Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft

II: The role of hydrogen chemistry in present experiments and in ITER edge plasmas

D. Reiter

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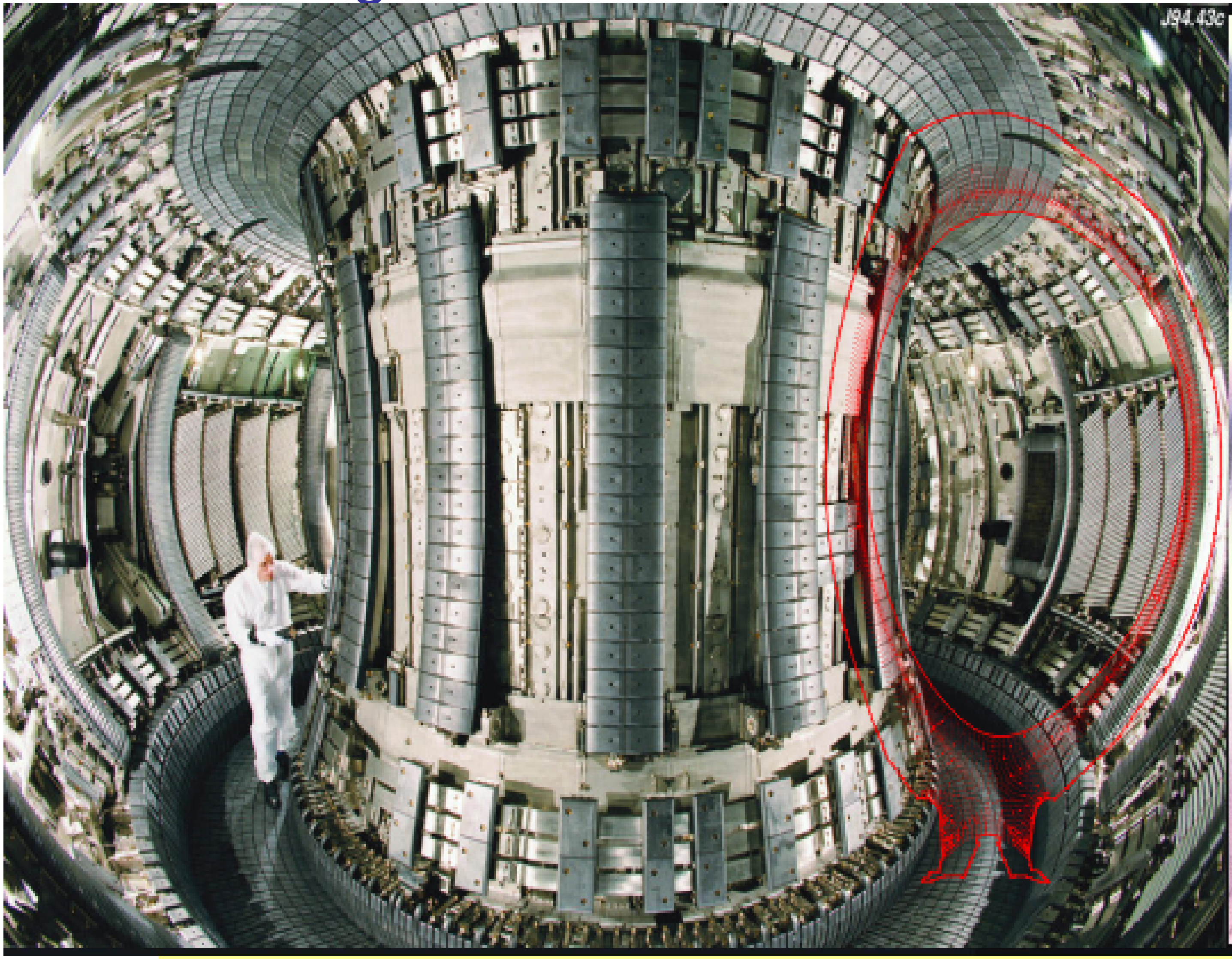
Atomic and Molecular Data for Fusion Energy research, Aug.-Sept. 2006, ICTP, Trieste

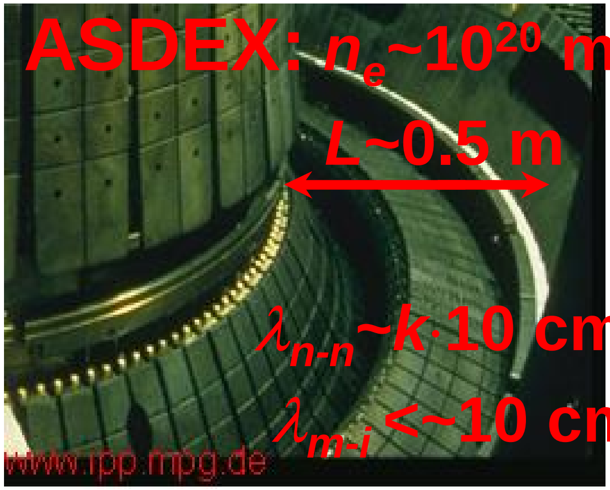
Main focus of coordinated European edge code model validation is on JET

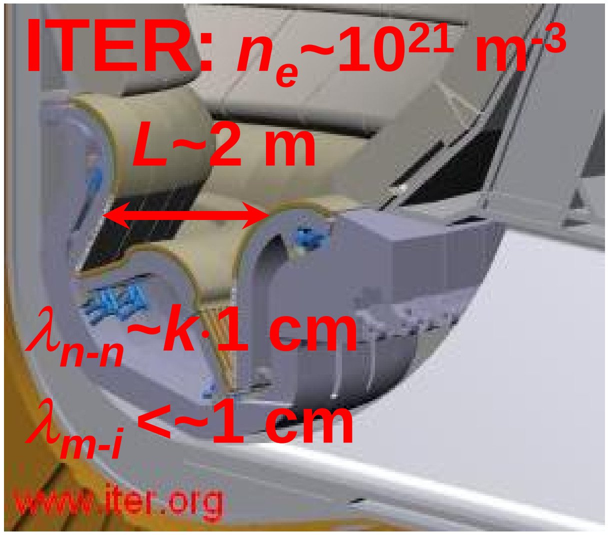


JET Furnace chamber:

Ø 8.5 m 2.5 m high 3.4 T 7 MA 1 min

Motivation





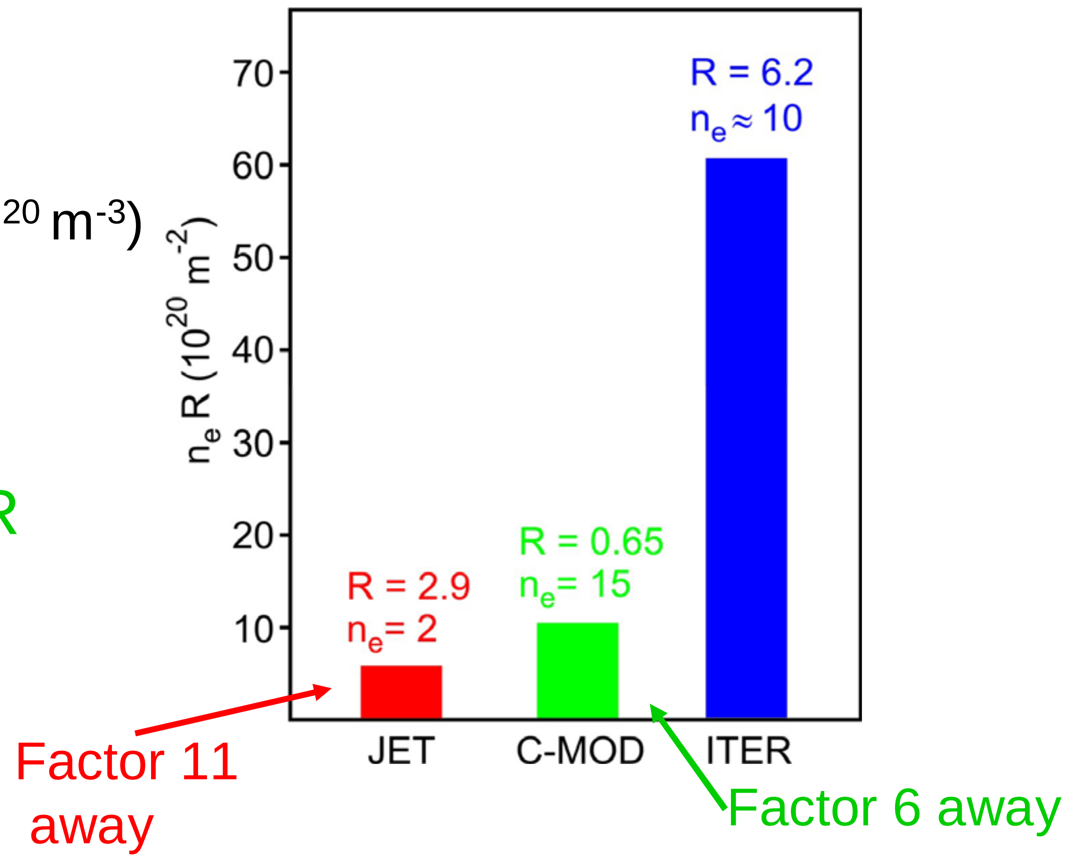
- ITER divertor will have much larger $L \cdot n$ then all existing tokamaks.
- It is necessary to take into account effects which have been safely ignored in divertor modelling for most present devices
- One such effect is *neutral-neutral collisions (viscous effects in gas)*
- Large regions of dense, low temperature plasma requires more accurate simulation of the *molecular reaction kinetics*, including *molecule-ion collisions*

Current hypothesis: in the "detached state" is the divertor dynamics and chemistry is controlled by "Collisionality"

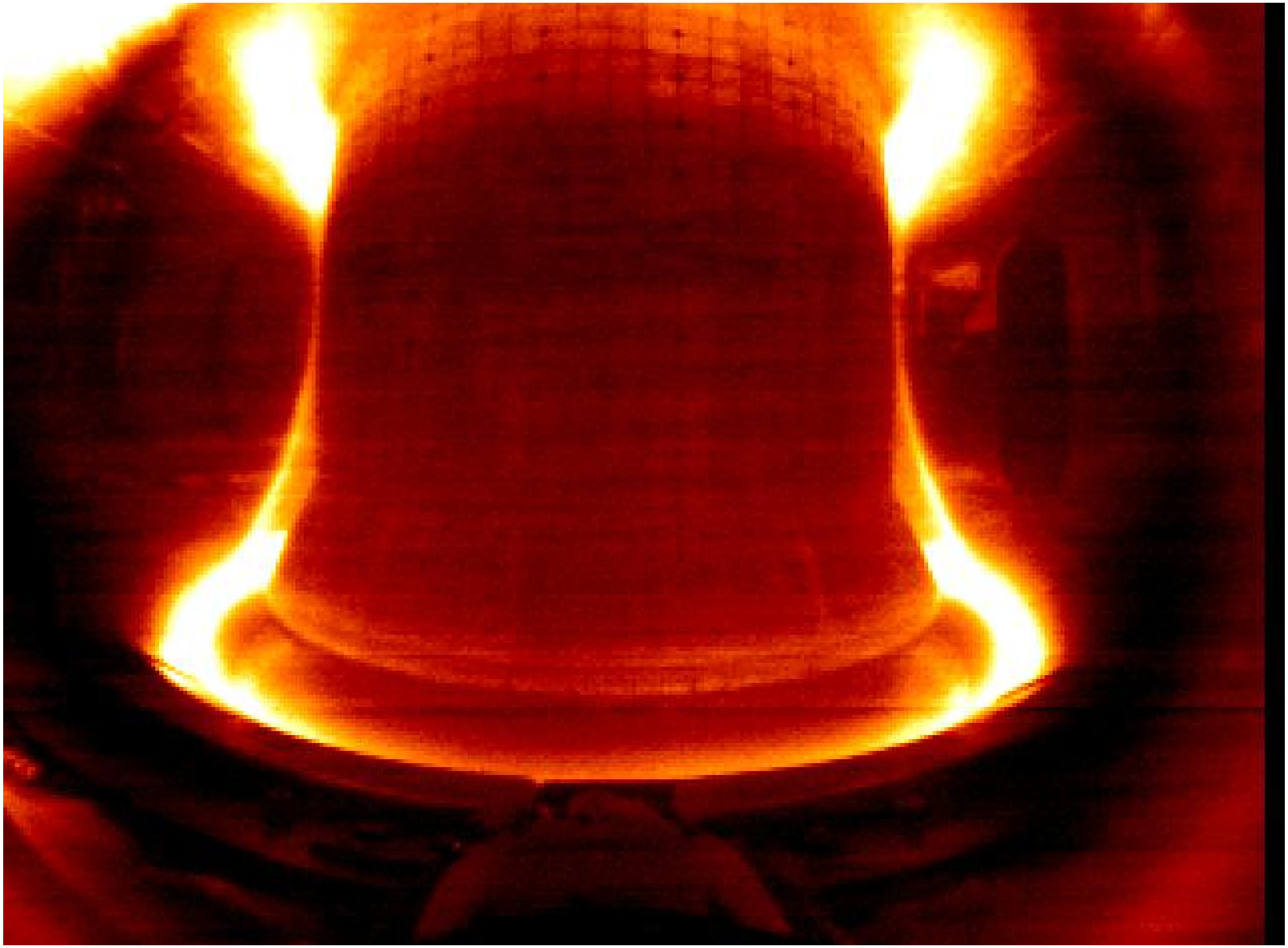
(inv. Knudsen number)

