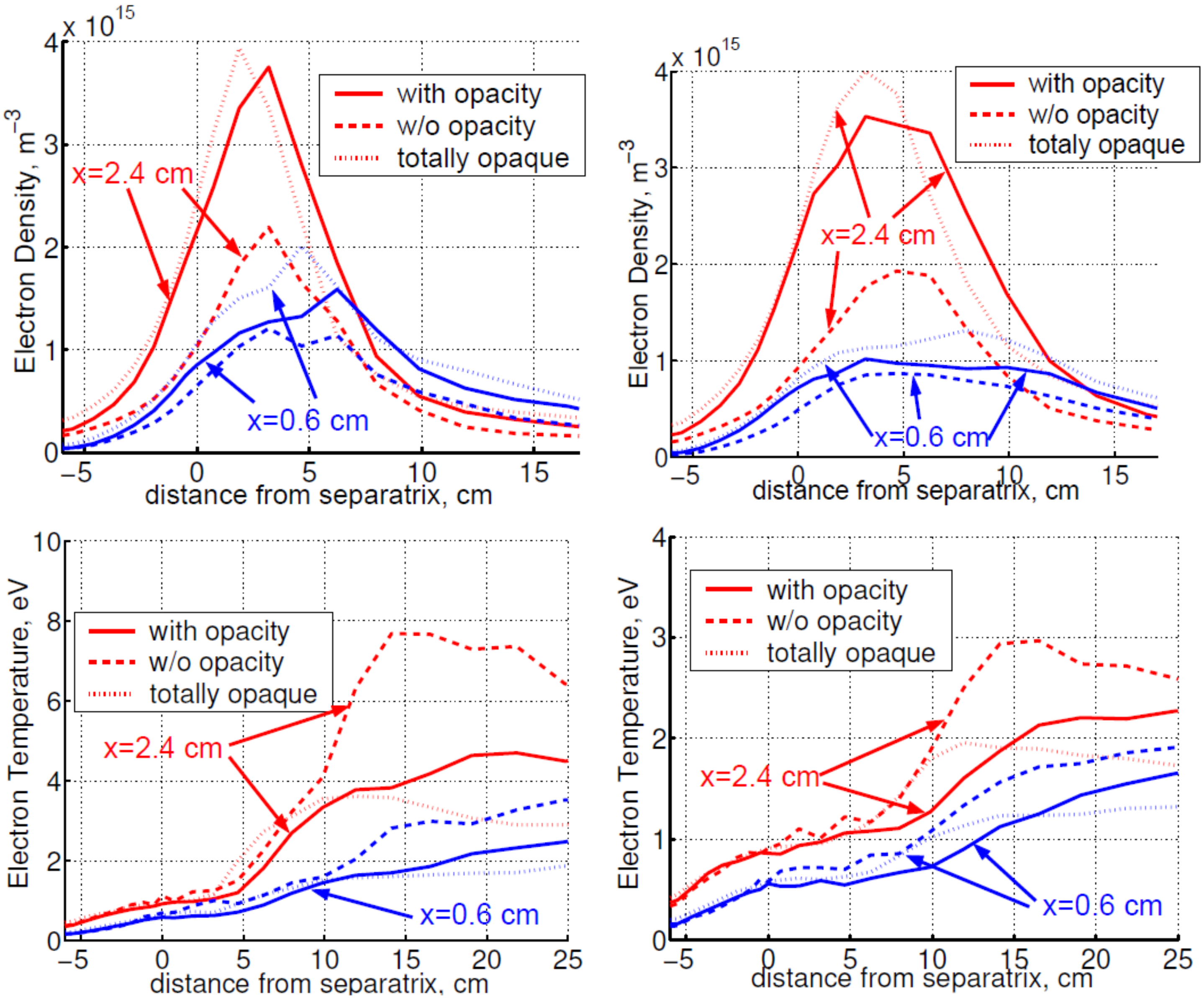
Figure 4.6: The regions in the inner and outer divertors for which the photo-induced ionization is greater than the ordinary ionization. Dashed line is the isotherm with $T_e = 2\ eV$, solid line is the contour of constant atom density $n_D = 5 \cdot 10^{14}\ cm^{-3}$

