Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft

III: Status of atomic and molecular data and data formats for fusion edge plasmas

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Atomic and Molecular Data for Fusion Energy research, Aug.-Sept. 2006, ICTP, Trieste

A decade ago we lacked a credible solution to the divertor problem.

With the discovery of the cold, detached, chemically rich divertor in the 1990s, we have now the (makings of) a divertor solution for high power magnetic confinement devices

Fusion research is an applied science: 3 questions what, why, how

What are the basic effects ?

Why (understanding the "What")

How can we make the application work

Long list of deficient understanding

- •Sources of impurities
- •Impurity transport
- •Elms
- •Private flux zone
- •Neutral behaviour outside the plasma
- •Edge flows
- •Carbon re-deposition, tritium co-deposition
- •Fueling
- •Long pulse operation

ITER is needed as soon as possible:
presently identified effects will be different (enough) and new effects will (probably) be found.

What are the basic effects ?

Some of the questions answered

Why (understanding the "What")

Just getting started

How can we make the application work

ITER urgendly needed to find out

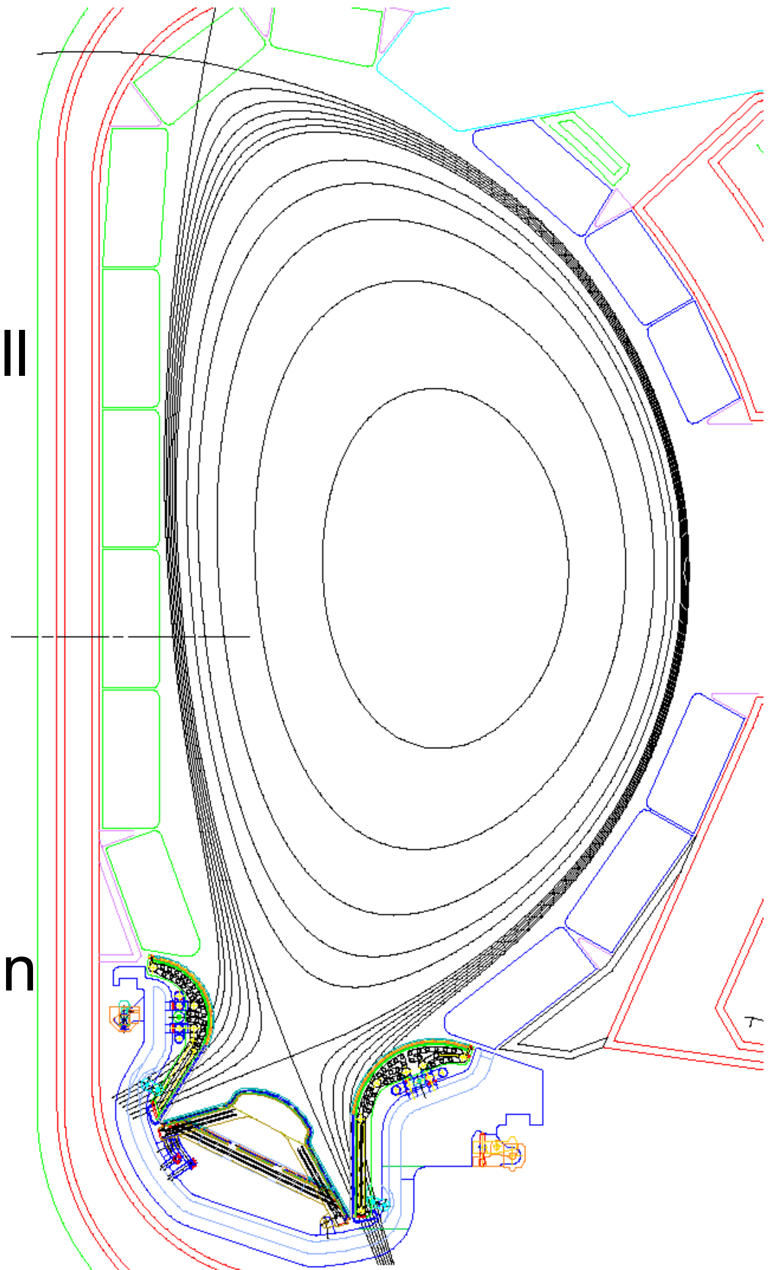
A specific research focus:

Tritium – Retention

•Hydrocarbon Sources,
•Transport,
•Flows,
•C:H films

And : flexible design of ITER edge and divertor

ITER



erosion

Graphite - a conservative choice
forgiving material, no melting,
3825 ºC sublimation temp

D peak flux 10^{24} m^{-2} s^{-1}
erosion yield about 1%
$\Rightarrow$ 10^{22} C-atoms m^{-2} s^{-1}
for steady state
$\Rightarrow$ 6 000 kg / year or 2.6 m/year

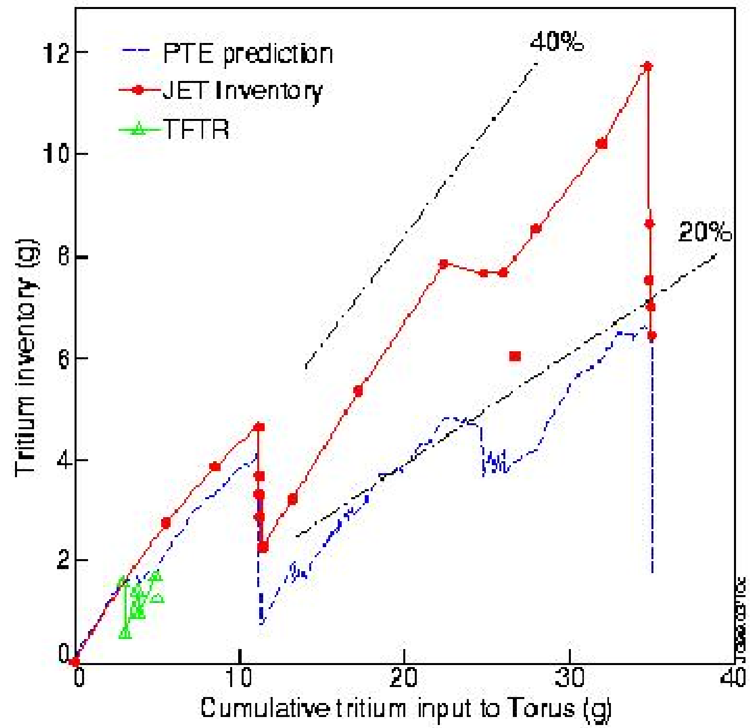
deposition

the tokamak - a closed system
essentially all eroded particles
are re-deposited

The tritium retention issue:

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

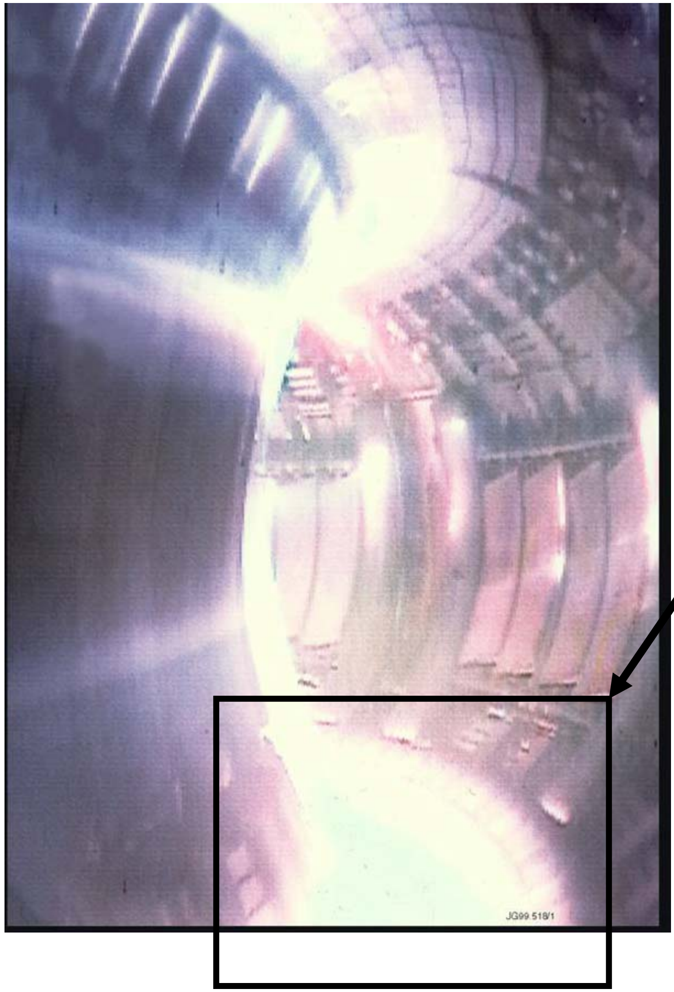
JET: Retained Tritium



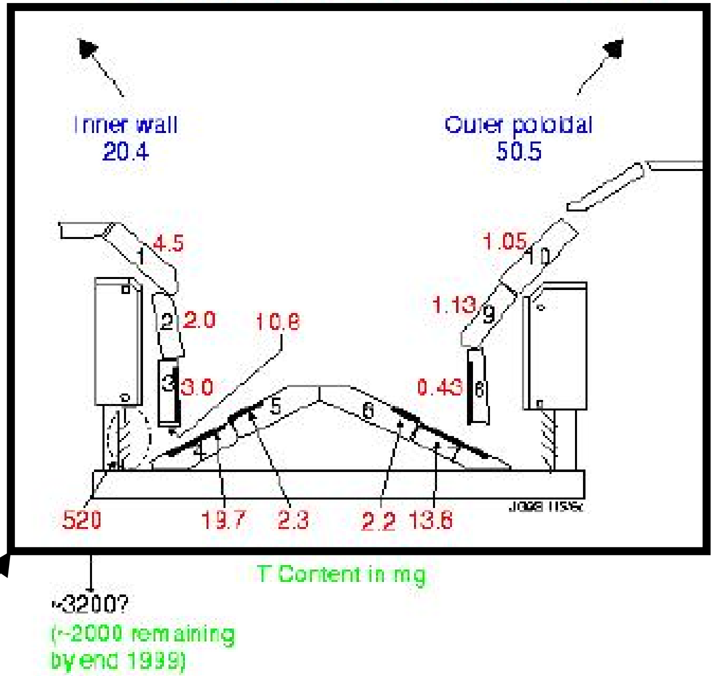
The rate of T retention in JET during DTE1 was 40% of input, reducible to 17% after cleanup in D, without sign of saturation.
P. Andrew, et al, FED 47 (1999) 233.

Extrapolation to Iter: the permitted in-vessel T-inventory, 0.5 kg, could be reached in 100 shots.

Carbon re-deposition,
Tritium –co-deposition



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.

On Jet, operated with tritium, the tritium inventory built up without saturation limit.

This problem may be so serious as to rule out the use of carbon in fusion devices.

That, however, would eliminate the leading candidate material, and the one that, by a considerable margin, we know most about.

It would be a setback to be driven to the extreme of not being able to keep the carbon option open.

This problem may be so serious as to rule out the use of carbon in fusion devices.

That, however, would eliminate the leading candidate material, and the one that, by a considerable margin, we know most about.