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

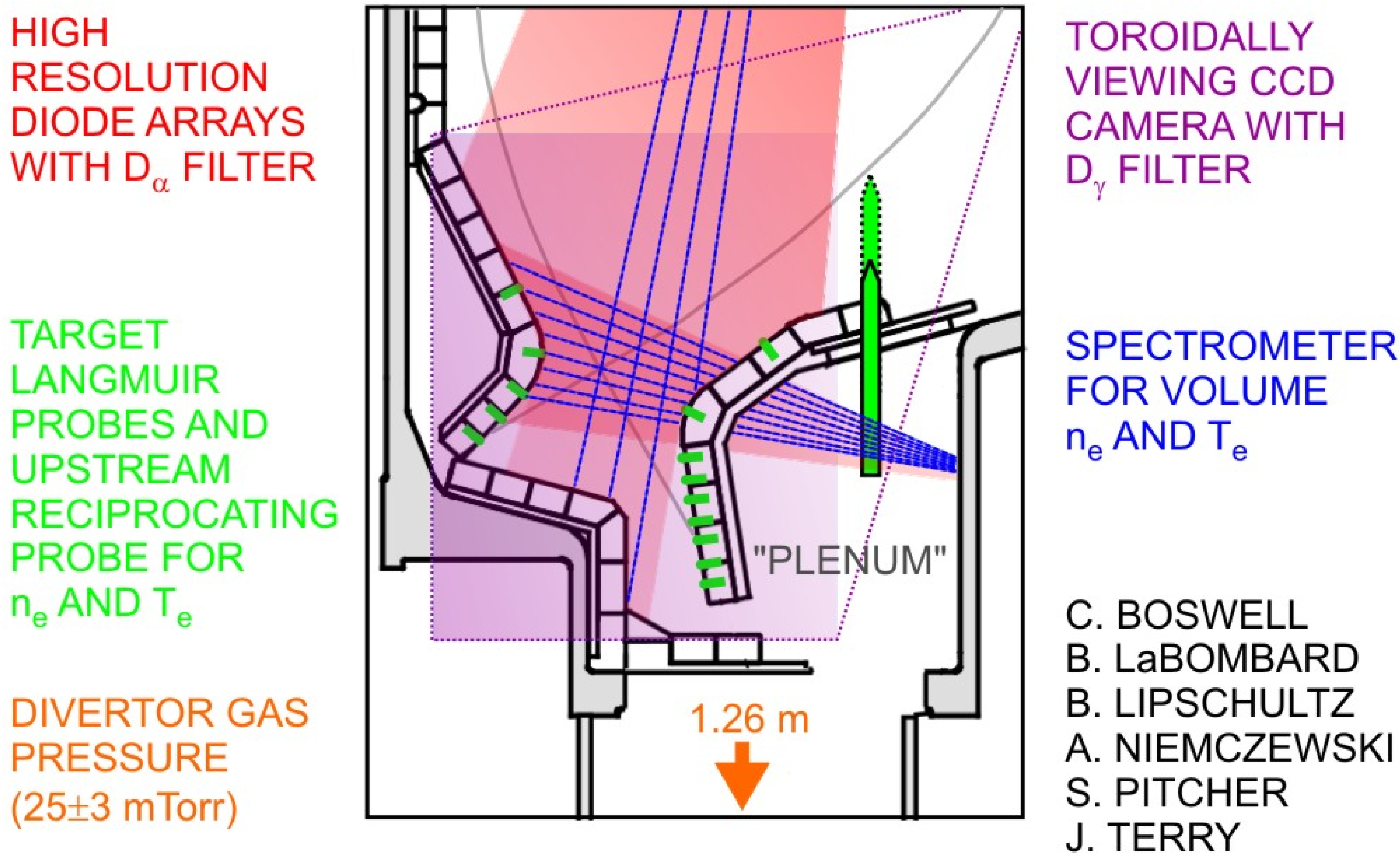
Alcator C-Mod (MIT)
10 times smaller than ITER
similar shape
higher density



Alcator C-Mod (MIT)



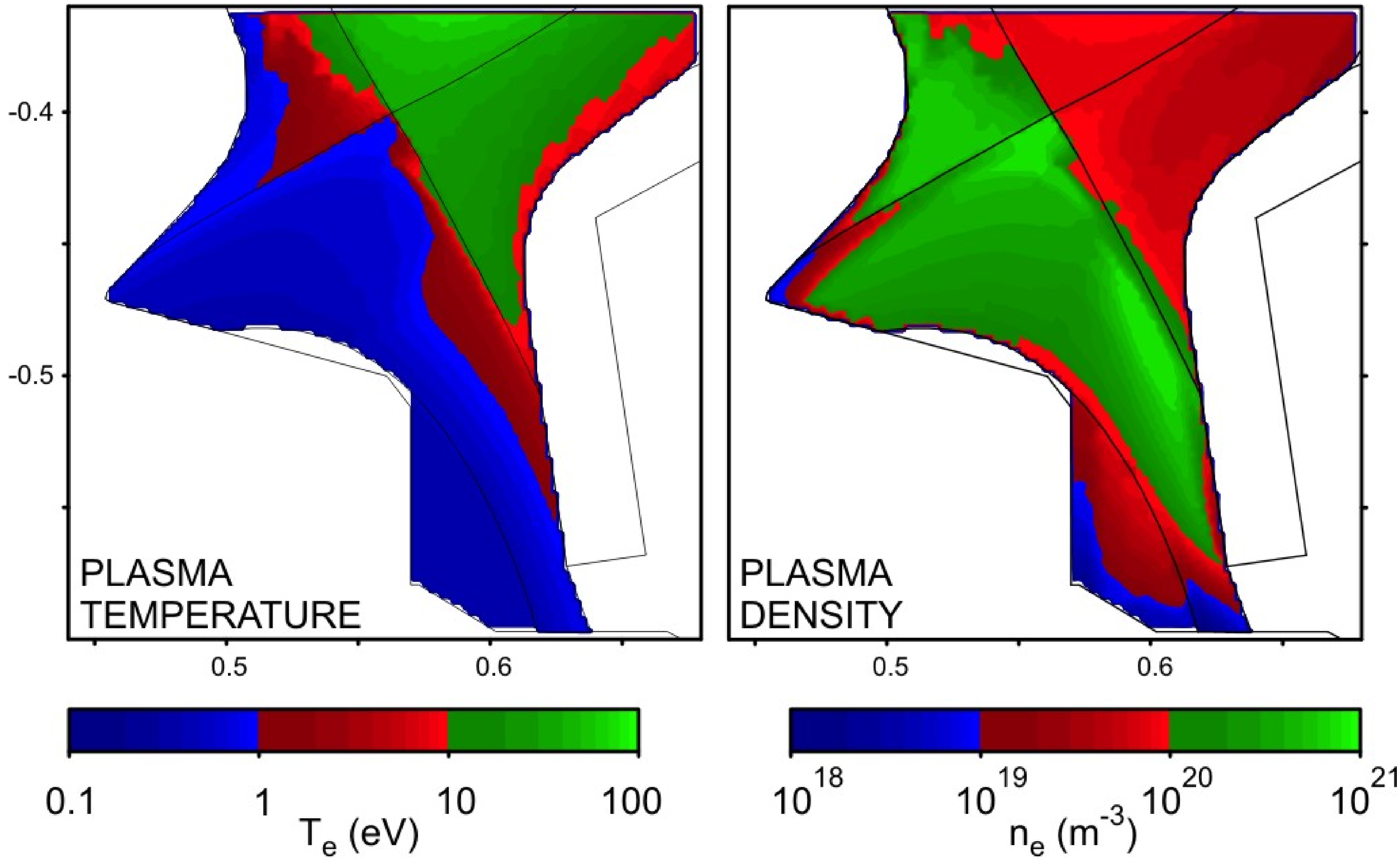
Predictive quality regarding „divertor chemistry“ ???
Separate plasma transport by replacing plasma transport modelling with OSM reconstruction

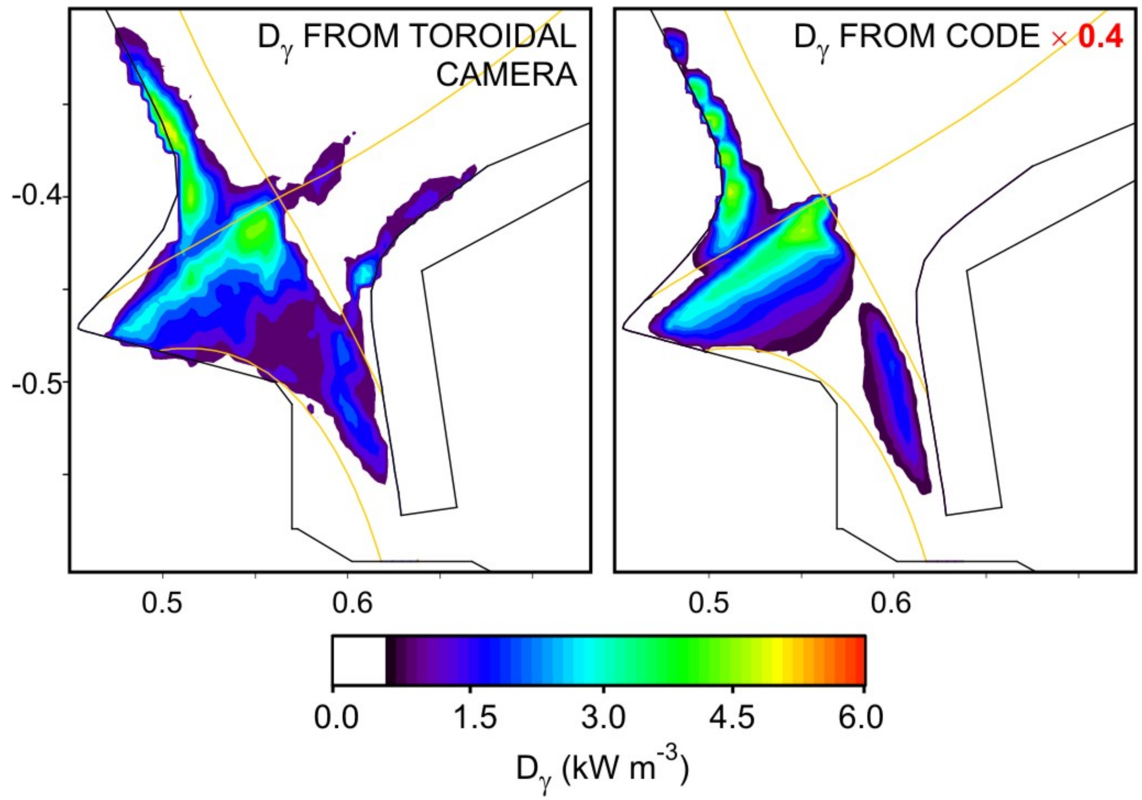


Shot: 990429019, at 950ms,

$\langle n_e \rangle = 1.5\ 10^{20}$, $I_P = 0.8$ MA, $B_{tor} = 5.4$ T

OSM reconstruction (Lisgo et al., 2004)





D_γ (from D, D_2, D^+,D_2^+):

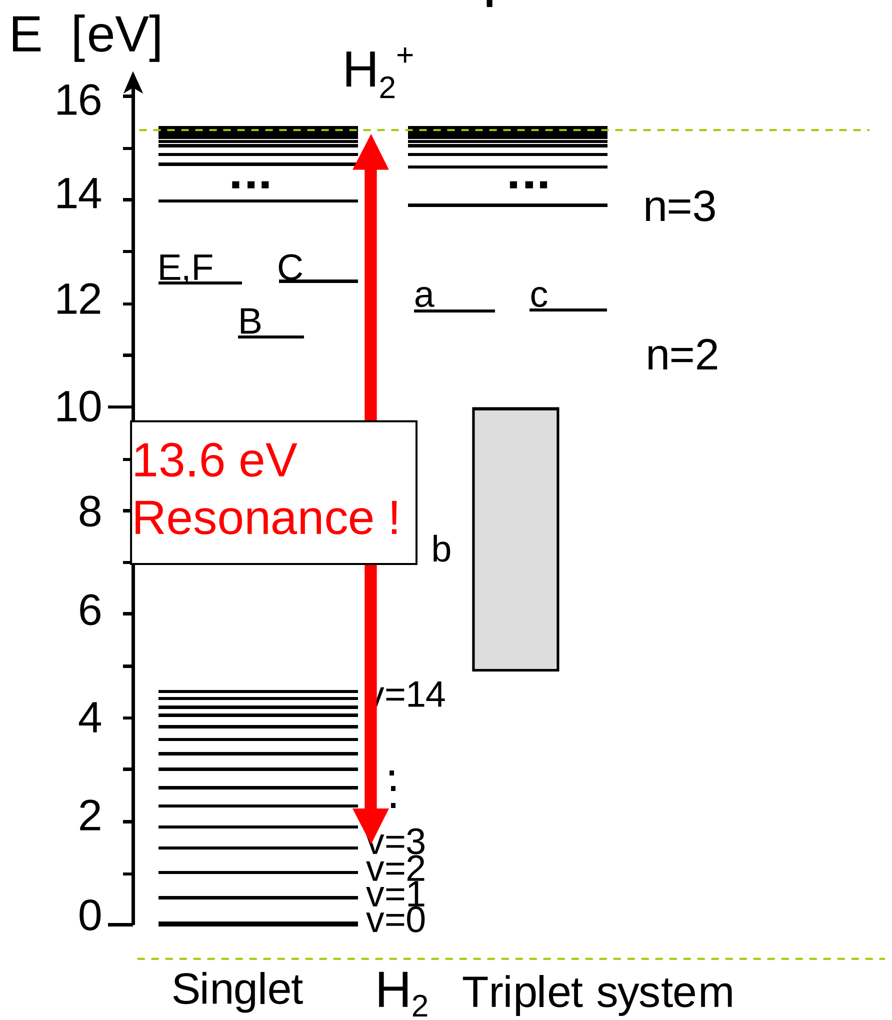
Profile matched, but high by factor 2

Calibration? Atomic Data? Plasma reconstruction?