Opaque ionisation rates exceed ordinary ones

Kotov, Reiter, Wiesen et al, 2006

ITER CASE

Kotov, Reiter,
Wiesen et al 2006



(a) Low Pressure (b) High Pressure

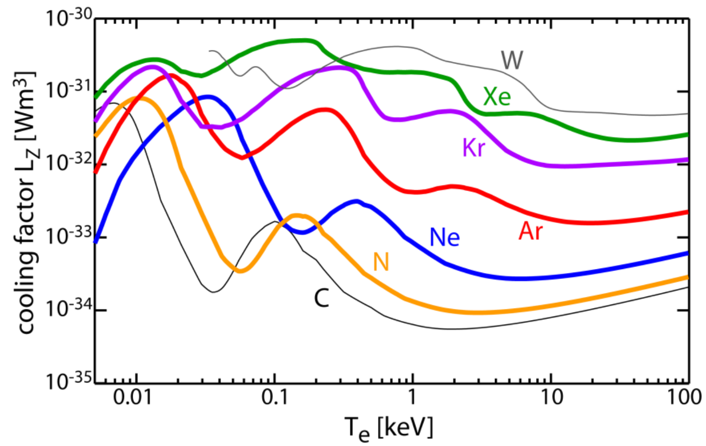
x = poloidal distance from target

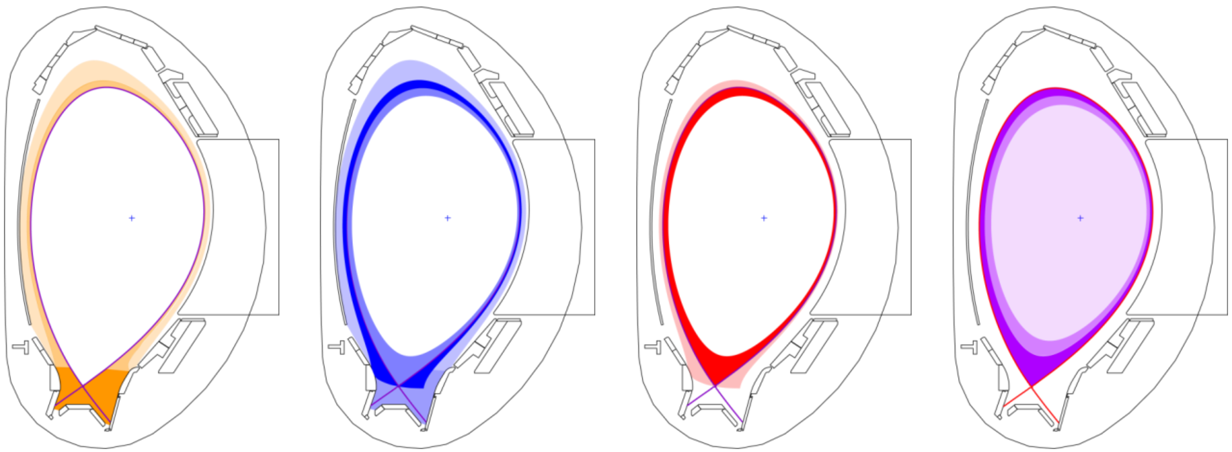
TAILORING OF THE OPTIMAL IMPURITY MIX FOR RELIABLE EXHAUST SCHEME FOR DEMO

$$q_{rad}^{imp} = n_e n_z L_z(n_e, T_e, \tau) l$$

Various seeding impurities possible

- Nitrogen: Divertor
- Neon: SOL
- Argon: SOL & pedestal
- Krypton: Pedestal & core
- Xenon: Future machines, pedestal