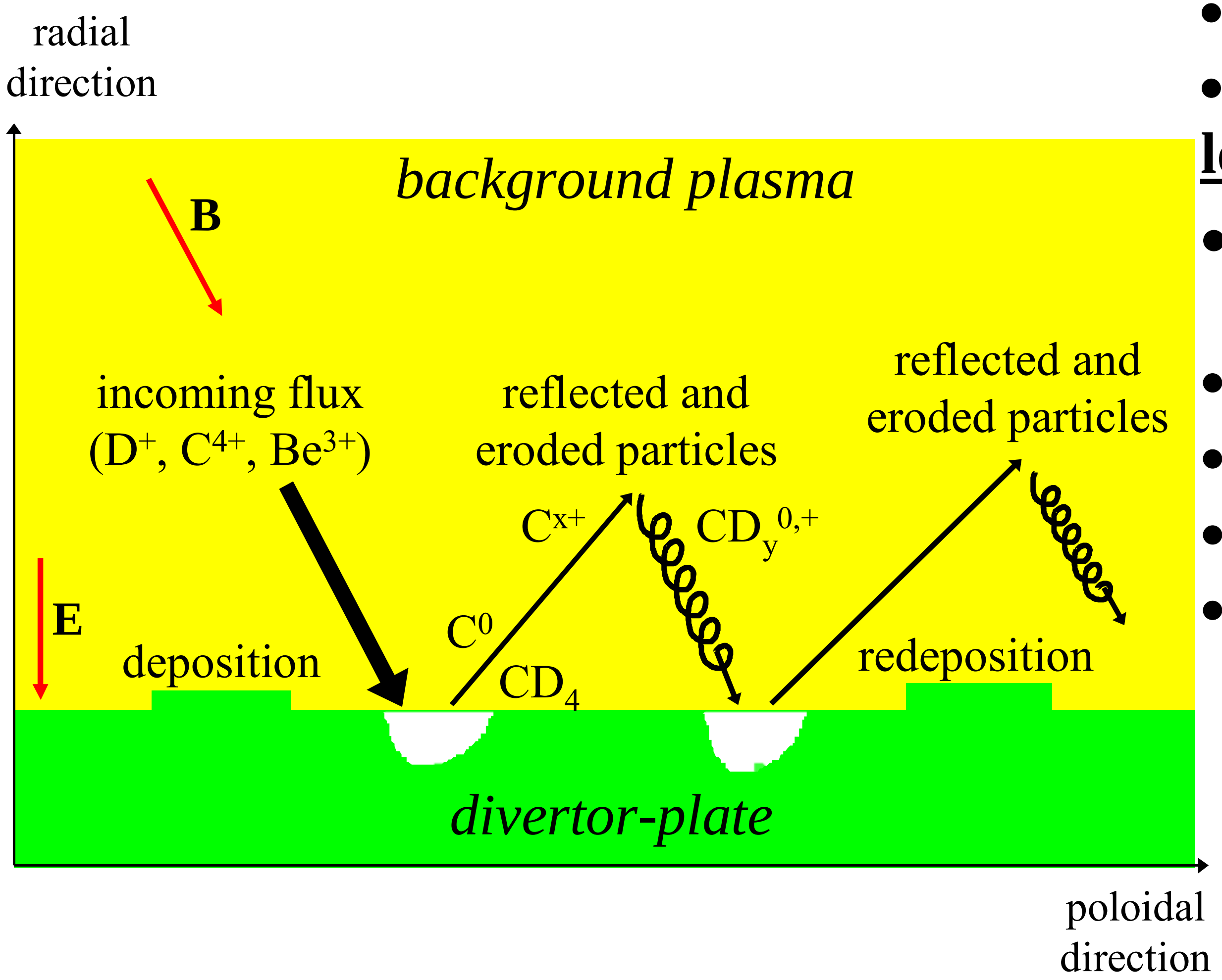
Key issues (see: “low temperature plasma physics”)

- Surface processes involving Hydrocarbons and their ions

- Role of Hydrocarbon chemistry and transport modelling in divertor plasmas

modelling of erosion and re-deposition processes

The ERO-TEXTOR/JET/ITER Code



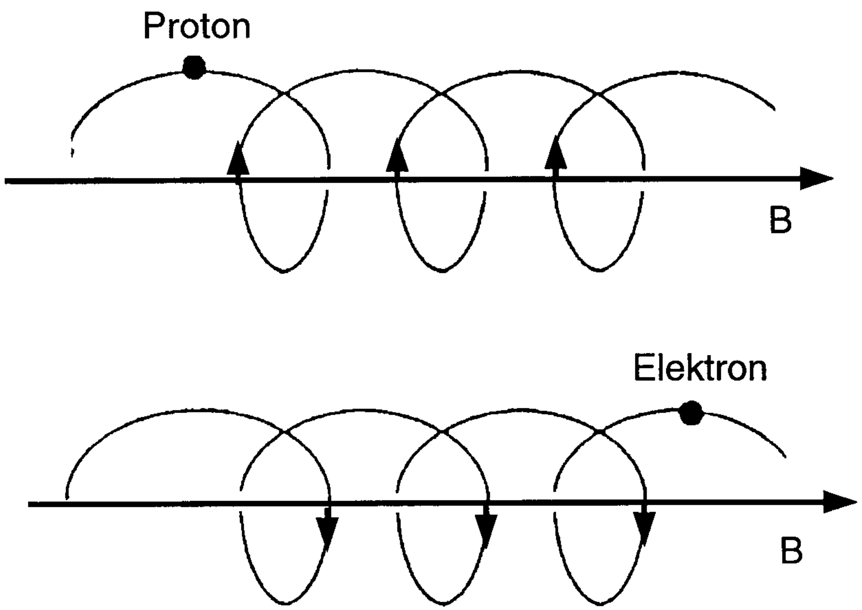
plasma-wall-interaction:

- **physical sputtering**
- **chemical erosion (CD_4)**
- **background deposition**

local particle transport:

- **Monte-Carlo → ionisation, dissociation**
- **Lorentz force**
- **friction (Fokker- Planck)**
- **thermal force**
- **diffusion**

Numerical complication: fast gyro motion in magnetic field



$$\omega_{ce} = 1.76 \times 10^{11} B[\mathrm{T}]$$

$$r_{Le}[\mathrm{m}] = 3.38 \times 10^{-6} \frac{\sqrt{T_e[\mathrm{eV}]}}{B[\mathrm{T}]}$$

B = 3 T

$f = \omega / 2\pi$

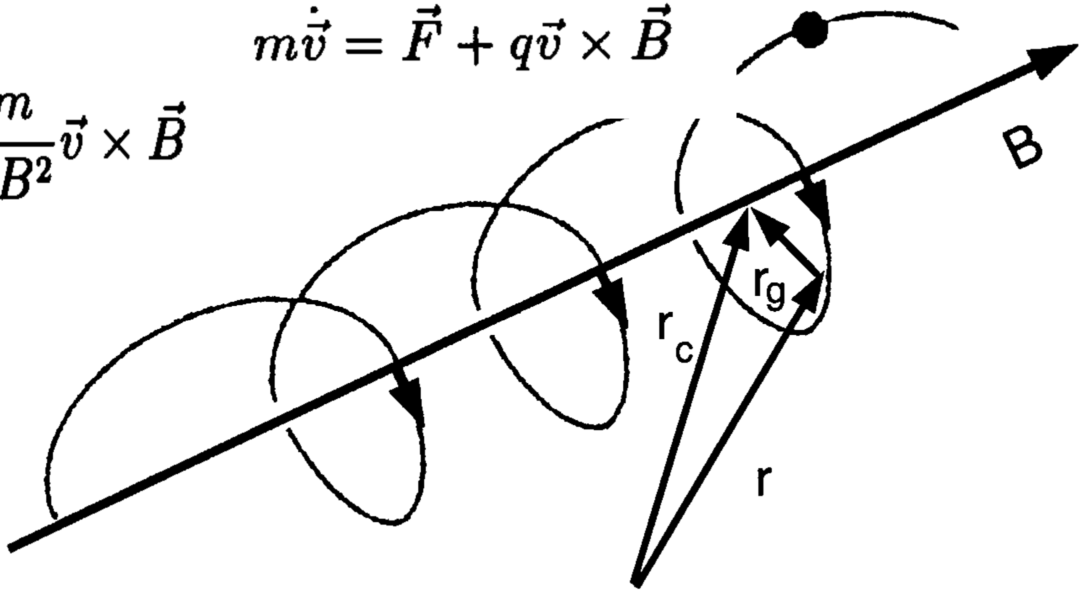
energy	electron larmorradius mm	ion larmorradius mm	electron cyclotron-frequency	ion cyclotron-frequency
10 keV	0.11	4.8	84 GHz	46 MHz
1 keV	0.035	1.5	84 GHz	46 MHz
10 eV	0.003	0.15	84 GHz	46 MHz

Gyro motion in magnetic field, cont.

guiding centre ansatz

$$m\dot{\vec{v}} = \vec{F} + q\vec{v} \times \vec{B}$$

$$\vec{r}_c = \vec{r} + \vec{r}_g \quad \text{mit} \quad \vec{r}_g = \frac{m}{qB^2}\vec{v} \times \vec{B}$$



Equation of motion for guiding centre

$$\vec{v}_c = \dot{\vec{r}}_c = \vec{v} + \frac{m}{qB^2}\frac{d\vec{v}}{dt} \times \vec{B} = \vec{v} + \frac{1}{qB^2}(\vec{F} + q\vec{v} \times \vec{B}) \times \vec{B}$$

$$\vec{v}_c = \vec{v} + \frac{\vec{F} \times \vec{B}}{qB^2} - \vec{v}_\perp = \vec{v}_\| + \frac{\vec{F} \times \vec{B}}{qB^2}$$

Slow drift-motion

Very stiff problem. Solution: “**Boris-solver**” (1960s)
Small Δt: solves for r(t), larger Δt: solves for $r_c(t)$

Reaction chain of methane molecules CH_4 (Erhardt/ Langer):

$CH_4^+ \longrightarrow CH_3^+ \longrightarrow CH_2^+ \longrightarrow CH^+ \longrightarrow C^+ \longrightarrow C^{2+}$

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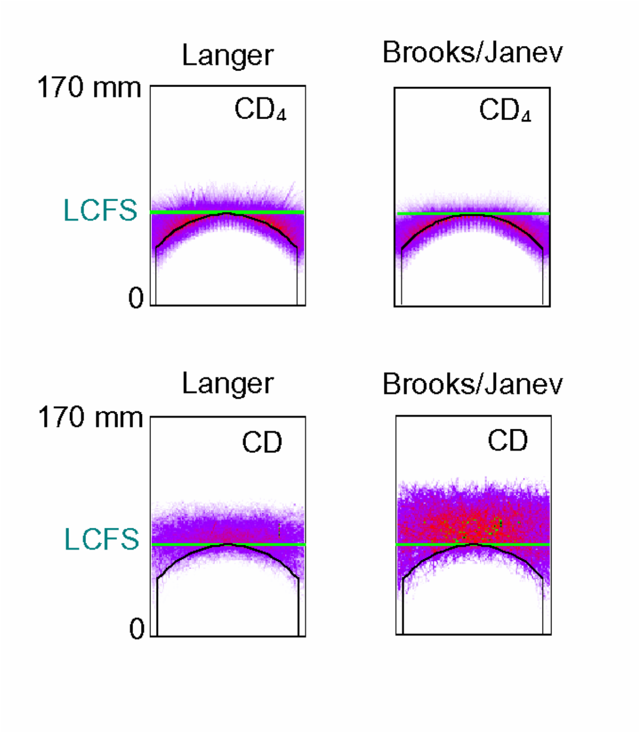
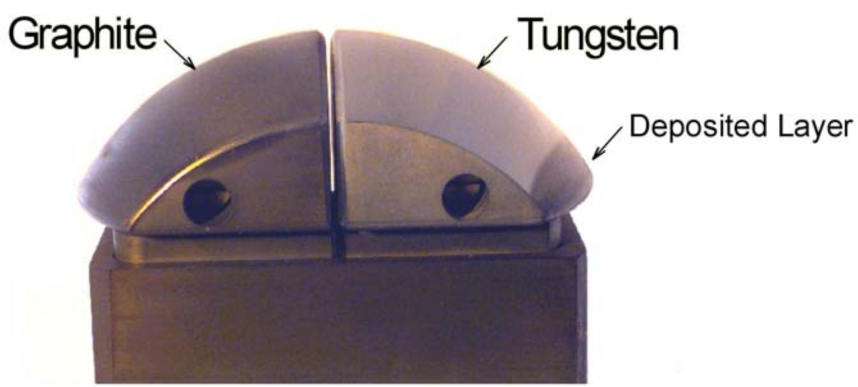