Results very sensitive eg. to T_e profile

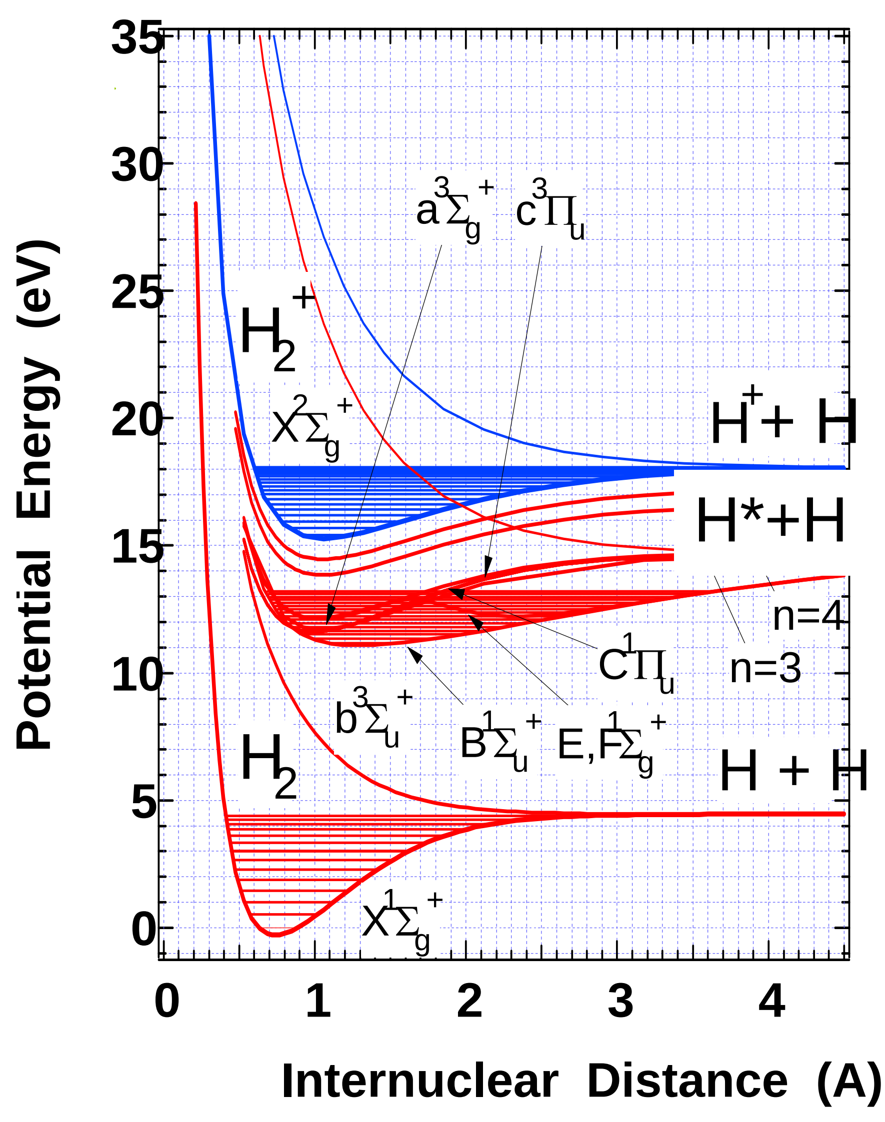
H_2 molecule, status in present divertor code

compiled 1997



More complete models available, still need to be integrated

compiled 2005

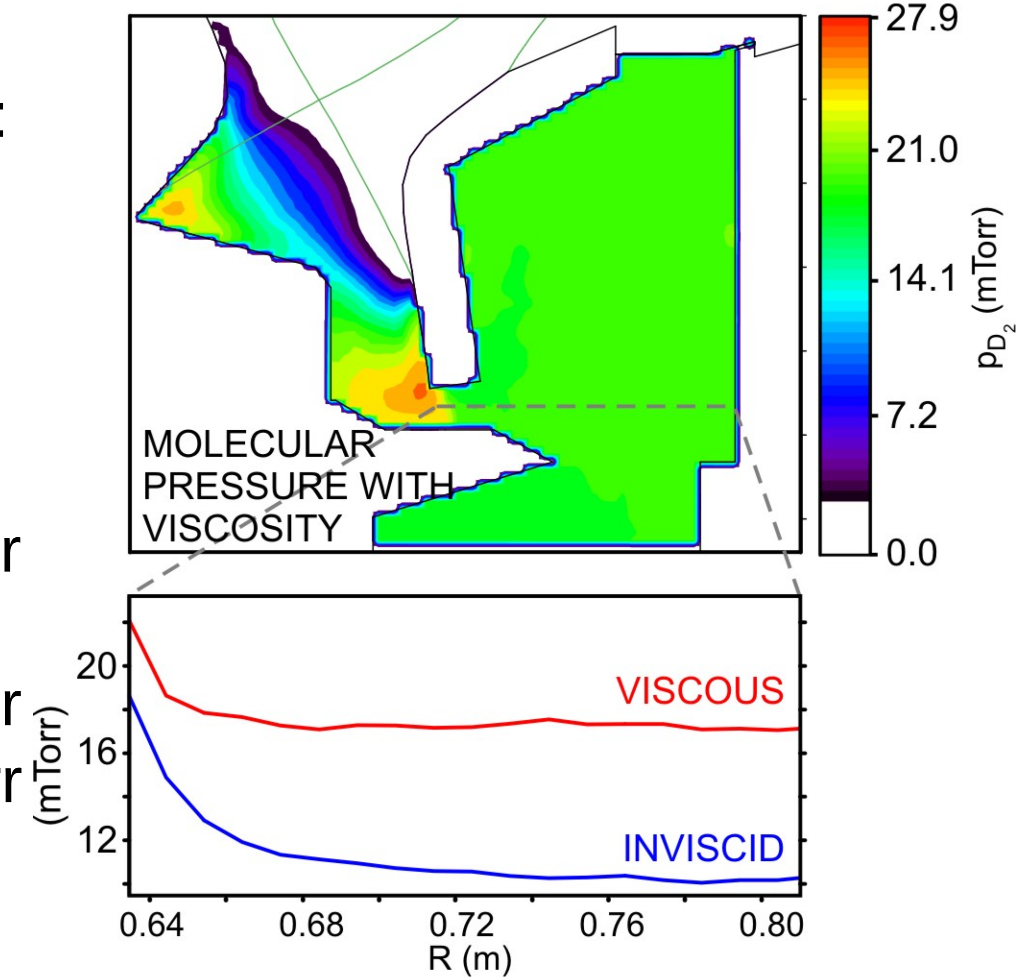


Critical for Particle Throughput (convection):

Neutral Plenum Pressure

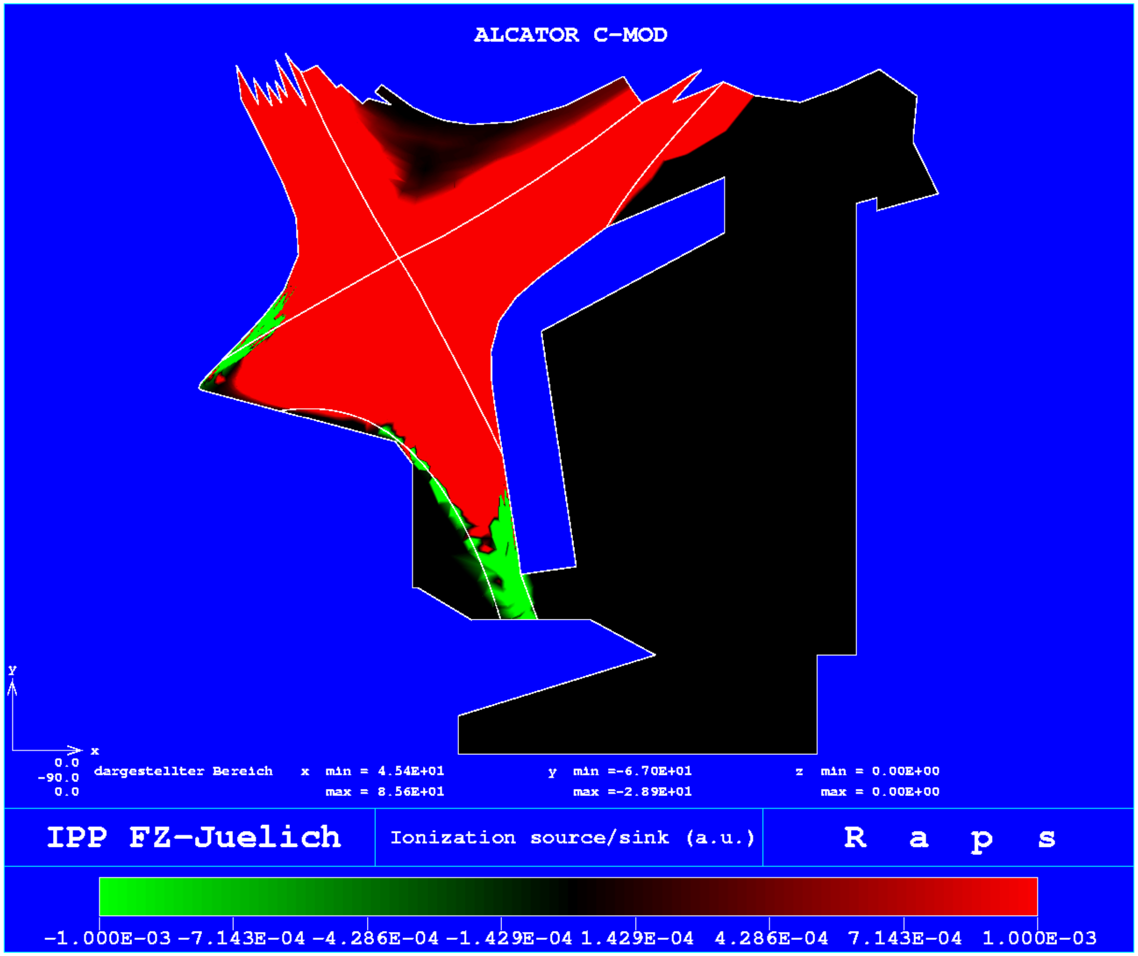
Experiment:	25 mTorr
Calc 2D (2000)	3 mTorr
Calc 2D (2003)	27 mTorr

(better A&M data,
better transport model,
better plasma data)



Good match to experiment in 2003, with full 2D kinetic detailed recycling model

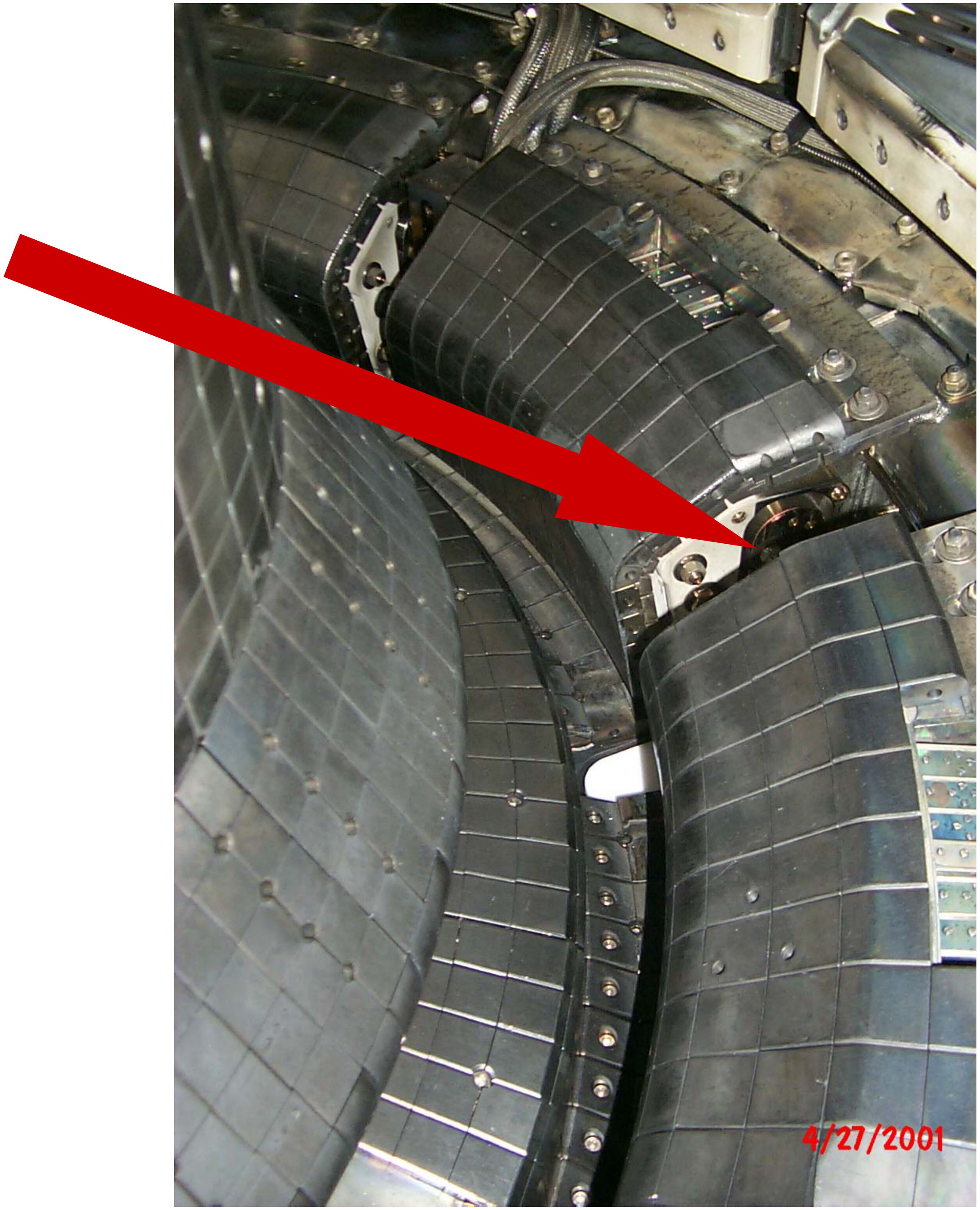
Ionizing area (red) , recombining area (green)