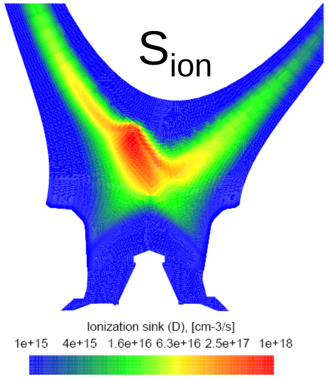


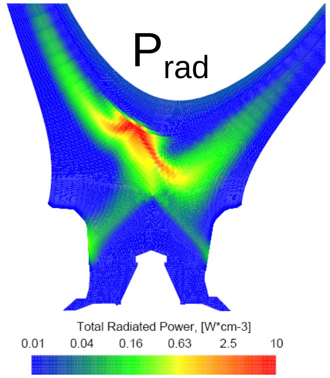
M.Bernert
PSI2016

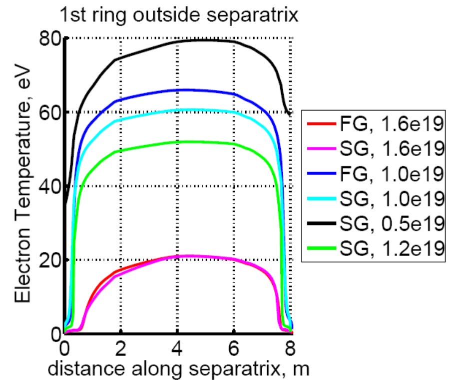
DEMO: 30% core radiation w/ X-point radiator

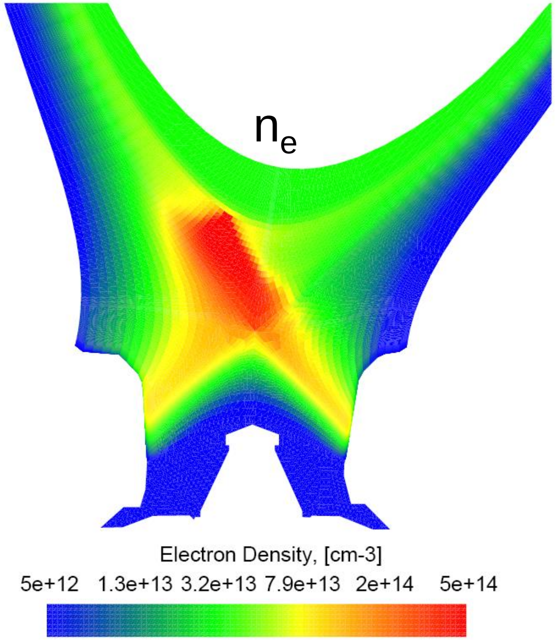
JET-C: LYMAN-OPACITY IMPORTANT FOR STABLE X-POINT RADIATOR IN SOLPS4.3

Reduction of upstream temperature (and increased density)





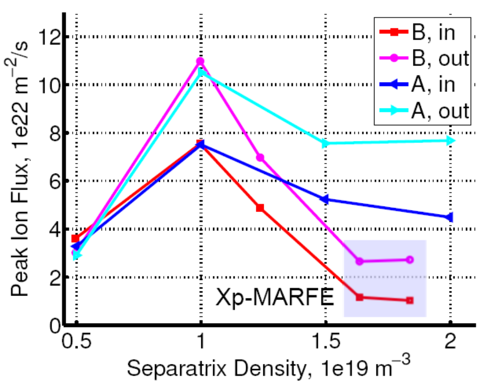


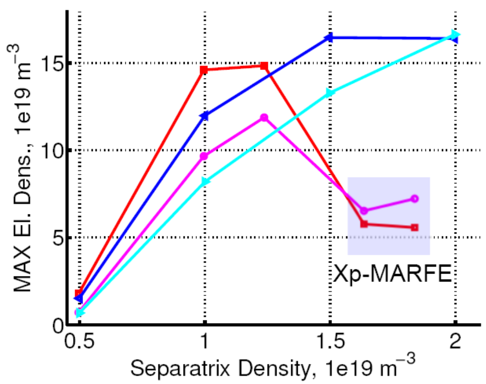


n_e^{mid}=1.6e19 m^{-3} f_{rad}=81 % (D: 28 %, C: 72 %) same drop for T_i

Ionization source ⇒ enhanced convective energy flux ⇒ reduced parallel gradient

n_e^{mid}=1.62e19 m^{-3}





Deeper detachment after formation of X-point radiatior

V. Kotov, D. Reiter, S. Wiesen
JNM2013

Model B=Model A + NNC + MAR + *transport of Ly photons and photo-excitation*

CONCLUSIONS

- The radiation transport MC module still exists in EIRENE
- Applications: dense tokamak divertors, also: industrial
- The module has been barely used after 2005
  → now being reactivated and applied in fusion
- EIRENE photon modul is currently being revised and updated at FZJ to make it generally available (again) to community: as stand alone or as part of e.g. SOLPS)
- New interesting applications in fusion emerging, e.g.:
  - interpretation of spectroscopy → validation of edge codes
  - diagnostics (e.g. metal wall reflections)
  - ITER (with metal wall) and DEMO (at large f_{rad})