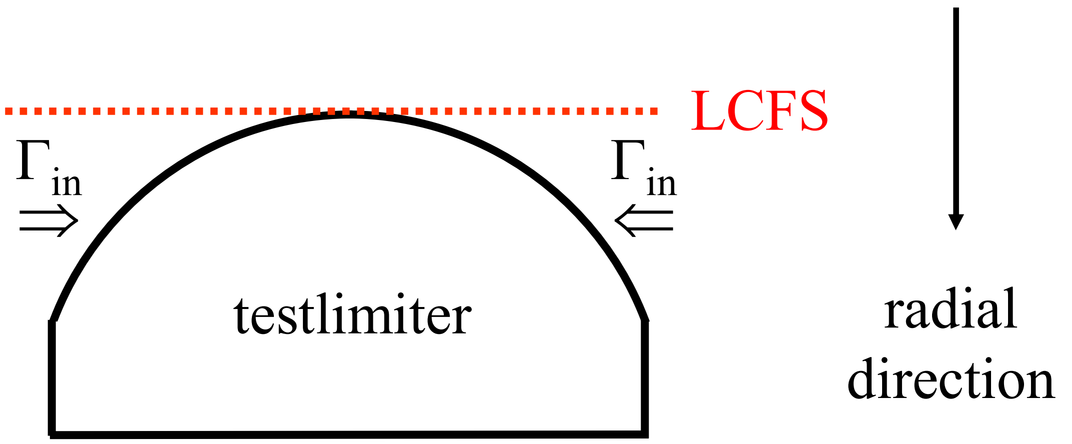
Ehrhardt-Langer, PPPL 2477, Sept 1987
Alman-Ruzic-Brooks, Phys.Plas. 7, 2000
Janev-Reiter, JUEL 3966, Feb 2002
Janev-Reiter, JUEL 4005, Oct 2002

<u>Hydrocarbon transport:</u> TEXTOR conditions

Chemical erosion of CD_4 and C_2D_4

<u>Assumptions for the calculations:</u>

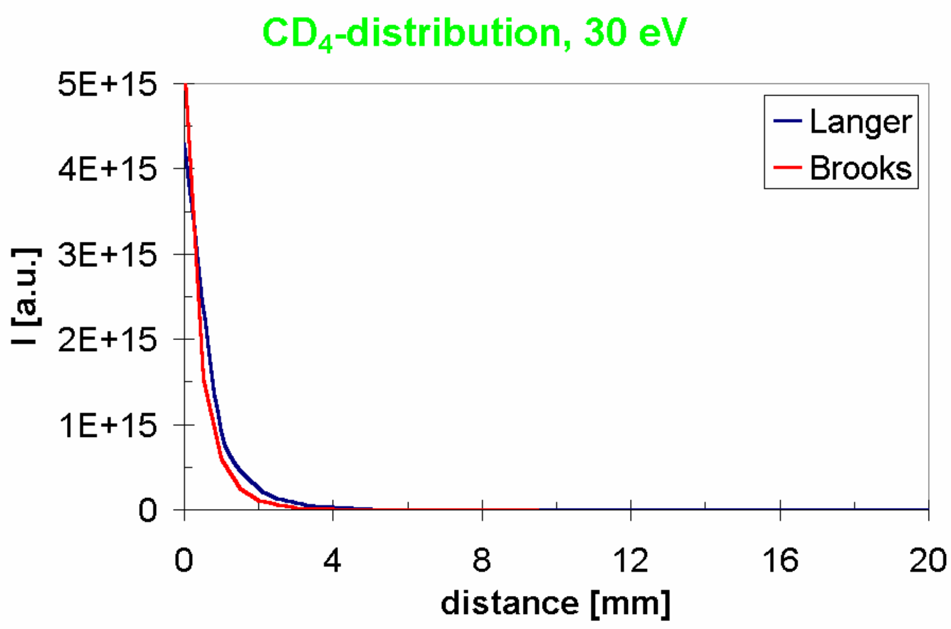
- carbon testlimiter with **spherical surface** (radius 70 mm)
- electron temperature **T_e(LCFS)** and density **n_e(LCFS)** at the last closed flux surface**:** input parameter
- decay lengths in radial direction: λ_{Te} **= 25 mm,** λ_{ne} **= 20 mm**

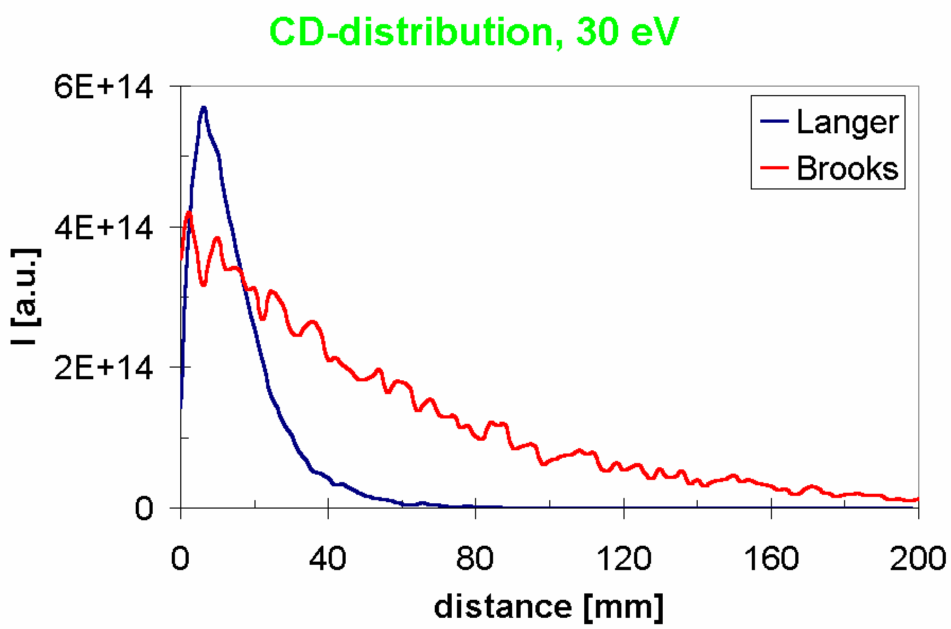


Parameter study: homogenous plasma, 30 eV, 1e13 cm^{-3}

Plane CD_4 source: Ehrhardt-Langer vs. Brooks/Janev data

Penetration of CD_4 and CD:



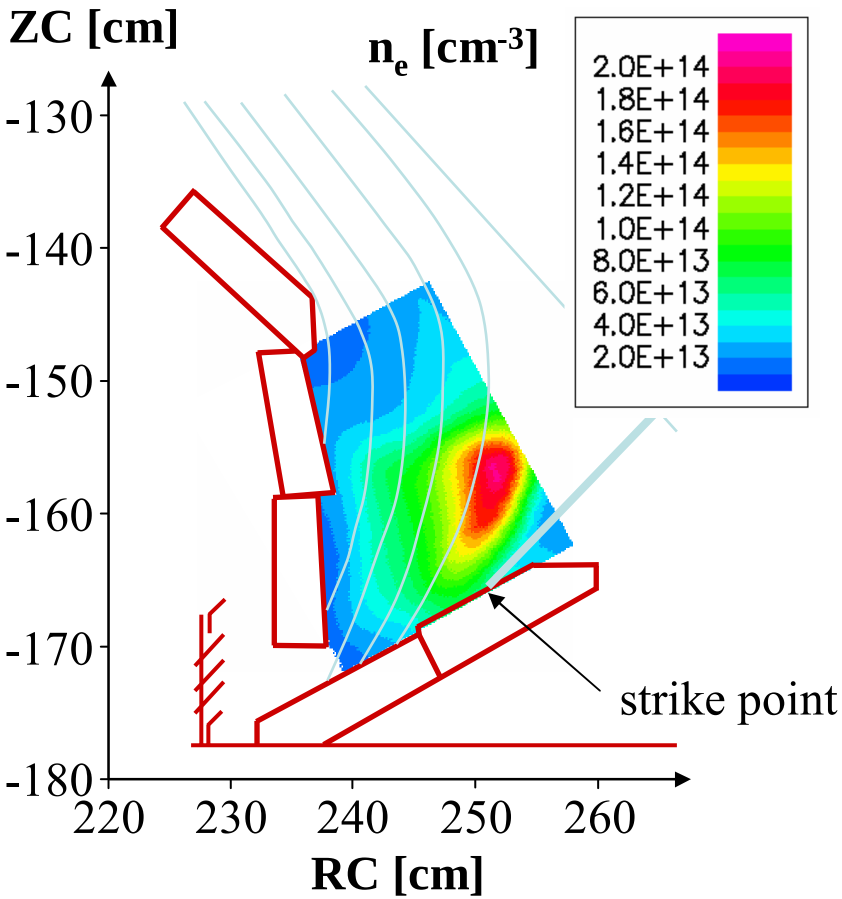


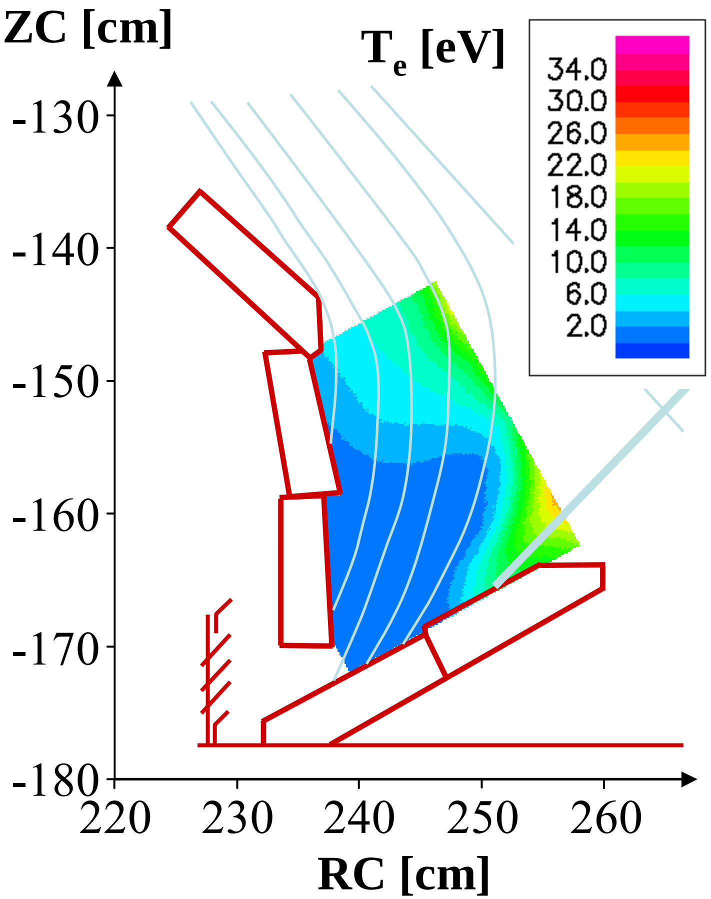
Similar penetration of CD_4 in "Brooks/Janev" and "Langer case": various differences in rate coefficients result in vanishing effect