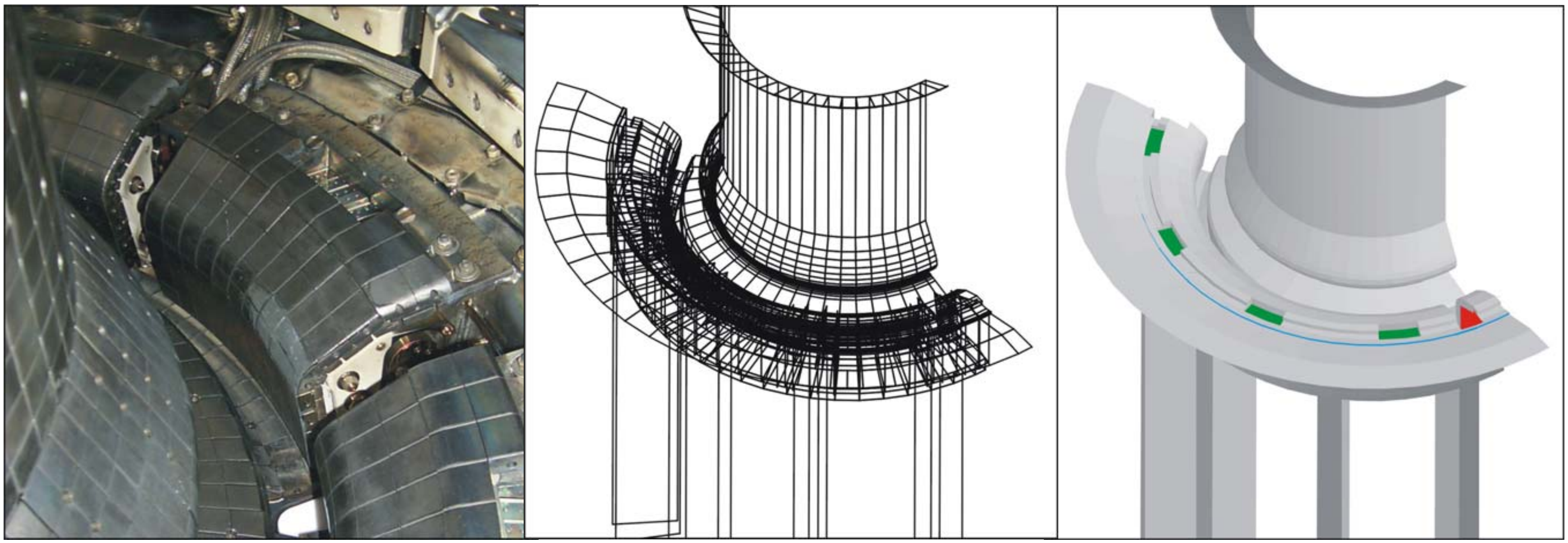
A quite cold edge plasma is sustained by recycling.
It “detaches” from the divertor targets (plasma pressure drop)

Additional
leakage pathways:

2D → 3D
(see later)



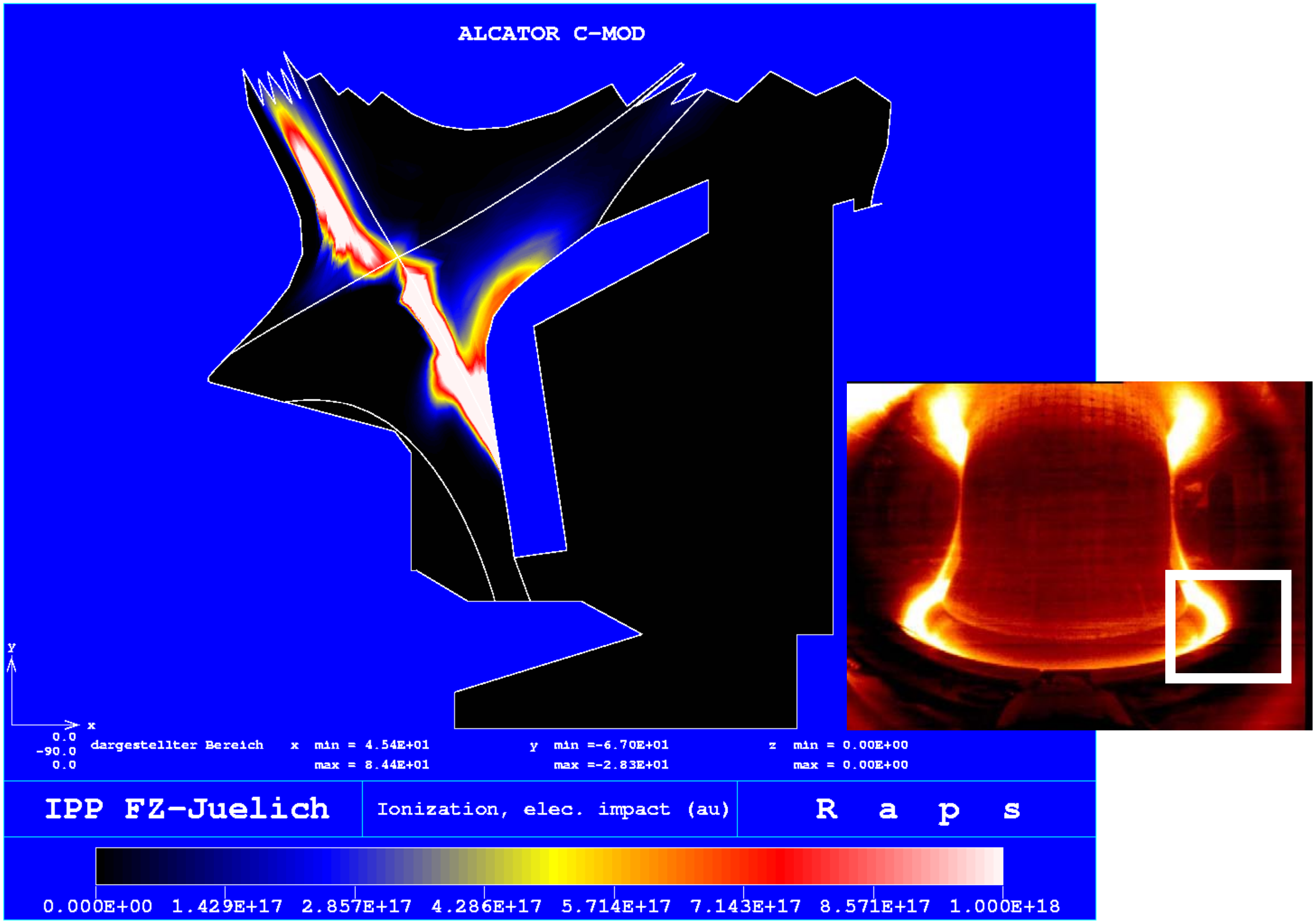
3D Neutral Gas, A&M and PSI Modelling



3D divertor structures (toroidal gap and gussets, bypass and poloidal gap)