MODEL NEEDS

- Revised CR models with (semi-) opaque lines, validation of opacity models (e.g. isoptope effects or collisional broadening in high density - DEMO)
- Wall reflection models for photons, e.g. on W/Be or deposited layers, how to parametrise a model for inclusion into EIRENE, e.g. roughness?
- Comparison with other codes for re-verification in 3D geometries, e.g. CHERAB vs EIRENE
- Code development: Improved Hybrid models for speed up of fully coupled models → EUROfusion TSVV-5

HYBRID METHODS

Hybrid Formulation of Radiation Transport in Optically Thick Divertor Plasmas*

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Received 9 September 2015, revised 20 October 2015, accepted 22 October 2015
Published online 08 July 2016

JÜLICH Forschungszentrum

HYBRID METHODS

Hybrid Formulation of Radiation Transport in Optically Thick Divertor Plasmas*

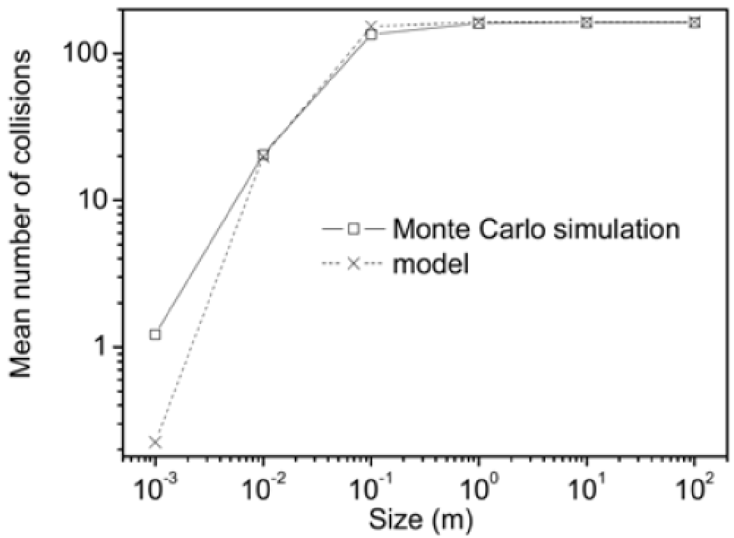

Fig. 3 Plot of the mean number of collisions calculated using the collision estimator (Monte Carlo simulation) and the model Eq. (10). The model is in a good agreement with the simulation in highly scattering media, i.e. if the mean number of collisions is large.

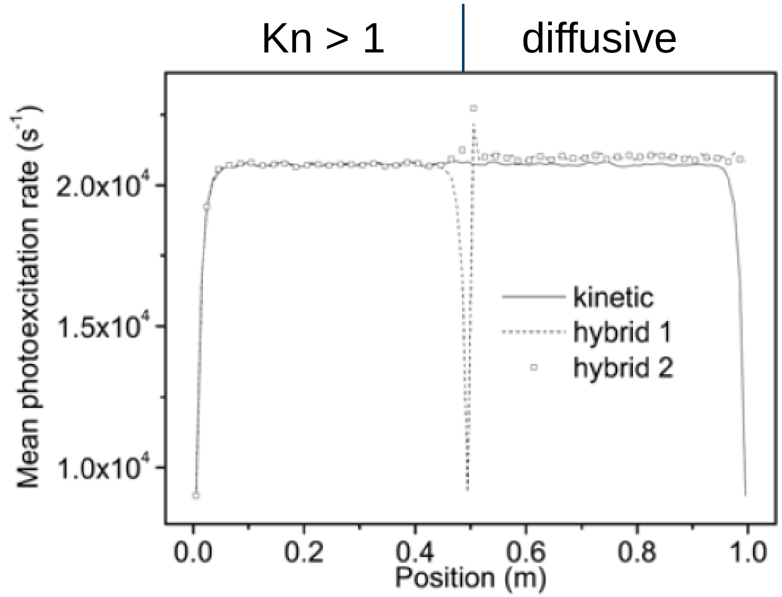

Fig. 4 A hybrid Monte Carlo simulation that combines the kinetic equation and a fluid equation can be devised, provided a suitable interfacing between the regions is done. In the second hybrid simulation, the amount of photons escaping from the diffusive region (right) to the kinetic region (left) has been estimated using an ad hoc model.