Significantly deeper penetration of CD in "Brooks/Janev case": missing reactions and smaller dissociation rates $\Rightarrow$ longer lifetime

JET MkIIa Modelling: *Background Plasma for ERO-JET (inner divertor)*

OSM for standard gas fuelled ELMy H-mode, 12 MW (#44029)

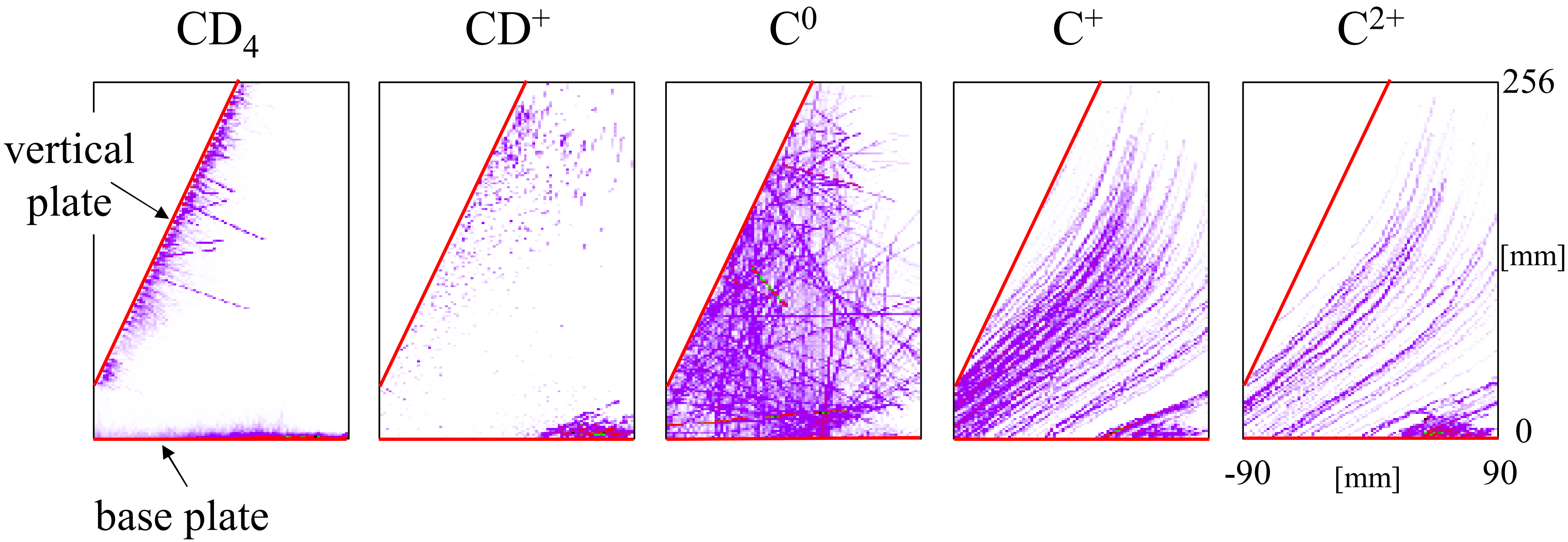




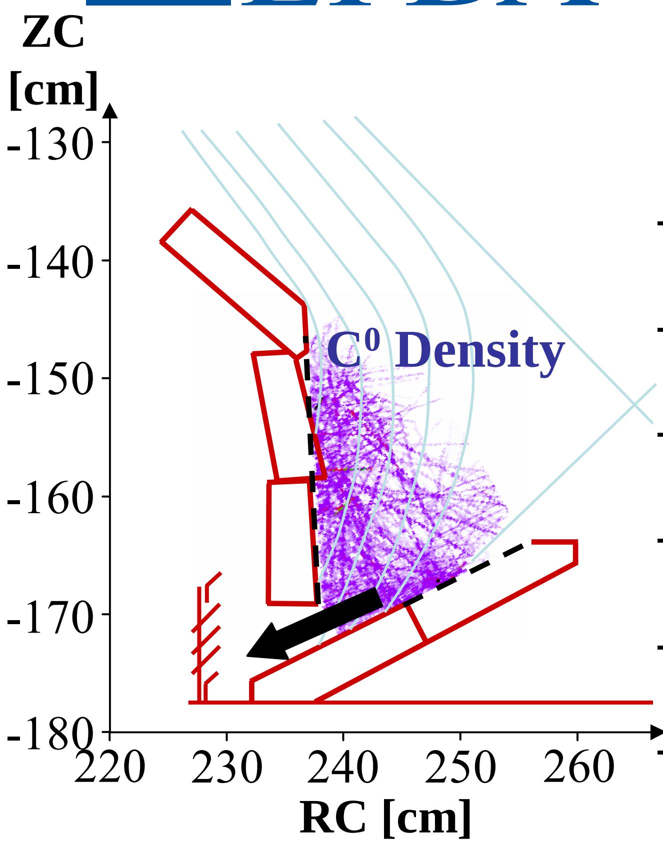
JET MkIIa Modelling: *Transport of chemically eroded CD_4 (inner divertor)*

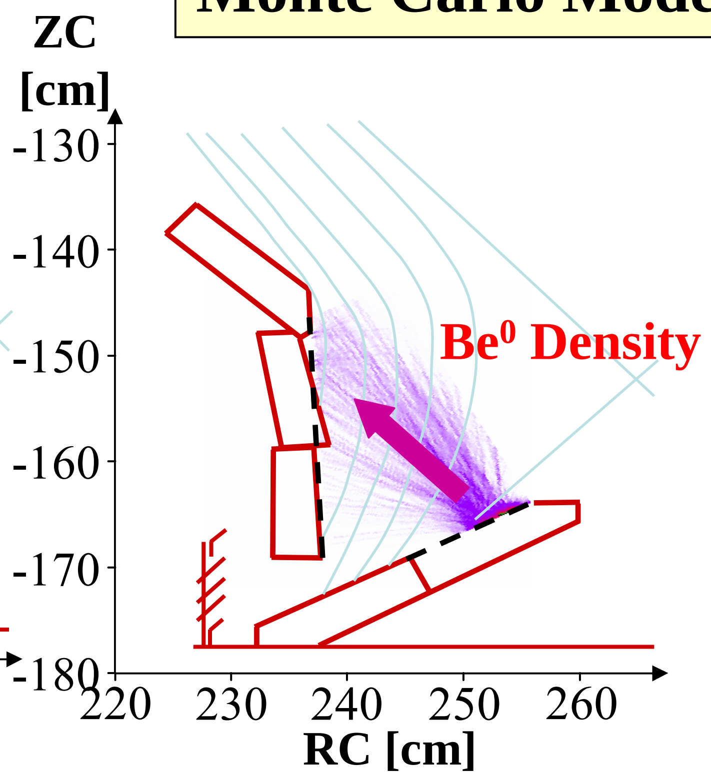
Spatial distribution of hydrocarbons and carbon

- Dynamic reflection of C–atoms and –ions (MolDyn)
- Zero sticking of hydrocarbons CD_y



Monte Carlo Modelling





far too little carbon flux towards louvre region,

C-H sources, transport and chemistry not in hand

Be distribution well reproduced

OSM interpretation code, atomic rates, phys. sputtering, transport, quite well established

ERO modelling, by A. Kirschner et al.

JET MkIIa Modelling: *Transport of chemically eroded CD_4/ C_2D_4 (inner)*

Particles to louver: Comparison with experiment

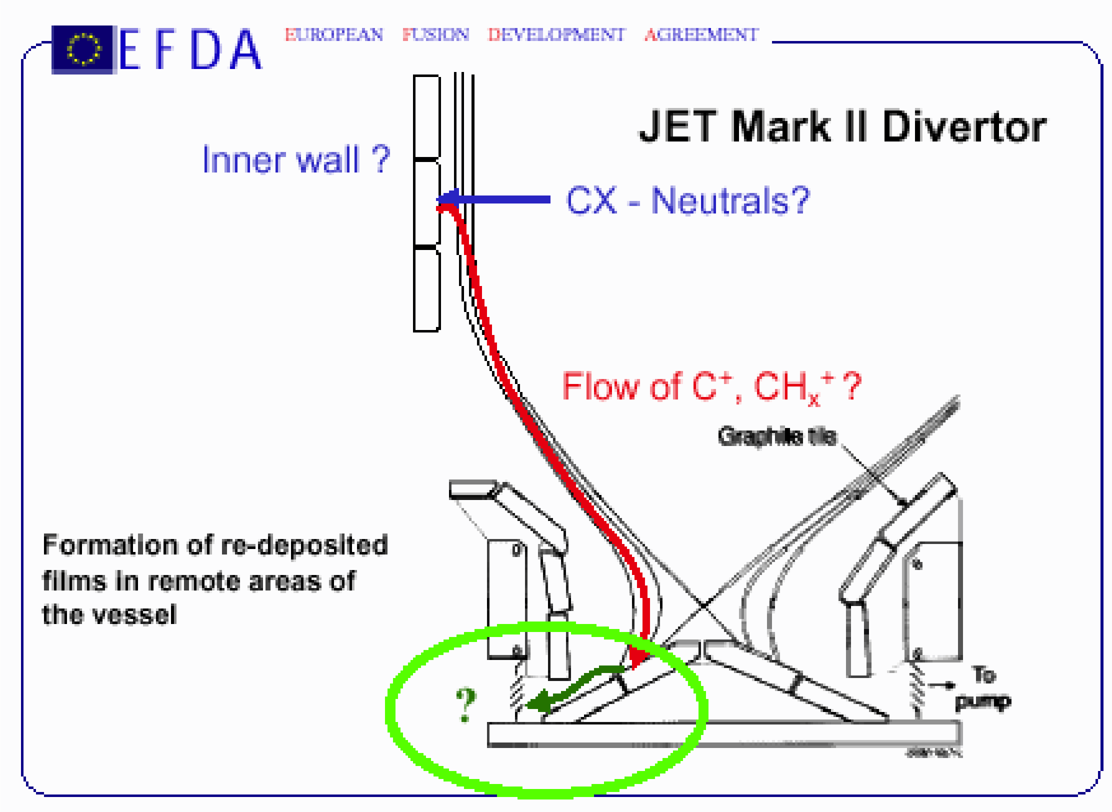
- **Measured** value of carbon particles entering louver region: **4% $\cdot\Phi_{D^+}$**

- **Simulations** with plasma parameter from OSM

- Chemical erosion of CD_4 with 1%:	$0.12\% \cdot \Phi_{D^+}$
- Chemical erosion of C_2D_4 with 1%:	$0.36\% \cdot \Phi_{D^+}$
- Background carbon flux with Γ_C = 1%:	$0.04\% \cdot \Phi_{D^+}$
	Σ **$0.52\% \cdot \Phi_{D^+}$**

- Stamp (PSI '00): Y_{CD4} = 5%, Y_{C2D4} = 7%
  and McCracken (NF 39, 1 (1999)): $\Gamma_C \cong 5\%$ ⇒ **$3.3\% \cdot \Phi_{D^+}$**