→strong toroidal variations in the divertor neutral pressure

Ionization by electron impact on neutral gas

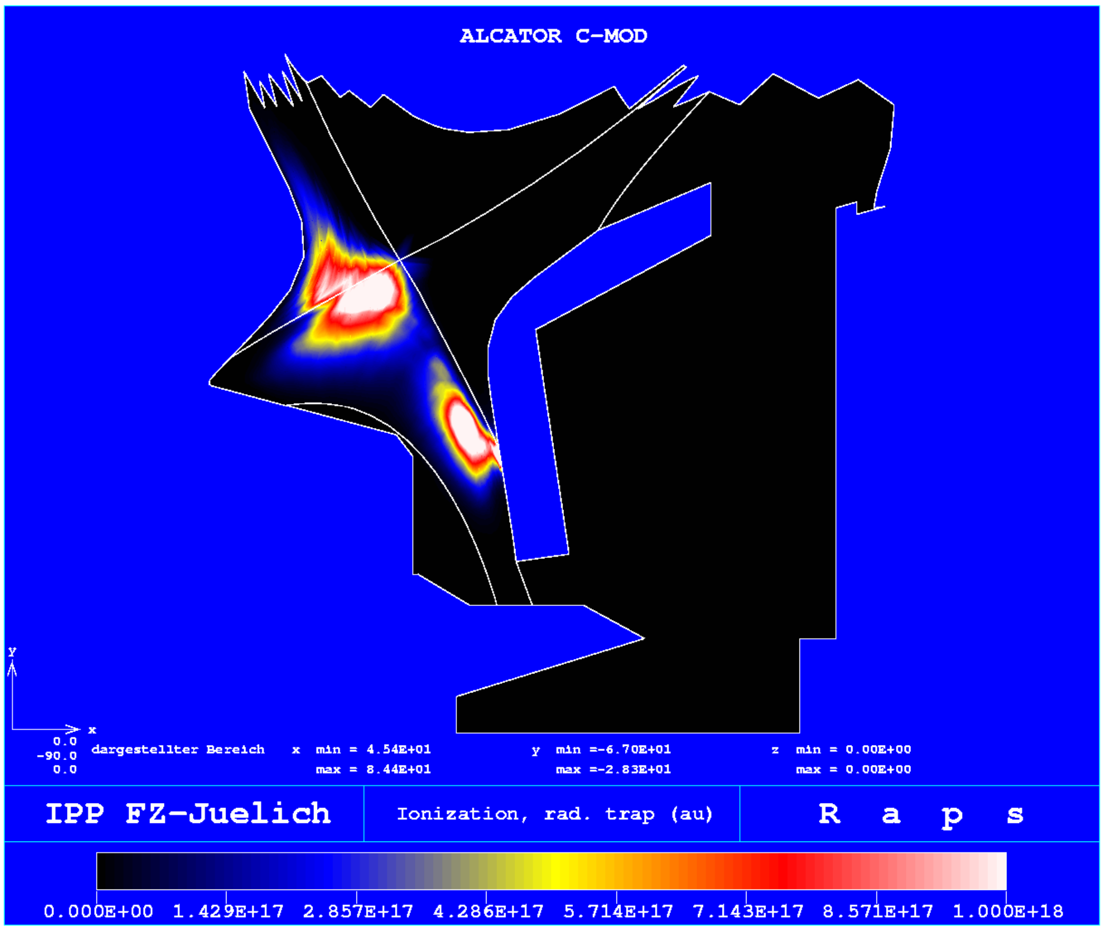


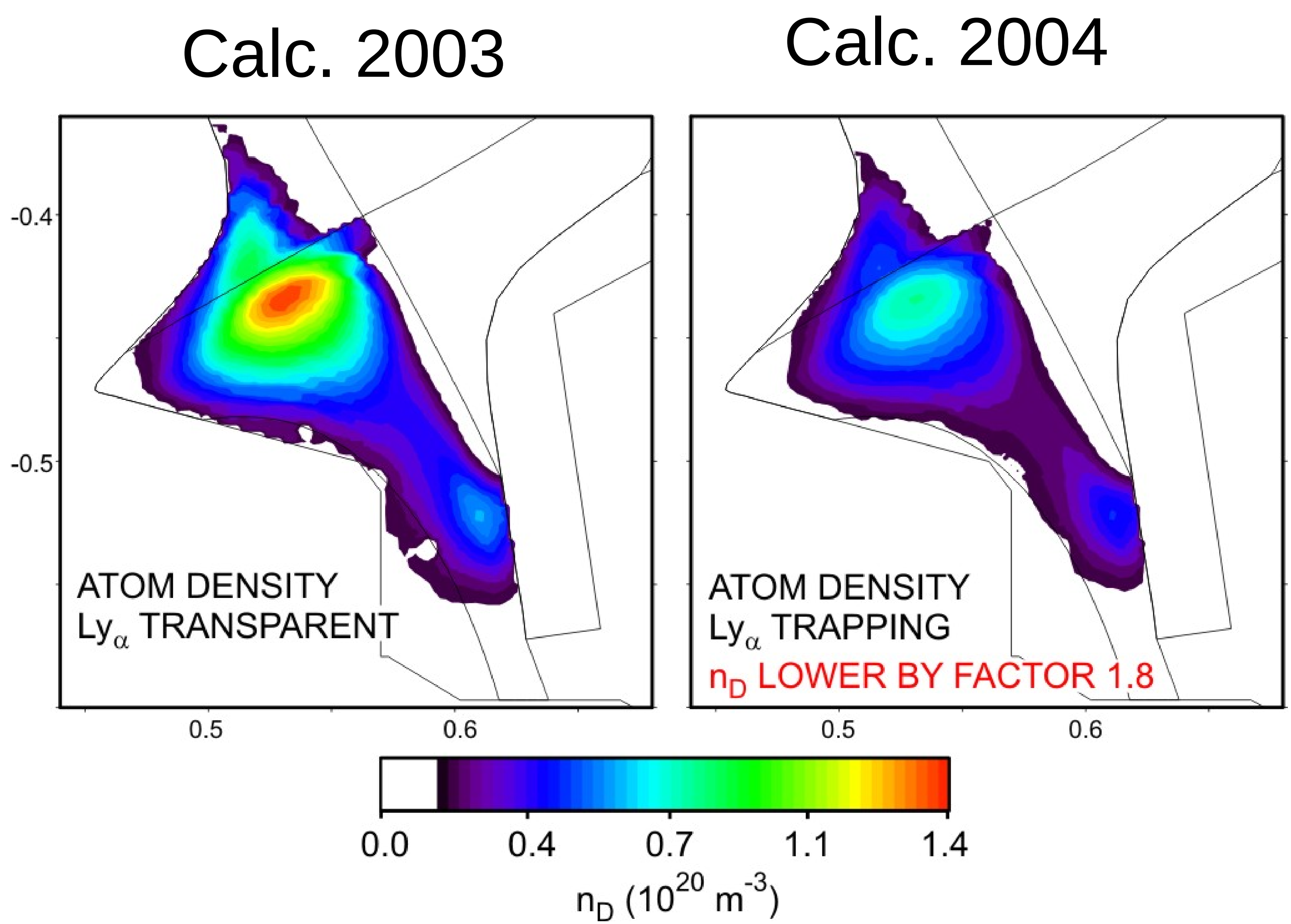
Radiation transfer: opacity of Ly-lines

(though completely elementary, has long remained unnoticed in divertor modelling)

$$h\nu + H(1) \rightarrow H^*, \quad H^* + e \rightarrow H^+ + 2e$$

(additional path for ionization in dense, low T_e divertors)

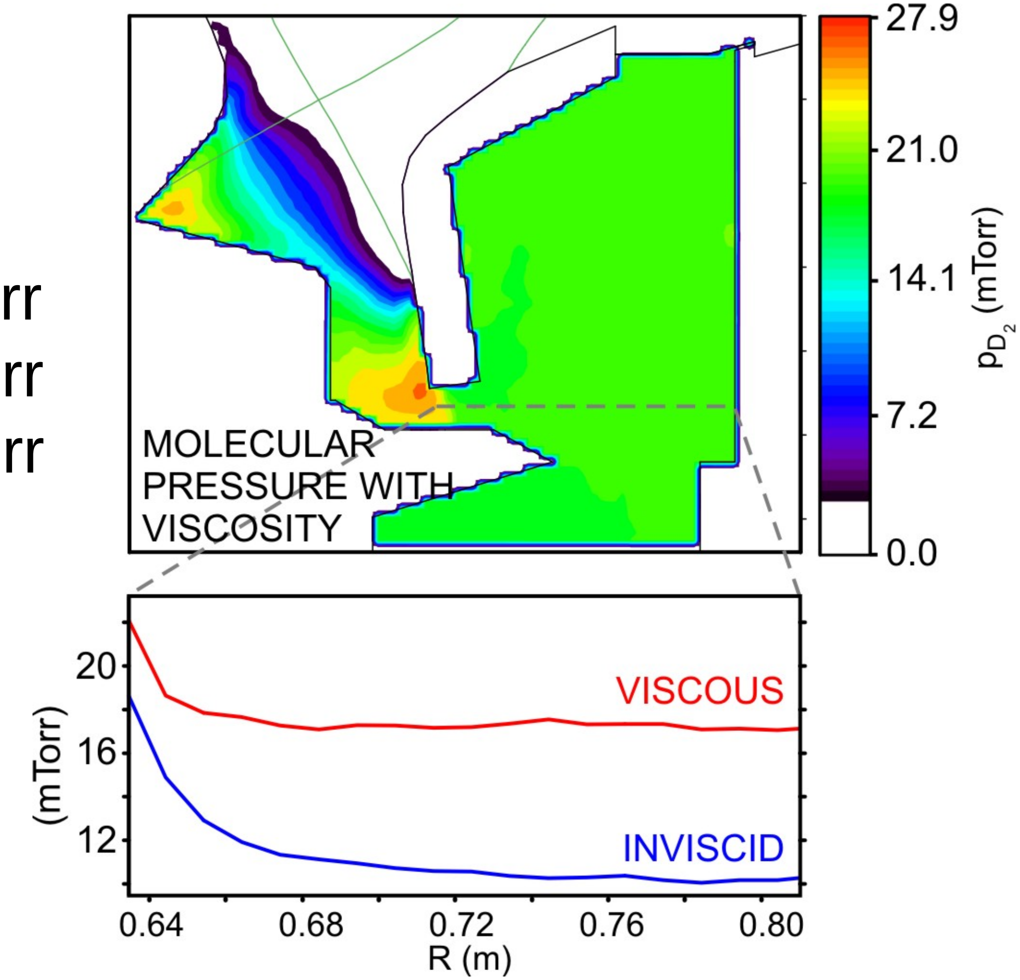



Calc. 2003
Calc. 2004
-0.4
-0.5
0.5
0.6
0.5
0.6
ATOM DENSITY
Lyα TRANSPARENT
ATOM DENSITY
Lyα TRAPPING
nD LOWER BY FACTOR 1.8
0.0
0.4
0.7
1.1
1.4
nD (10^20 m^-3)

Neutral Pressure

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

However
Ly-opacity: 17 mTorr
3D: 11 mTorr



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

Example 2:
Hydrogenic ionisation-recombination balance

The full database must contain a large number (~ several 100) of individual processes

Fortunately: very different timescales are involved (numerically stiff problem):
$\Rightarrow$ an underlying reduced model exists.

This is often referred to as:
Collisional radiative models (Astrophysics)
Multistep ionisation and recombination models (Plasma physics)
Condensed case approximations (Semiconductor physics)
Lumped species concepts (Atmospheric research)
Intrinsic low dimensional manifolds (combustion flames)

Atomic and Molecular Database for EIRENE:
see: www.eirene.de/htmlseiten/amjuel/

ionisation – recombination – transport balance: atoms

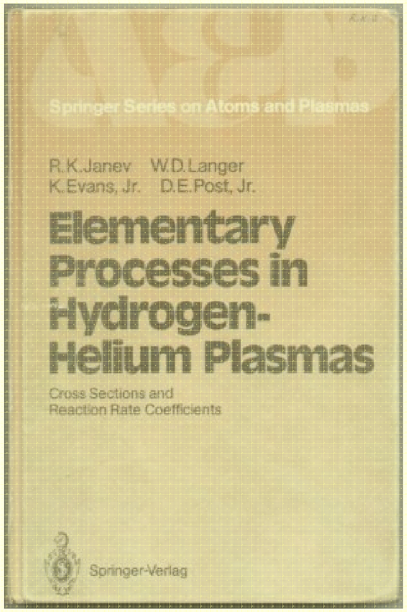
multi	direct	Path	Comment	File
gscr		e + H(n=1) $\rightarrow$ H^+	via H^*	fort.10 (sum)
gscr2		e + H(n=2) $\rightarrow$ H^+	via H^*	fort.101 (sum)
gscr21		e + H(n=2) $\rightarrow$ H(n=1)	via H^*	fort.102 (sum)
gscr12		e + H(n=1) $\rightarrow$ H(n=2)	via H^*	fort.103 (sum)
	bel	e + H^+ $\rightarrow$ H(n=1)	rad.rec (2.1.8)	fort.11.1
alcr-bel		e + H^+ $\rightarrow$ H(n=1)	via H^*	fort.11.2
alcr		e + H^+ $\rightarrow$ H(n=1)		fort.11.3 (sum)
alcr2		e + H^+ $\rightarrow$ H(n=2)		fort.111 (sum)

conventional multistep model

Extensions for Lyman-α radiation transfer (photoexcitation)

Extension for (future) photoionisation simulations

ionisation – recombination - transport : molecules



+

Sawada/ Fujimoto CR-Model

multi	direct	Path	Comment	File
	bq1	e + $H_2 \rightarrow H_2^+$	direct (2.2.9)	–
gscrh2		e + $H_2 \rightarrow H_2^+$	via H_2^*	fort.12 (sum)
	bq7	p + $H_2 \rightarrow H_2^+ + H$	from H_2(v=0)	
	bq8	p + $H_2 \rightarrow H_2^+ + H$	from H_2(v≥1)	
	bq6	e + $H_2 \rightarrow H + H^-$	from H_2(v=0)	
	bq5	e + $H_2 \rightarrow H + H^-$	from H_2(v≥1)	
	bq2	e + $H_2 \rightarrow$ p + H(n=1)	direkt (2.2.10)	
gs2c		e + $H_2 \rightarrow$ p + H(n=1)	via $H_2 \rightarrow H + H^*$	
missing		e + $H_2 \rightarrow$ p + H(n=1)	via $H_2^* \rightarrow$ p + H	
missing		e + $H_2 \rightarrow$ p + H(n=1)	via $H_2^* \rightarrow H + H^*$	
total		e + $H_2 \rightarrow$ p + H(n=1)		fort.14 (sum)
—	—	e + $H_2 \rightarrow$ p + H(n=2)	above H_2^+	—
	h1s (bq4?)	e + $H_2 \rightarrow H + H$(n=1)	direkt (2.2.5)	
gs2d		e + $H_2 \rightarrow H + H$(n=1)	via $H_2 \rightarrow H + H^*$	
h2r1		e + $H_2 \rightarrow H + H$(n=1)	via $H_2^* \rightarrow H + H$	
missing		e + $H_2 \rightarrow H + H$(n=1)	via $H_2^* \rightarrow H + H^*$	
total		e + $H_2 \rightarrow H + H$(n=1)		fort.13 (sum)
	h2s	e + $H_2 \rightarrow H + H$(n=2)	direkt	
missing		e + $H_2 \rightarrow H + H$(n=2)	via $H_2^* \rightarrow H + H$(n=2)	
gs2e		e + $H_2 \rightarrow H + H$(n=2)	via $H_2 \rightarrow H + H^*$	
missing		e + $H_2 \rightarrow H + H$(n=2)	via $H_2^* \rightarrow H + H^*$	
total		e + $H_2 \rightarrow H + H$(n=2)		fort.131 (sum)
	tq3	e + $H_2^+ \rightarrow$ p + p	direkt (2.2.11)	
gstq1		e + $H_2^+ \rightarrow$ p + p	via p + H^*	fort.16 (sum)
	bq3	e + $H_2^+ \rightarrow$ p + H(n=1)	direkt (2.2.12)	
gstq2		e + $H_2^+ \rightarrow$ p + H(n=1)	via $H + H^*$	fort.15.1
gstq1m		e + $H_2^+ \rightarrow$ p + H(n=1)	via p + H^*	fort.15.2
total		e + $H_2^+ \rightarrow$ p + H(n=1)		fort.15.3
	h3s	e + $H_2^+ \rightarrow$ p + H(n=2)	direkt	
gstq1mm		e + $H_2^+ \rightarrow$ p + H(n=2)	via p + H^*	fort.151 (sum)
	—	e + $H_2^+ \rightarrow H + H$(n=1)	direkt: not possible	
gstq2m		e + $H_2^+ \rightarrow H + H$(n=1)	via $H + H^*$ (2.2.14)	fort.17
	h4s	e + $H_2^+ \rightarrow H + H$(n=2)	direkt	
gstq2mm		e + $H_2^+ \rightarrow H + H$(n=2)	via $H + H^*$ (2.2.14)	fort.171
	bq9	e + $H^- \rightarrow H$ + 2e	direkt, (7.1.1)	
missing		p + $H^- \rightarrow$ p + H	direkt (7.2.1)	
gstq3		p + $H^- \rightarrow$ p + H	via $H + H^*$	
missing		p + $H^- \rightarrow H + H$(n=1)	direkt	
gstq3m		p + $H^- \rightarrow H + H$(n=1)	via $H + H^*$	
	h5s	p + $H^- \rightarrow H + H$(n=2)	direkt (7.2.2)	
gstq3mm		p + $H^- \rightarrow H + H$(n=2)	via $H + H^*$	

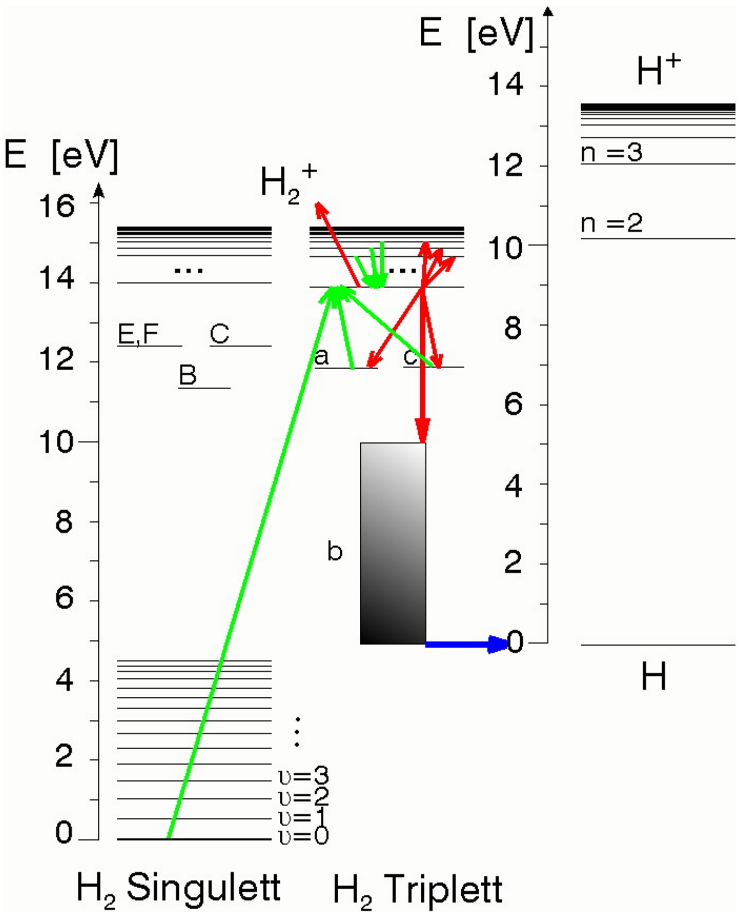
(MAR_1)

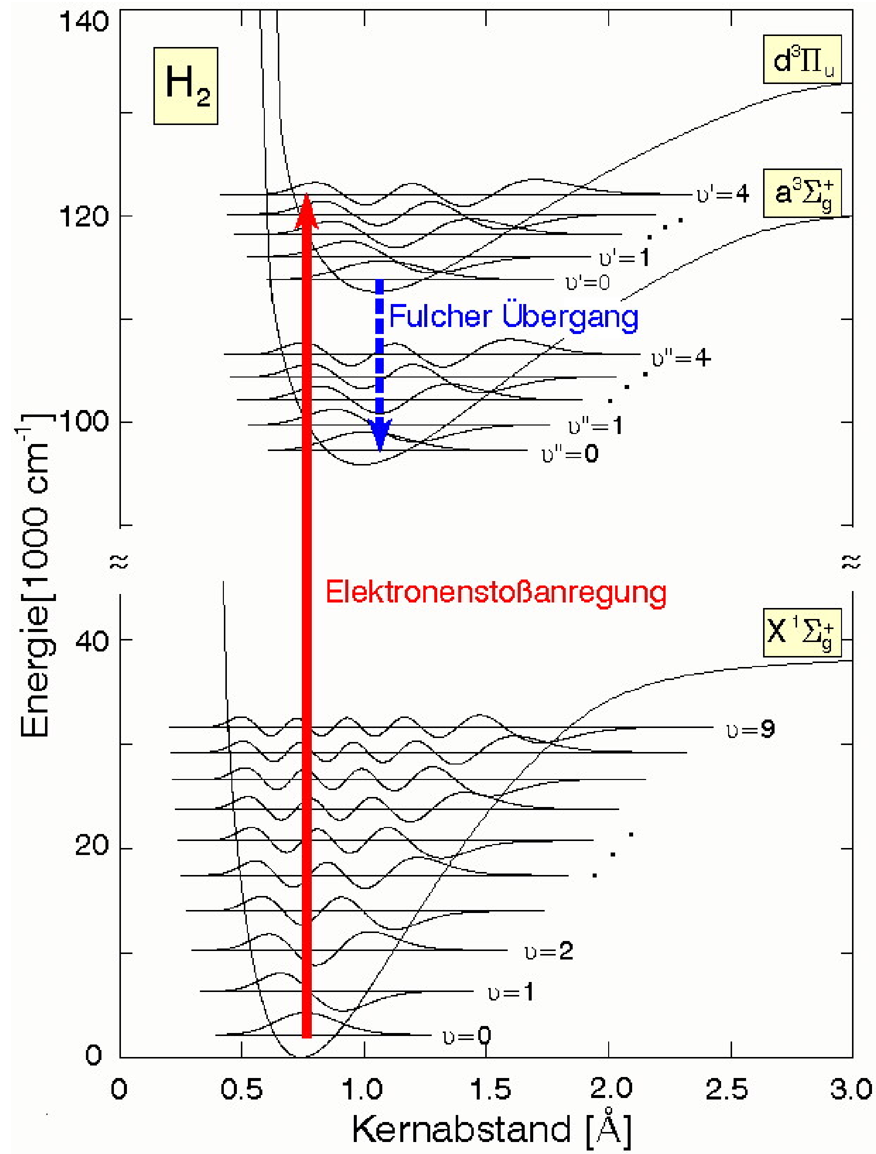
(MAD_2)

(MAR_2)

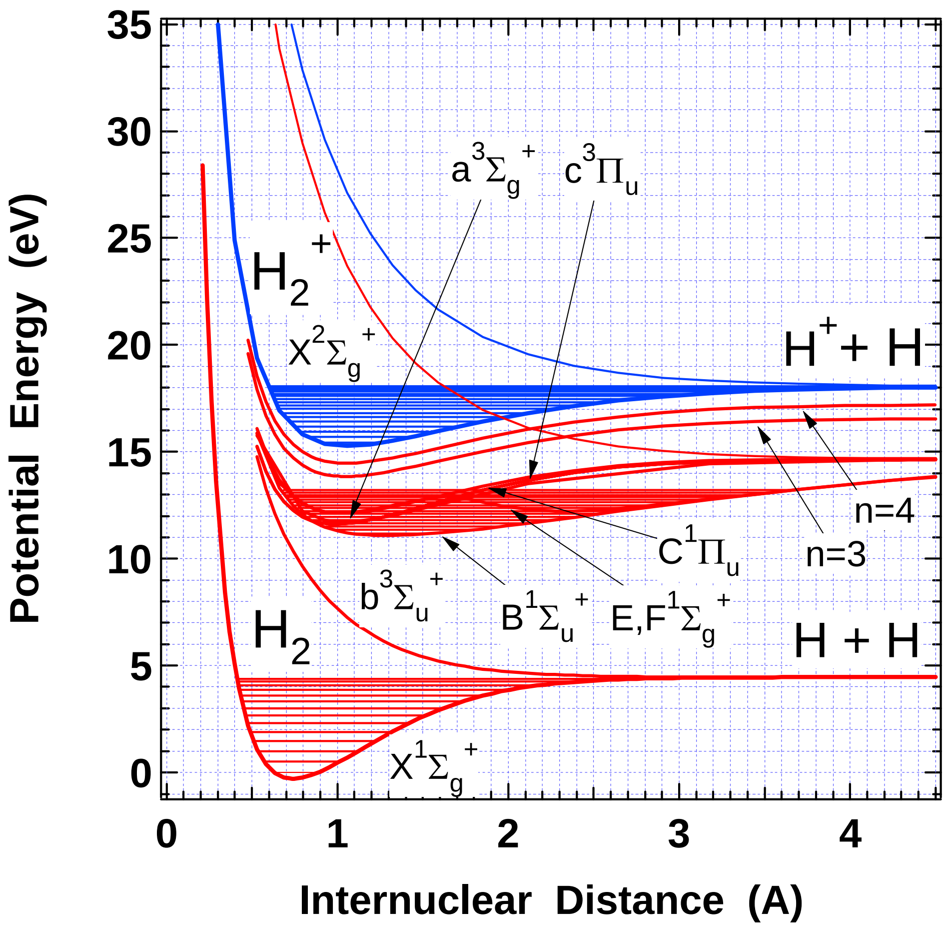
Molecule spectroscopy (late nineties): identification of important role of molecule reaction kinetics on overall Divertor dynamics

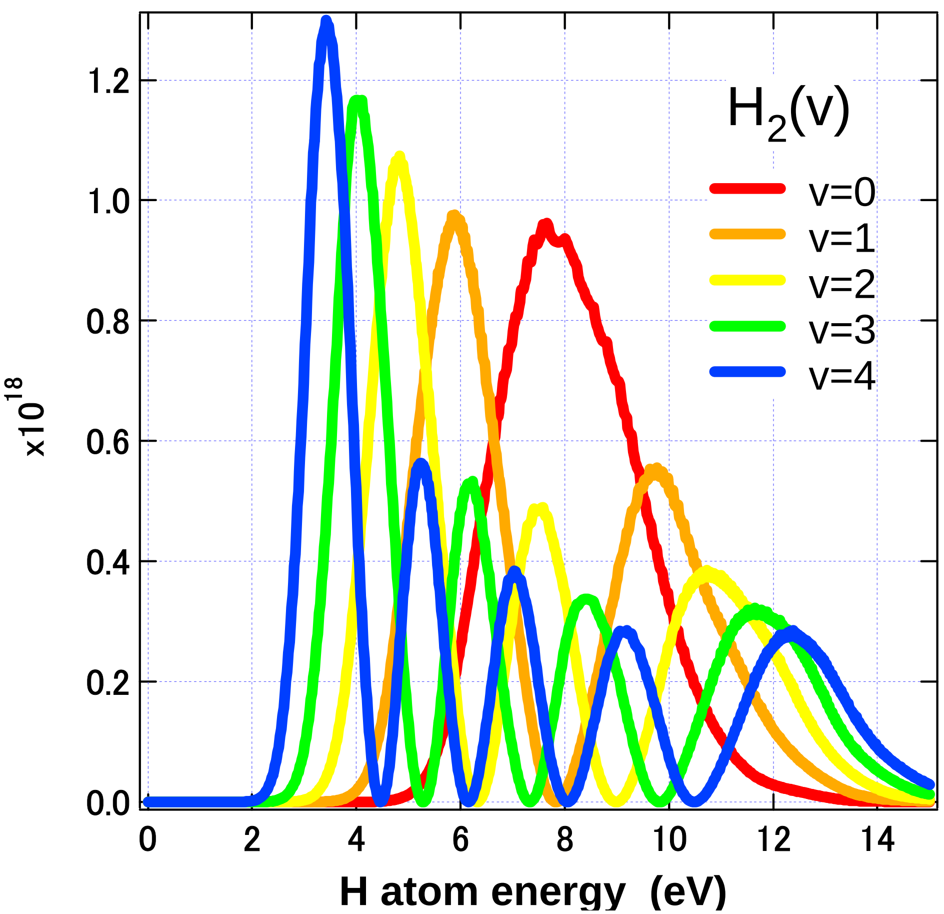
U. Fantz et al.