- in addition "shifted plasma" (~8 cm to louver): ⇒ **$4.6\% \cdot \Phi_{D^+}$**

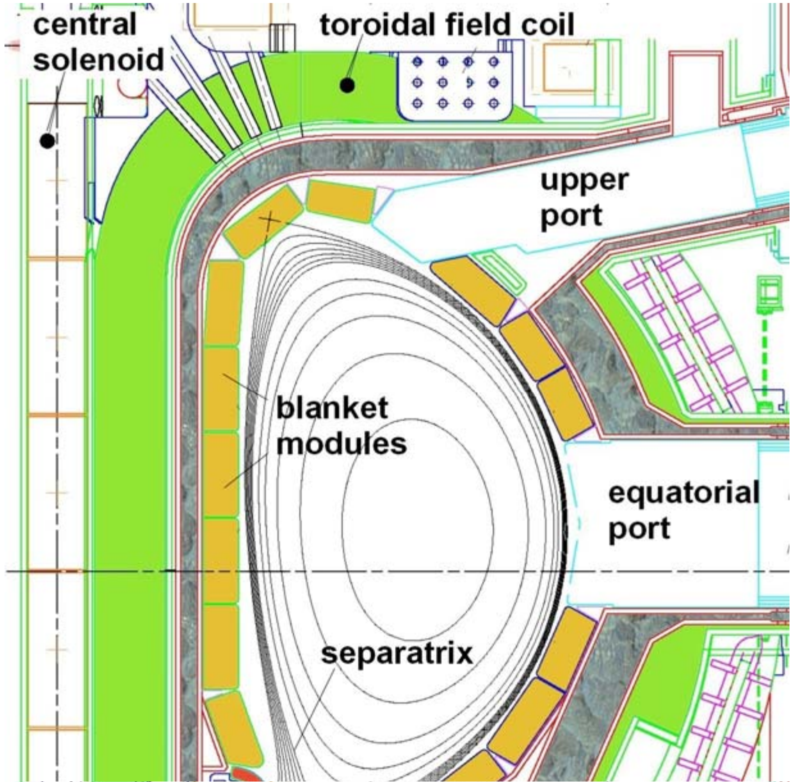


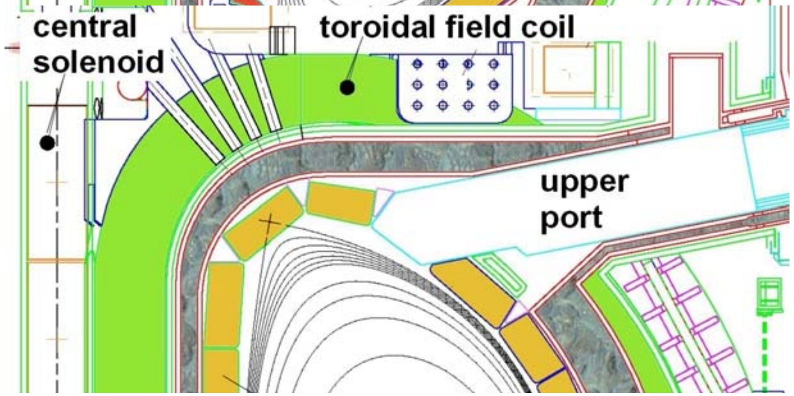
Present „understanding“ of erosion and deposition

- **carbon and beryllium is eroded in the main vessel (by ions and neutrals)**
- **Transport by SOL-flows towards inner divertor**
- **deposition of C and Be on strike zone area**
- **further transport of carbon to remote (cold) areas**
- **chemical processes, in particular with soft carbon films are important**

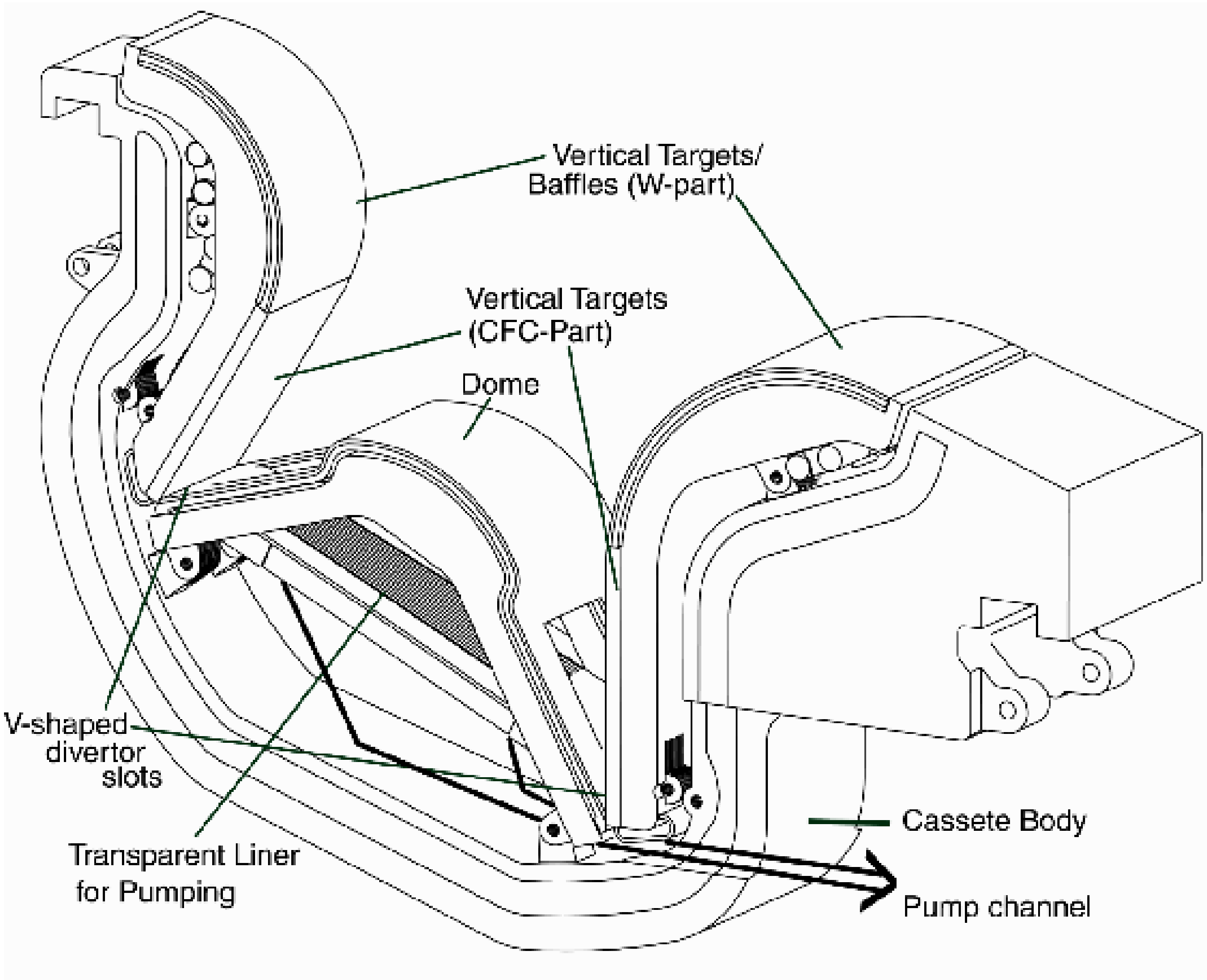
ITER will have a Be-wall how will this change the tritium retention ?

ITER

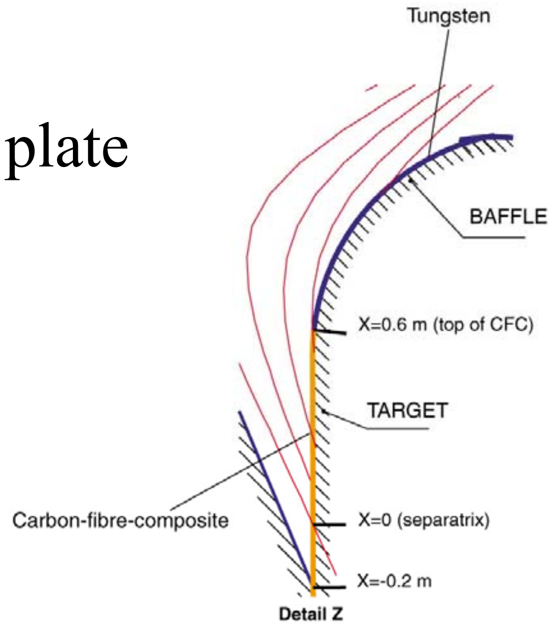

central
solenoid
toroidal field coil
upper
port
blanket
modules
equatorial
port
separatrix


central
solenoid
toroidal field coil
upper
port

ITER divertor cassette



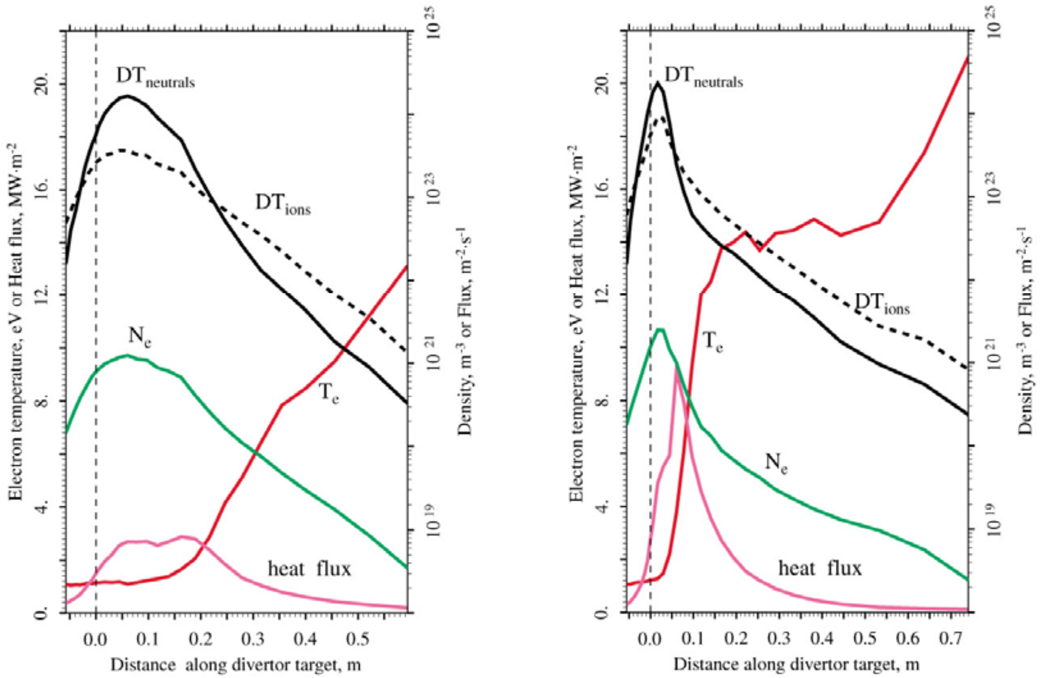
ITER divertor
plasma parameters along plate



(a)

inner
divertor

outer
divertor

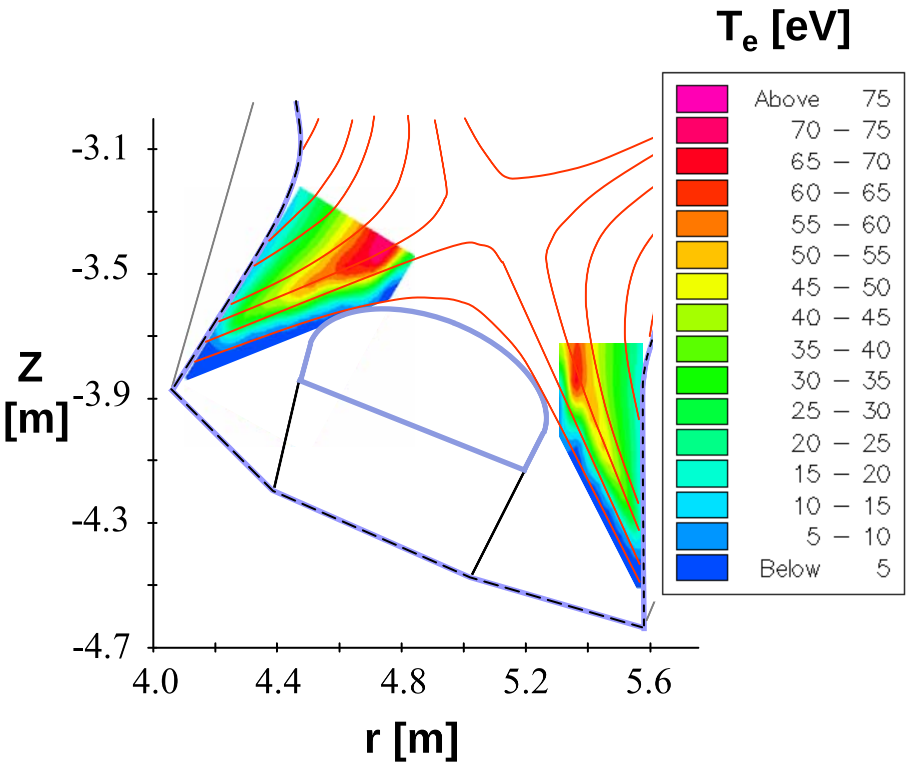


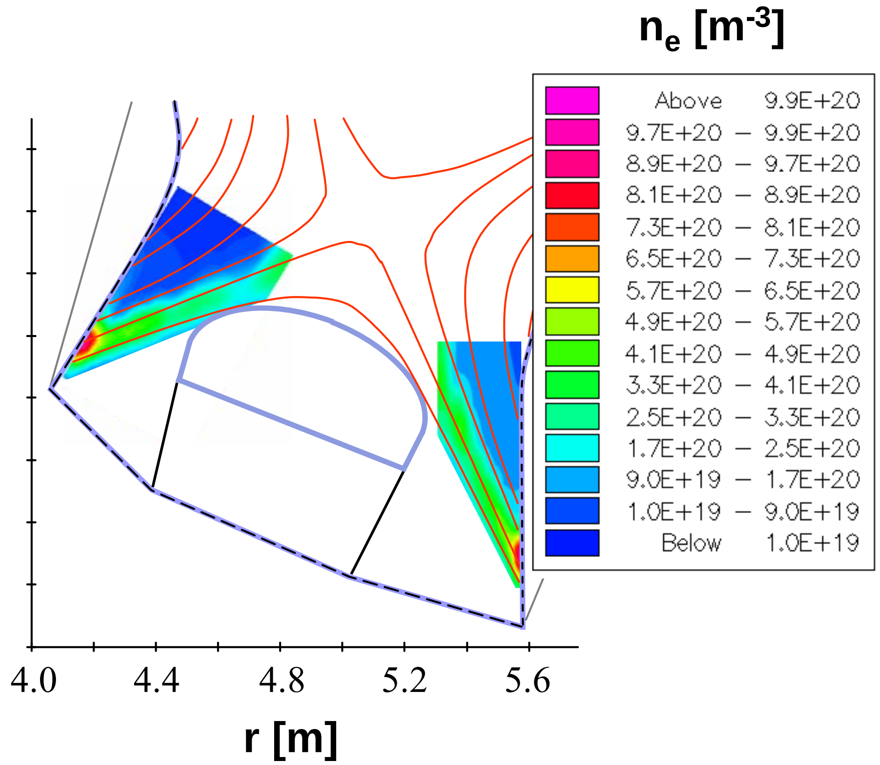
(b)

ITER: tritium retention and lifetime predictions (1)

Background Plasma from B2-Eirene

Reference case 345 (410 MW fusion power at Q=10, 30% radiated from core)



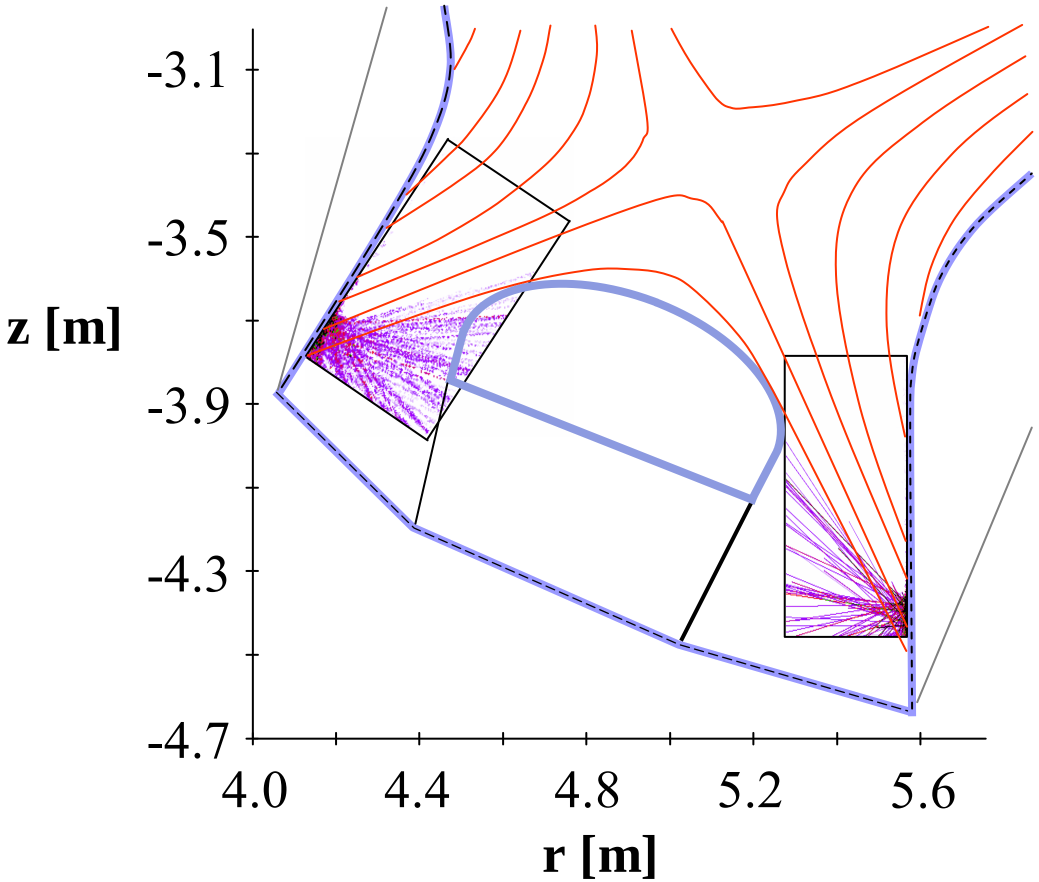


ITER: tritium retention and lifetime predictions (2)

Transport of chemically eroded CD_4

Spatial distribution of C^O

- **Zero sticking** of hydrocarbons CD_y, no background flux included



Loss of neutrals to PFR

⇓

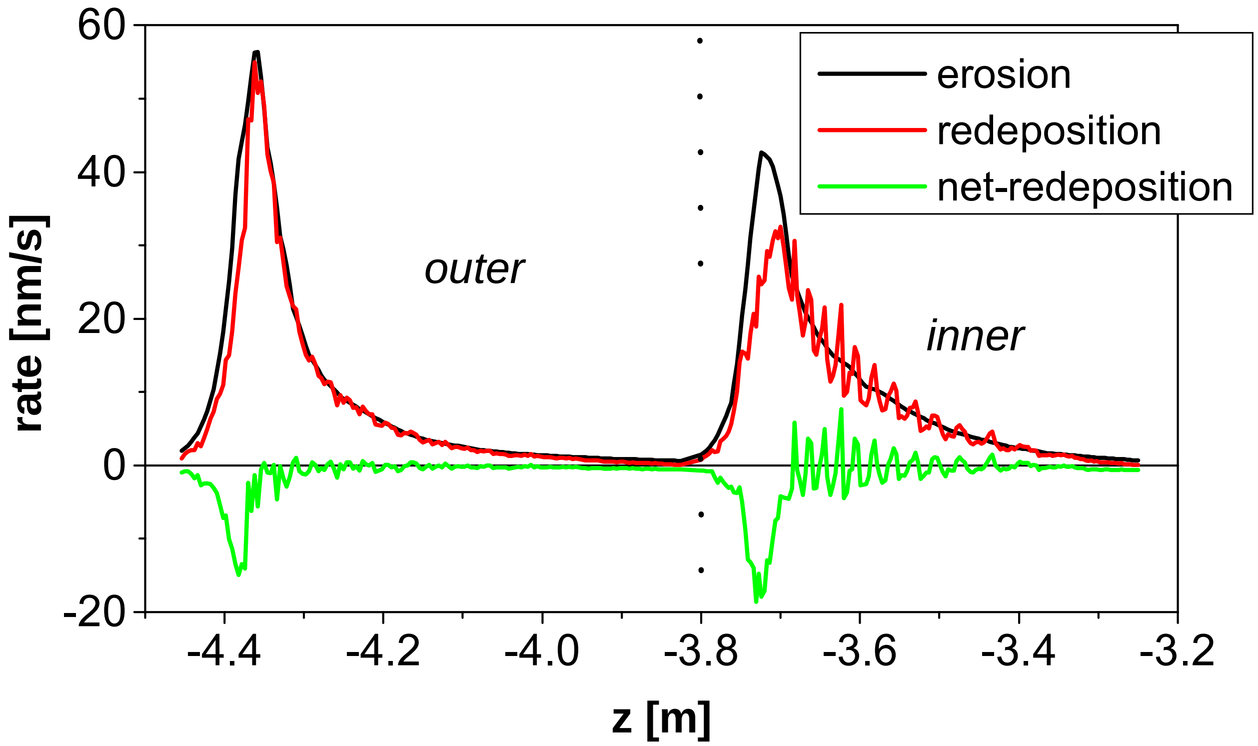
Net erosion

ITER: tritium retention and lifetime predictions (3)

Transport of chemically eroded CD_4

Erosion and re-deposition profiles along the plates

• **Zero sticking** of hydrocarbons CD_y, no background flux included



• High amount of re-deposition (84% inner, 88% outer)

• Net-erosion (or balanced) along the plates, ~15 nm/s near strike points

The consequences of tritium retention for ITER

Extrapolations of tritium retention results to ITER

after how many ITER pulses do we reach the limits for tritium retention ?