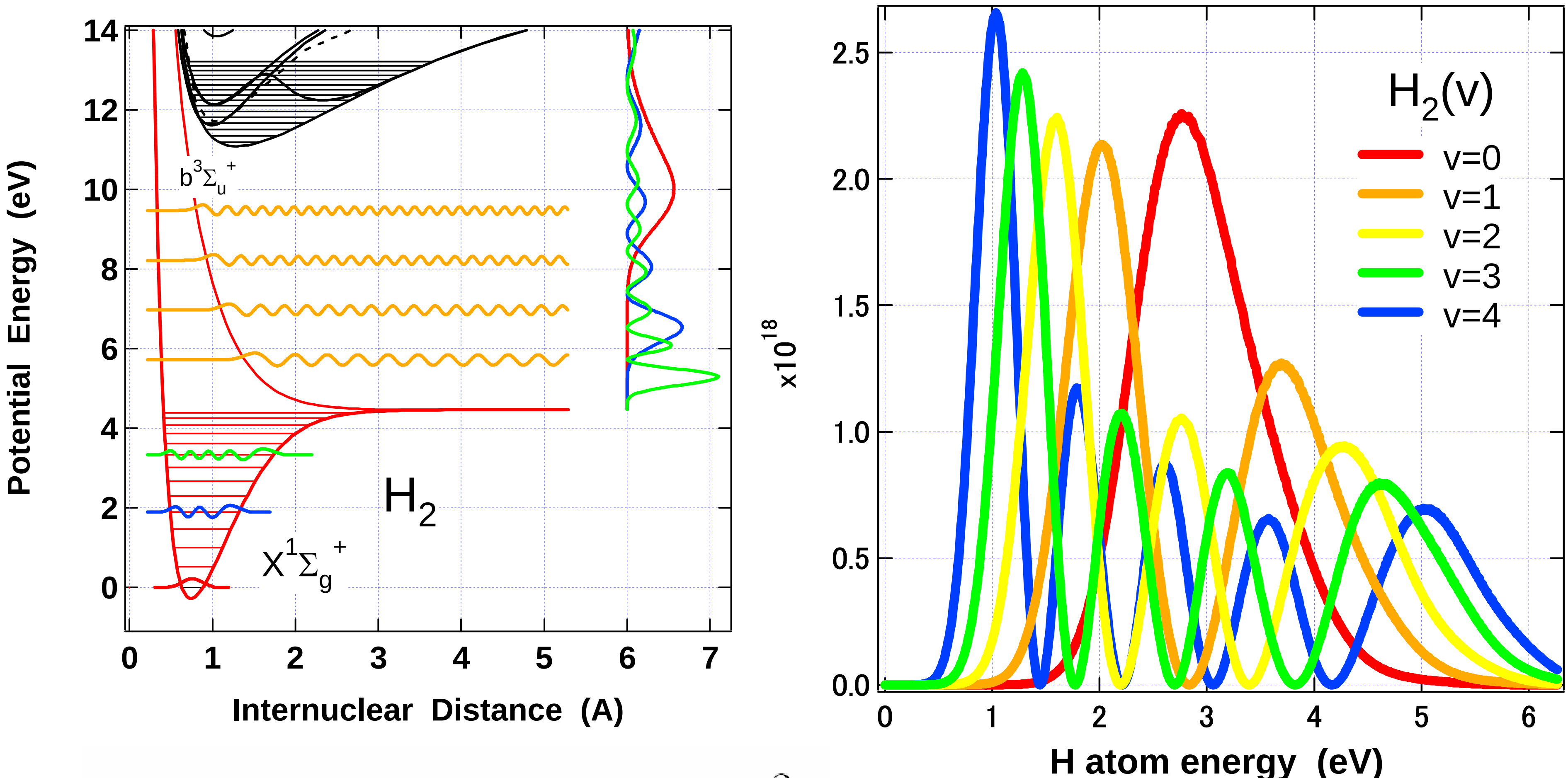


$H_2(X)$ -> H_2^+(repulsive) -> H + H^+
$H_2(X)$ -> H_2^*(repulsive) -> H + H^*





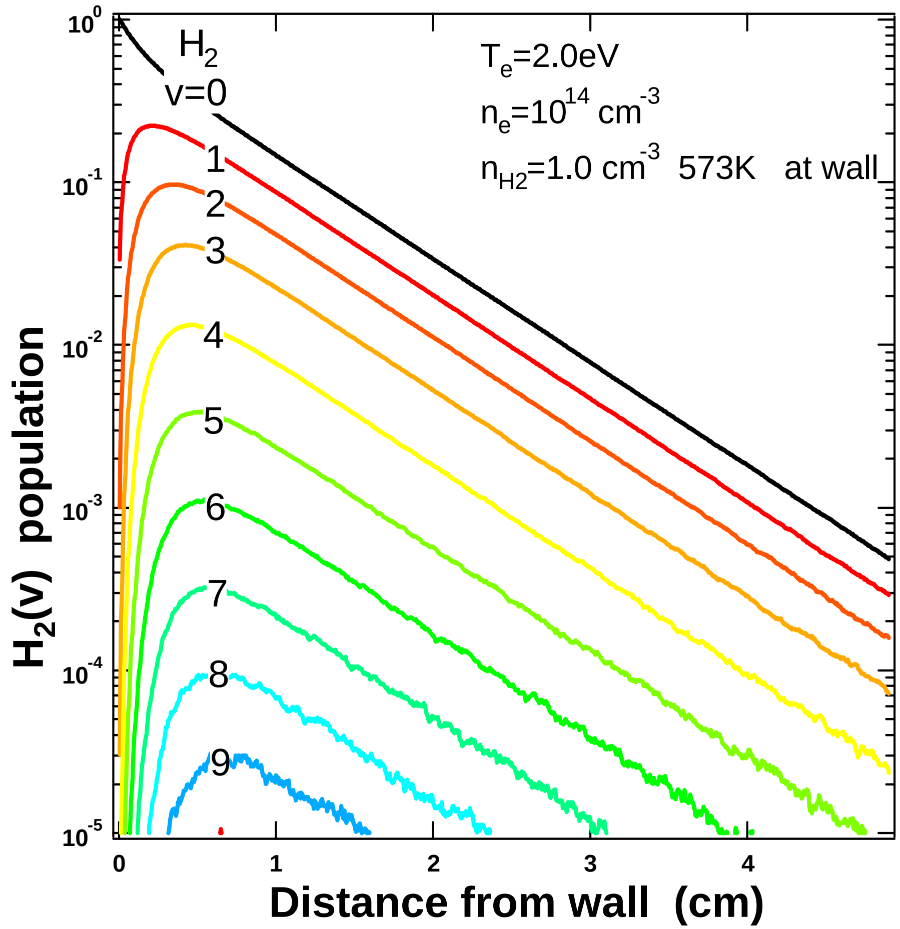
Calculation of H atom velocity
$H_2(X) \rightarrow H_2(b) \rightarrow H + H$



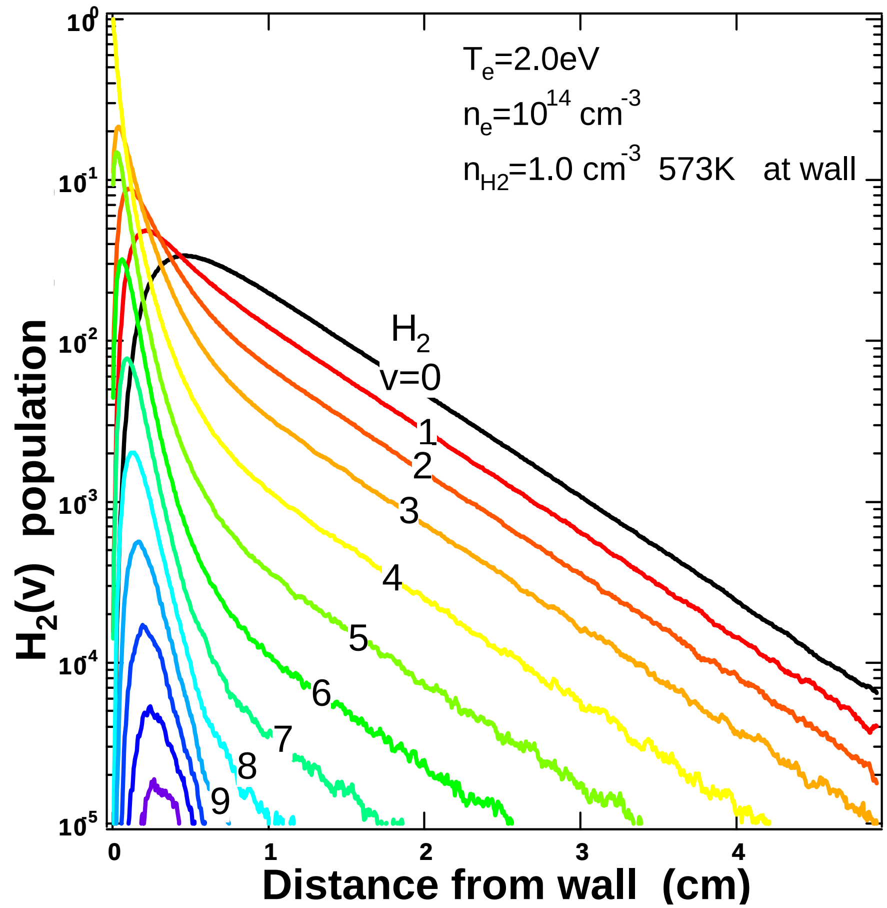
$$q_{\kappa v} = \left| \int \chi_{\kappa}^{b}(R) \chi_{v}^{X}(R) dR \right|^2$$

Sensitivity to surface produced vibr. excitation

1-D Monte-Carlo Model of Neutral-Particle Transport (K. Sawada)

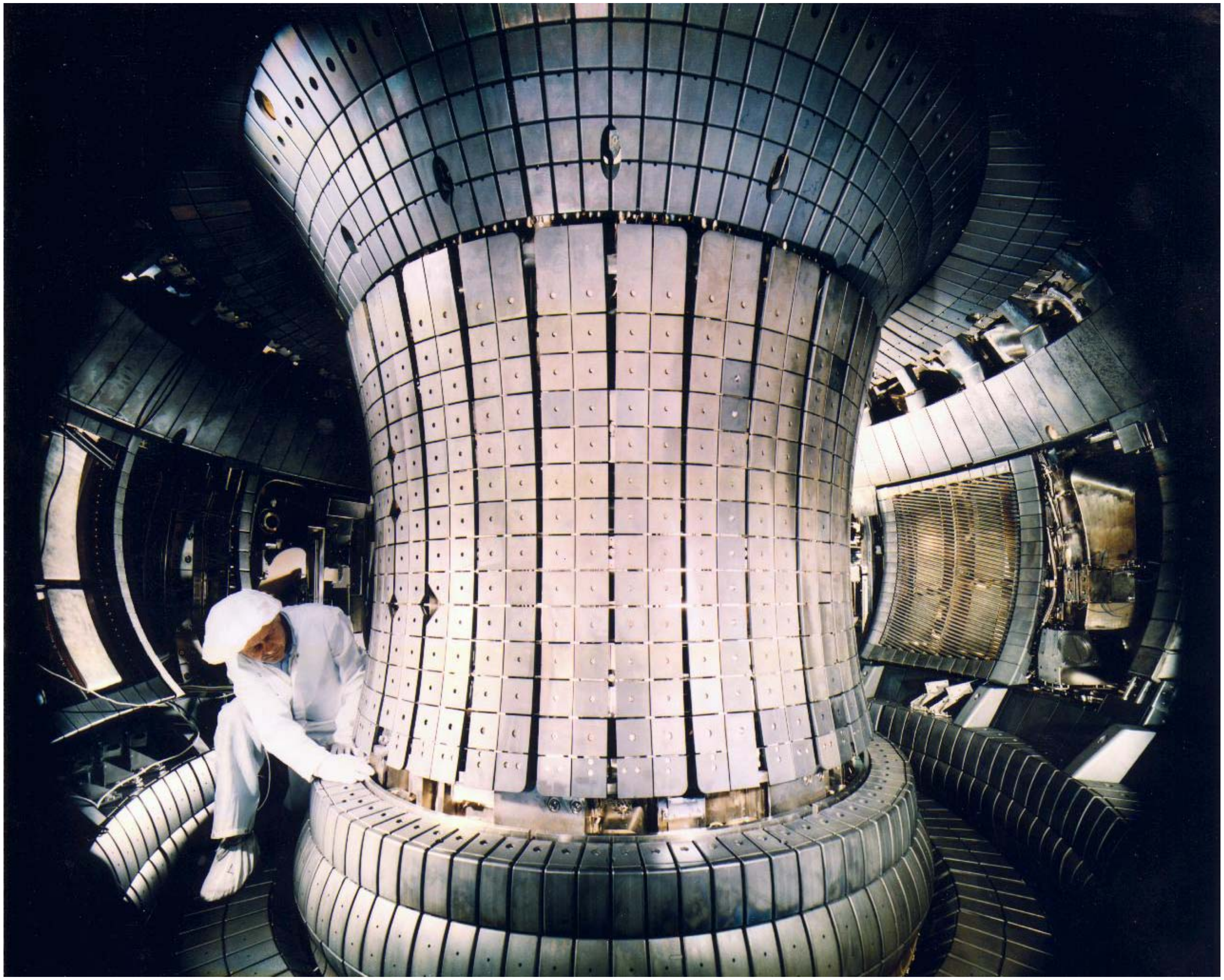


All H_2 from wall: v=0

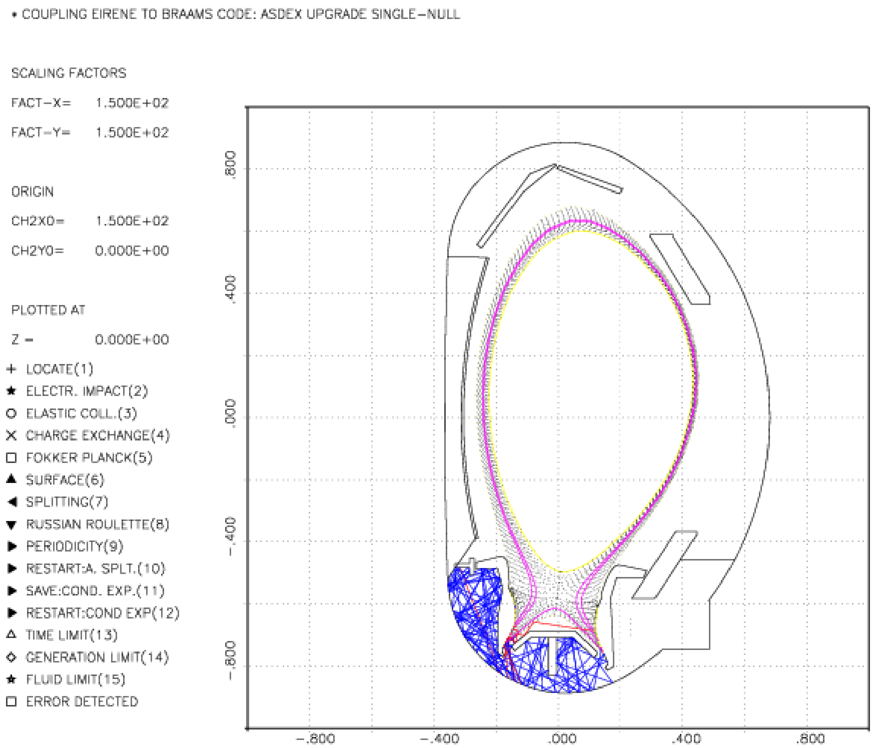


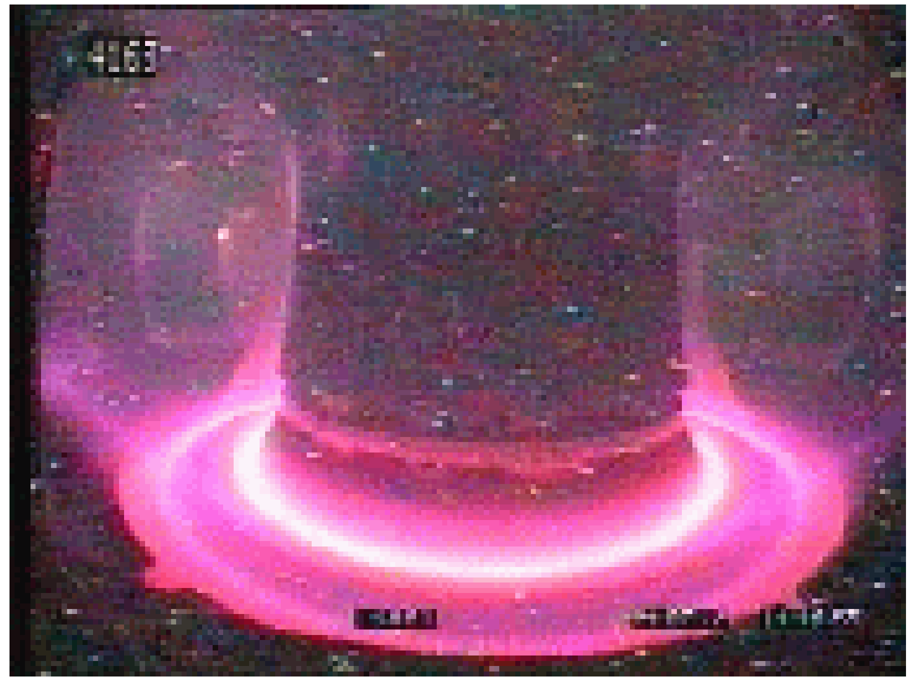
All H_2 from wall: v=4

ASDEX-UPDRADE (IPP Garching)