Extrapolation from experiments	D,T flux (#/s)	T-retention rate (T/ion)	ITER retention gT/s extrapolation (flux: $1.8\ 10^{24}$/sc)	shots /T-limit (400 sec)
TEXTOR	$5\ 10^{20}$/s	$6.4\ 10^{-4}$	0.0064	136
JET T experience	$1.2\ 10^{22}$/s (inner only)	$1.75\ 10^{-2}$ (only louver)	0.10g	9
JET GB on tiles	$2\ 10^{22}$/s	$2.7\ 10^{-3}$	0.024	36
JET C5 on louver from QMB	$1.9\ 10^{22}$/s	2.9 10-4	0.0026	340
Modelling				
ERO-code (2% CxHy er.)			0.006	145
WBC code			0.007	125

large uncertainties, but in any case critical

ITER: tritium retention and lifetime predictions (4)

Transport of chemically eroded CD_4

estimated tritium retention and target lifetime from ERO-ITER

· Plasma parameter of reference **case 345**

· **Zero sticking** of hydrocarbons, $\mathbf{Y_{chem} = 2\%}$

⇒ **T-retention** (inner + outer): **~ 6 mg/s**

⇒ **Safety limit** (350g) reached after: **~ 60 discharges** of 1000s

⇒ **Target lifetime** (erosion of 0.5cm): **~ 600 discharges** of 1000s

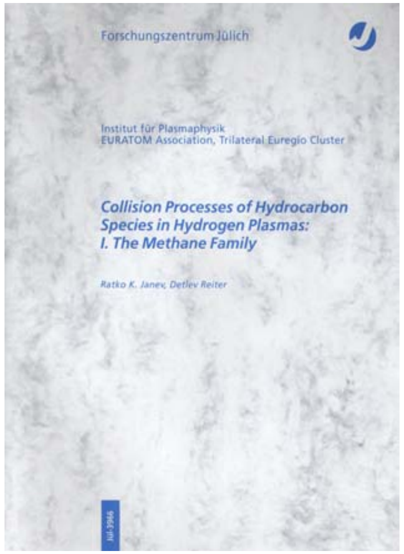
Effect of Beryllium?

New Hydride Collision Databases
for Technical Plasmas and Fusion Plasmas

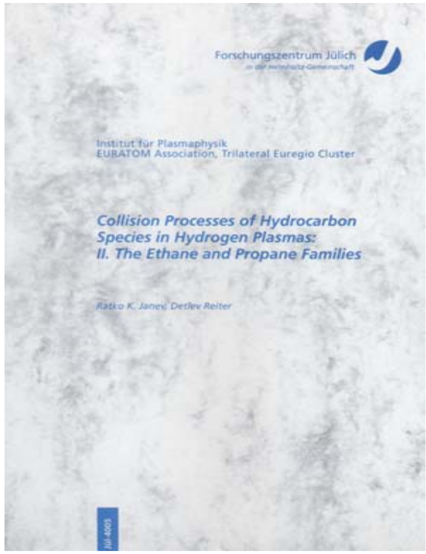
Databases used in (fusion) applications are sometimes
either entirely obsolete, or, at best, incomplete and largely empirical

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

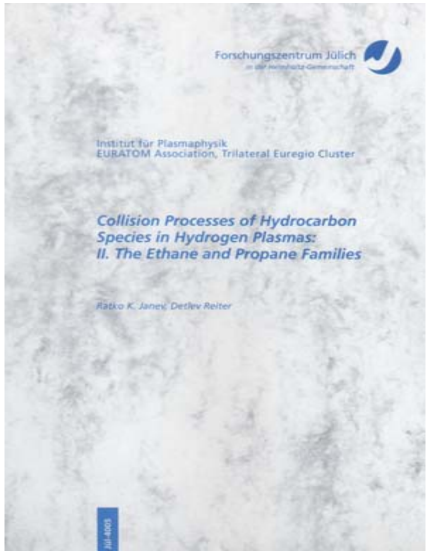
Methane (CH_y) | C_2H_y | C_3H_y | Silane (SiH_y) | $p, H, H^-, H_2, H_2^+, H_3^+$



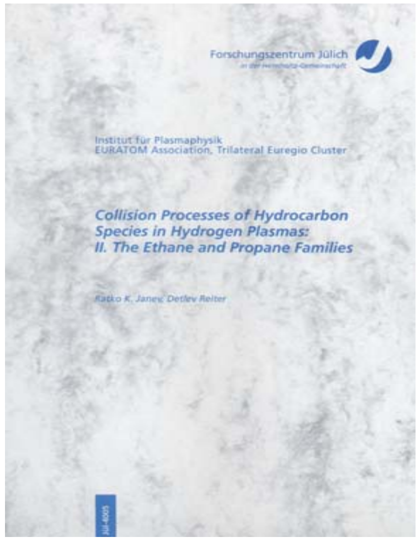
JUEL 3966, Feb 2002
Phys. Plasmas,
Vol 9, 9, (2002) 4071



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

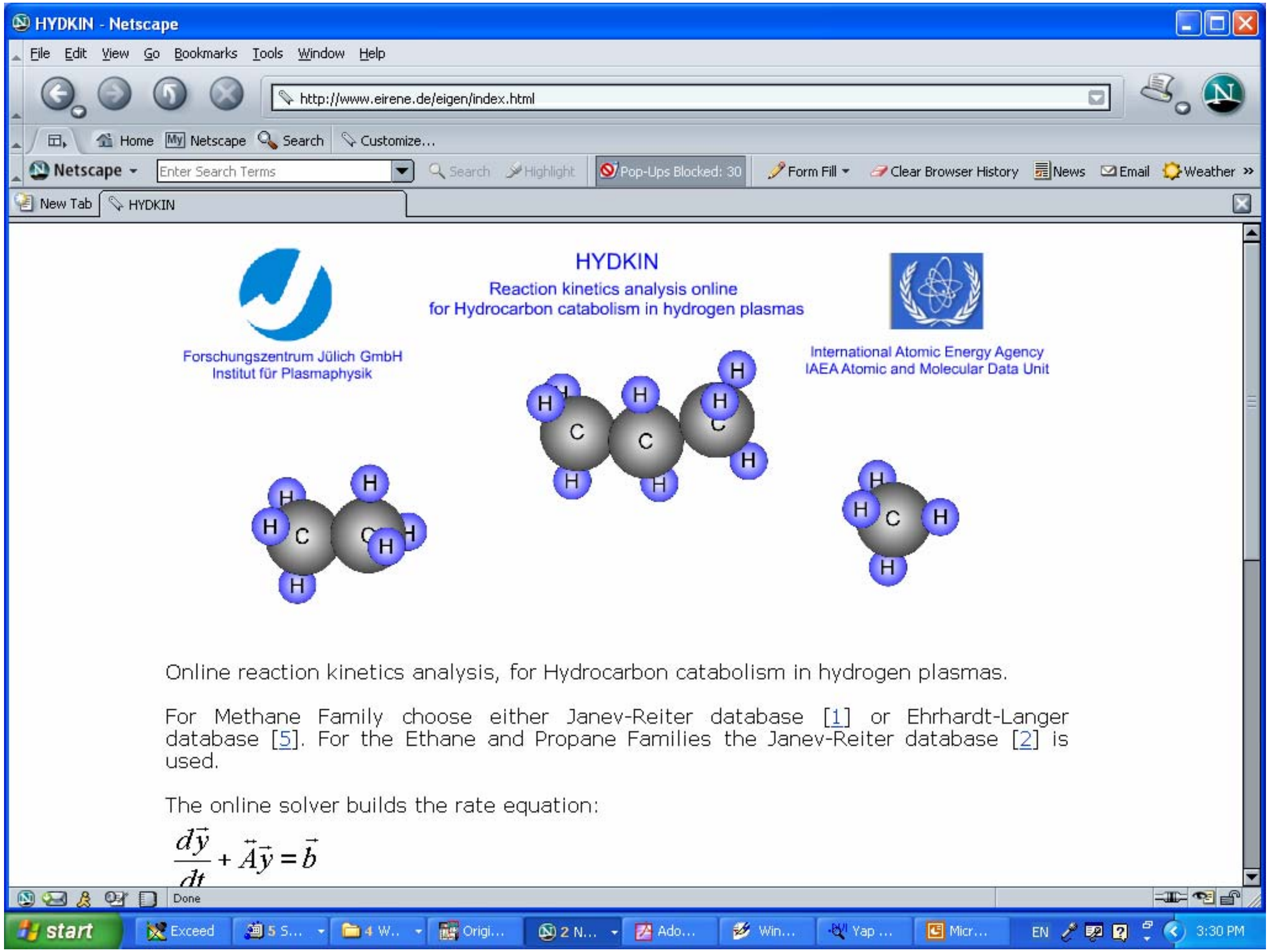


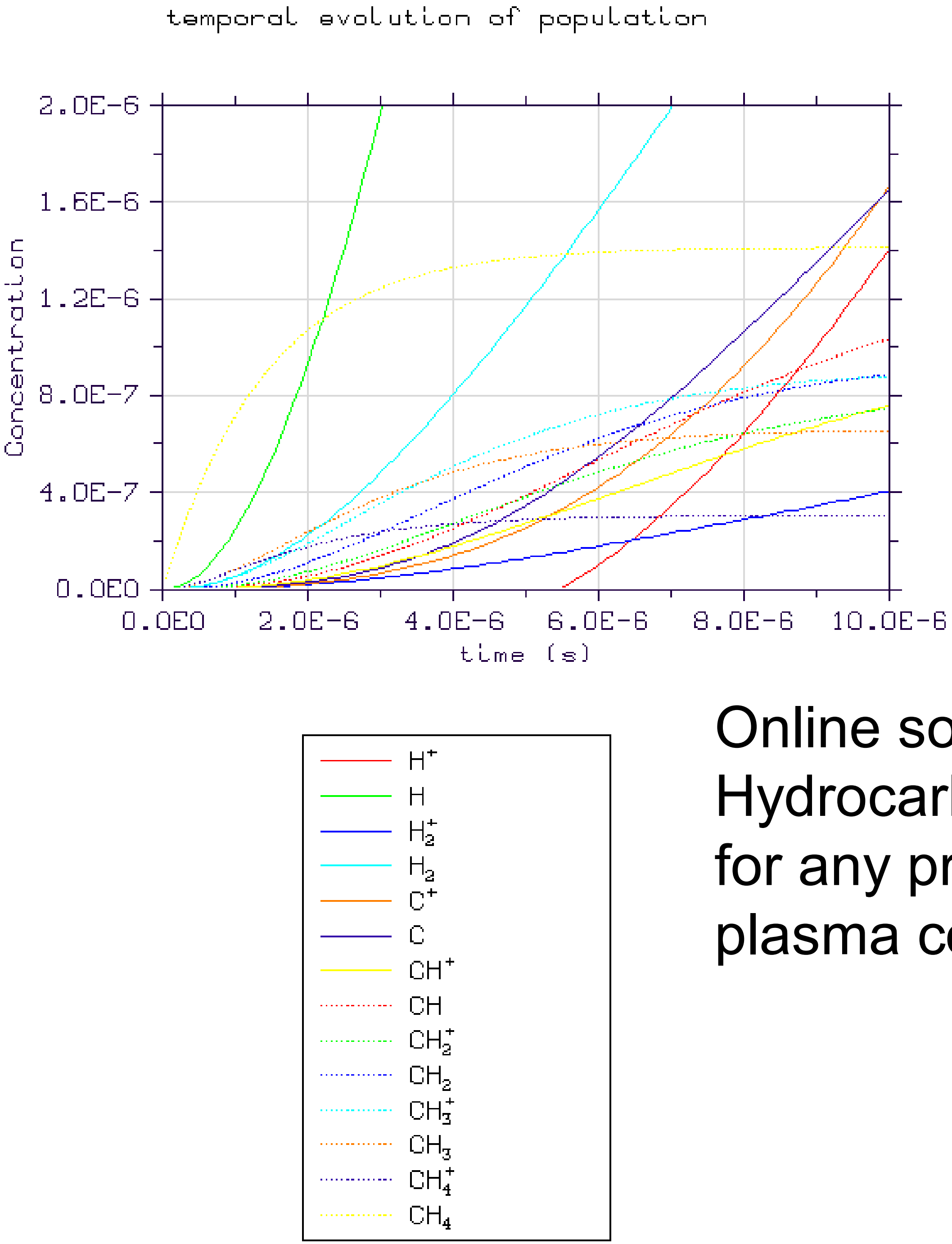
JUEL 4038, Mar. 2003
Contr. Plas.Phys,
47, 7, (2003) 401-417



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

Analysis tool for hydrocarbon catabolism in fusion edge plasmas
Online evaluation of cross sections σ(E), rate coefficients K(T), rate equations and S/XB, based upon recent database (2004)
www.eirene.de/eigen/index.html





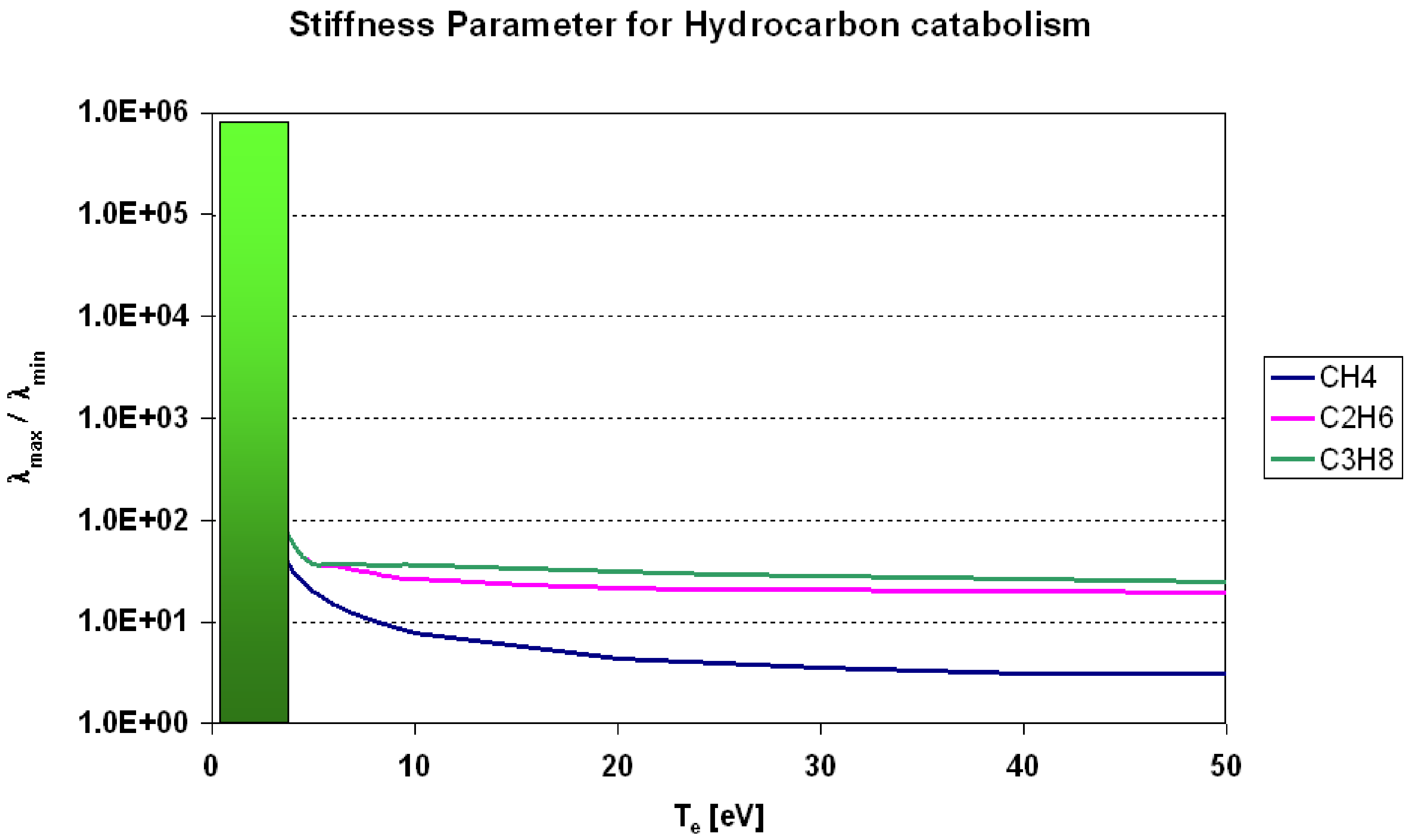
Online solution of time-dep. (1D) Hydrocarbon brake-up, for any prescribed divertor plasma conditions, up to C_3H_8

Very complex reaction chains (approx. 500 individual processes) in fusion plasmas: catabolic sequence dominant, little: anabolism

→Eigenmode analysis of reaction rate equations very simple:

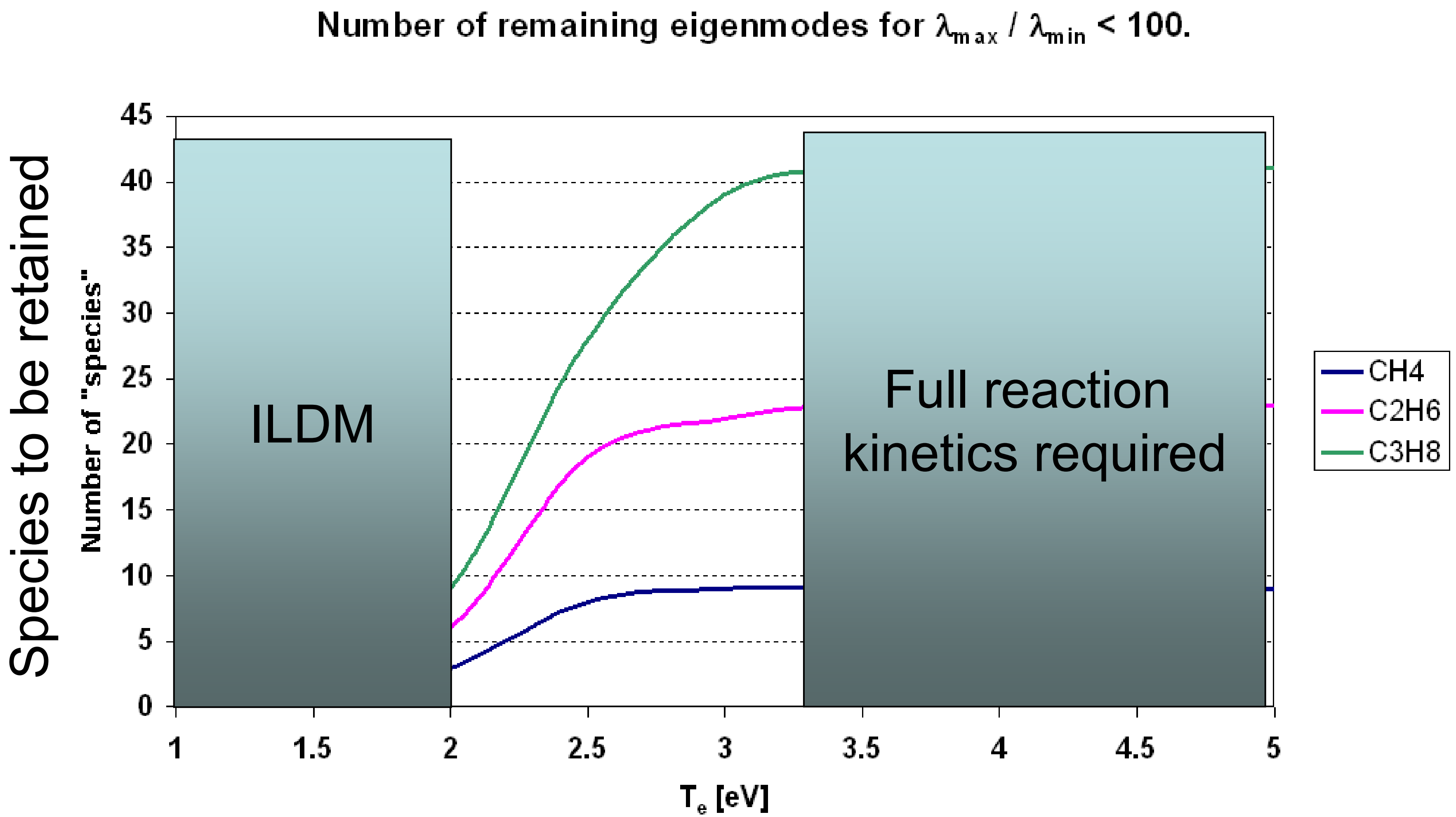
→Define "Stiffness parameter": λ_{max}/ $\Lambda_{min,}$, ratio of max. to min. eigenvalues

fast slow



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



Data Needs for Modelling

- reflection/sticking coefficients

in particular at at low energies

transport of eroded material to remote areas in ITER ?

- properties of deposited films,

in particular with mixed materials

how does a beryllium wall change the overall erosion/deposition ?

- tritium content and release mechanisms

how to minimise retention and how to recover the tritium ?

- rate coefficients for dissociation,

ionisation, recombination

reliable transport modelling from source to sink needed

- radiation properties, D/XB values

radiation cooling
combined effect of C, Be, W, Ne, Ar ?
recycling, release mechnisms ?
diagnostics improvements needed

The Status of Fusion

ITER Objectives

EU Domestic Assessment of the ITER-FEAT final design report in May 2001

main conclusions:

confidence to achieve the nominal plasma current of 15MA,
a significant window for long-pulse operation (about 8 min),
at a fusion amplification factor Q of at least 10,

capability for investigating steady-state plasma operation,
a range of plasma parameters which should allow Q=5,

'Hybrid' scenarios to extend the pulse length to periods of order 30 min,

design with significant flexibility to allow it to exploit progress made
in various areas aiming at performance beyond today's expectations.

ITER is an Experiment for investigating also plasma-wall interaction issues to prepare a viable solution for the steady state ractor (DEMO)

CONCLUSIONS

Magnetic confinement is now effective enough to contain the main fusion flame, but it is too good for the plasma edge (SOL): very narrow heat-footprints on targets.

n, T upstream (core) fixed by burn criteria, density limit, etc.

Detached regime: decrease particle flux to target for given upstream conditions: self sustained neutral cushion (reactive plasma) controlled by PMI and A&M

Experimental signatures (real and numerical experiments):

- **pressure drop along B-field**
- **Target particle flux drop with increasing n-upstream**
- **anti-correlation of Balmer emission of target flux**
- **very low T_e at target (1-3 eV)**
- **increased D_γ /D_α ratio (recombination?)**

CONCLUSIONS, cont.

Magnetic Confinement Fusion Reactors must operate at reduced target fluxes and temperatures ("detached regime").

The plasma regime in the Divertor (near target region) is then that of (high electron density) technical gas discharges / fluorescent lamps / RF discharges.

Divertor detachment physics involves a rich complexity of plasma chemistry not otherwise encountered in fusion devices.

A simple universal model seems unlikely. Synergism between:

- **ion neutral friction**
- **volume recombination**
- **radiation trapping**
- **supersonic flows, sheath physics**
- **thermal instability, . . .**