Trapping of neutral particles in the Divertor: high recycling and detachment regime

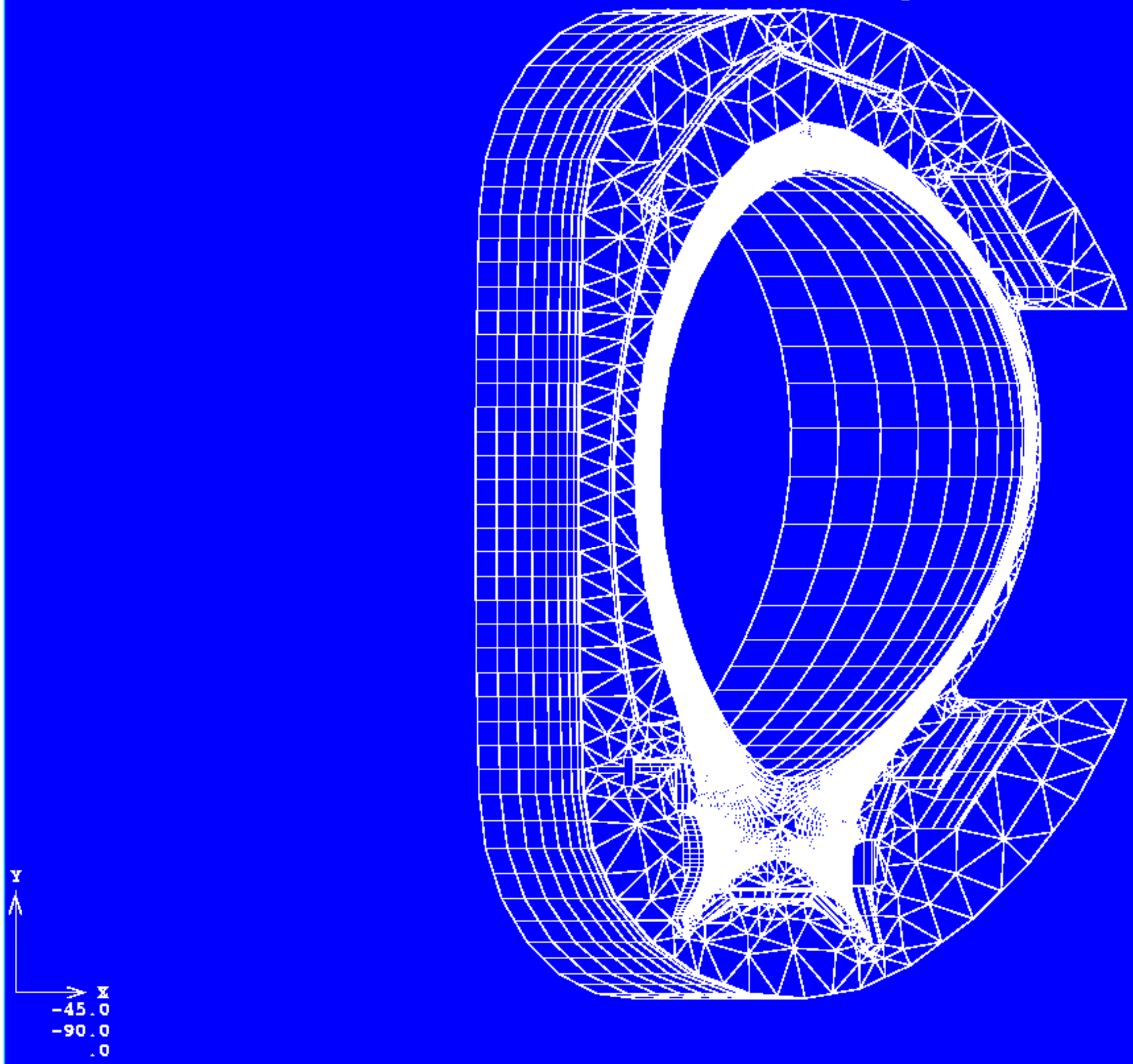




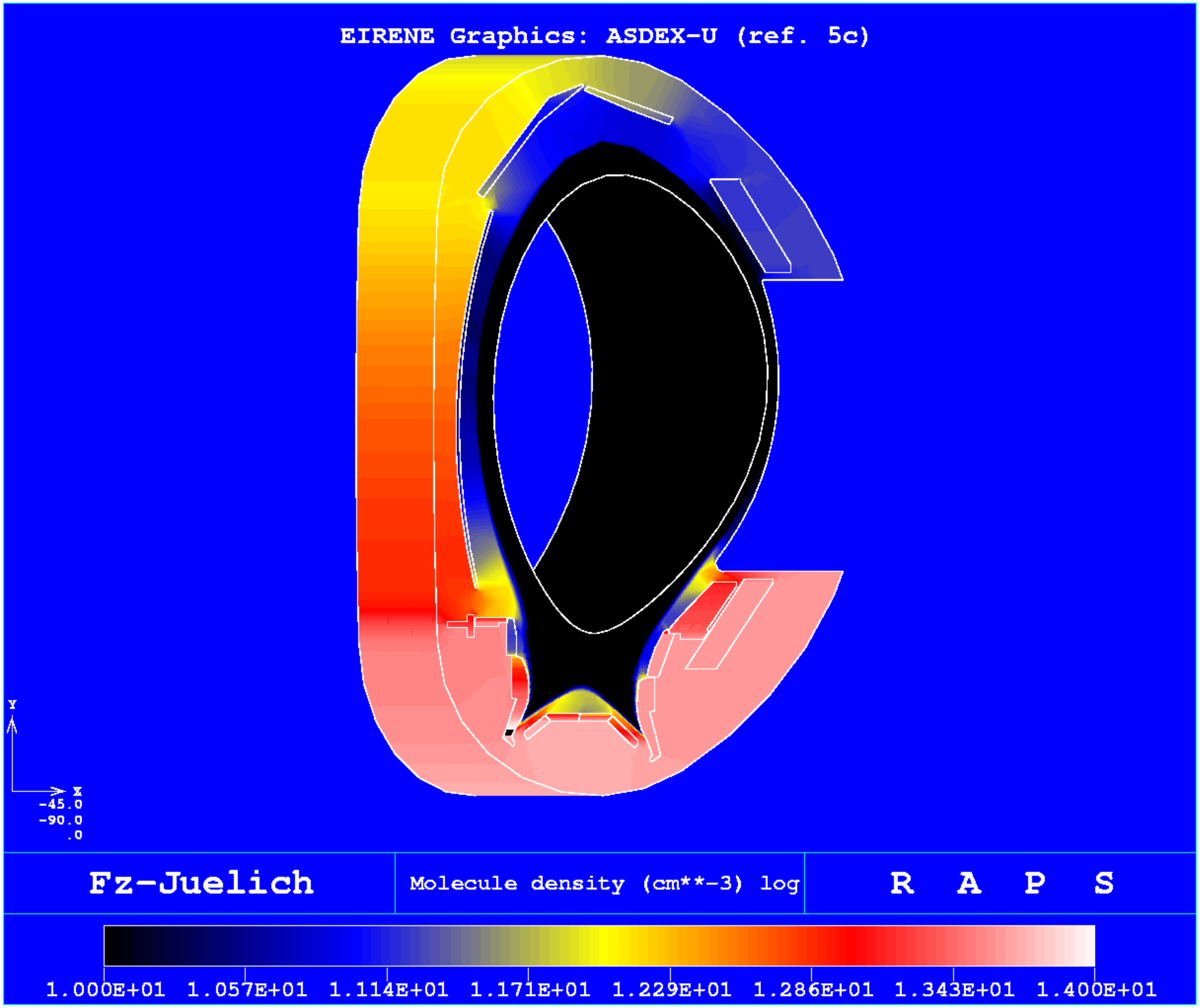
Particle Simulation: PMI, A&M

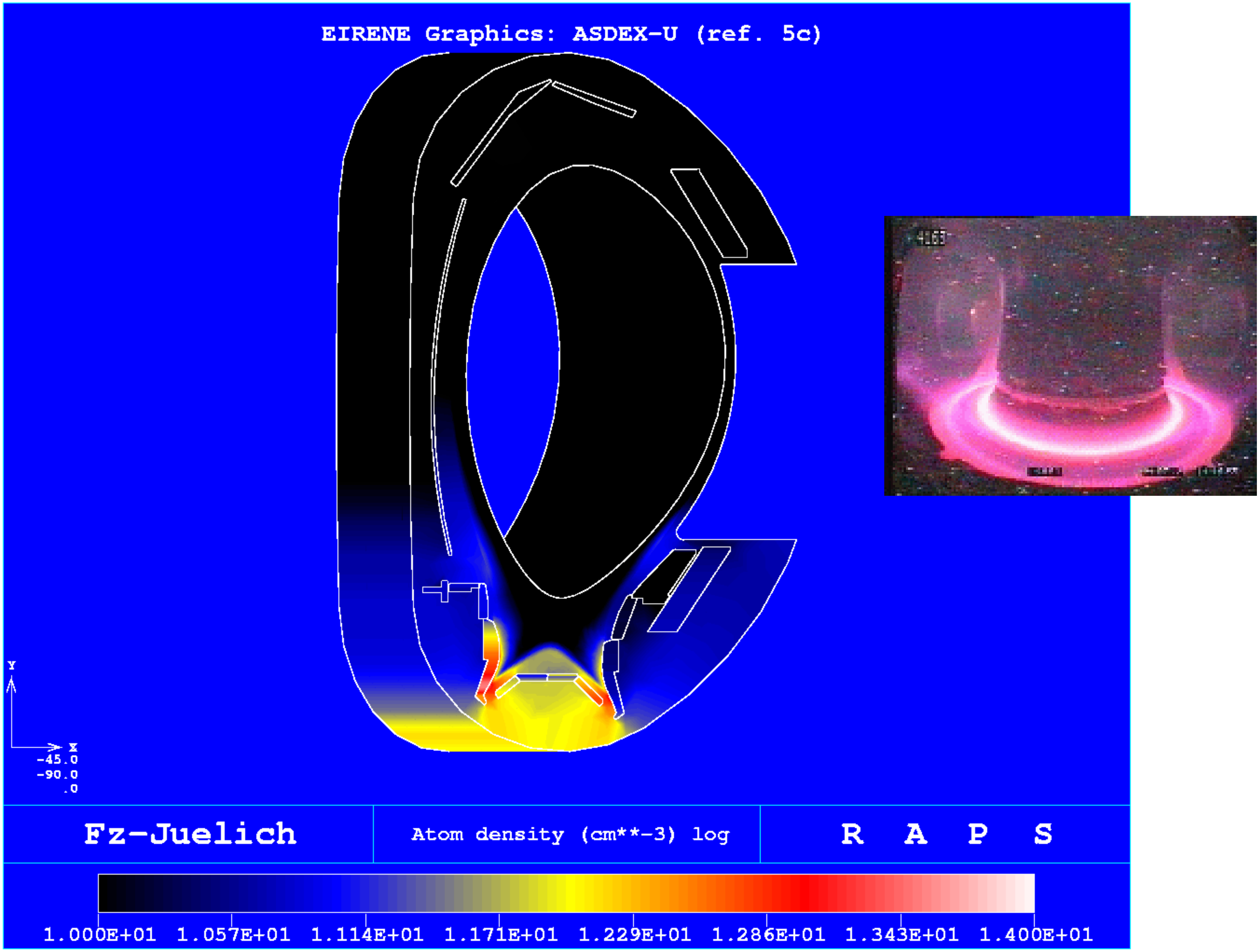
Visible light from ASDEX-U Divertor

EIRENE Torus-option

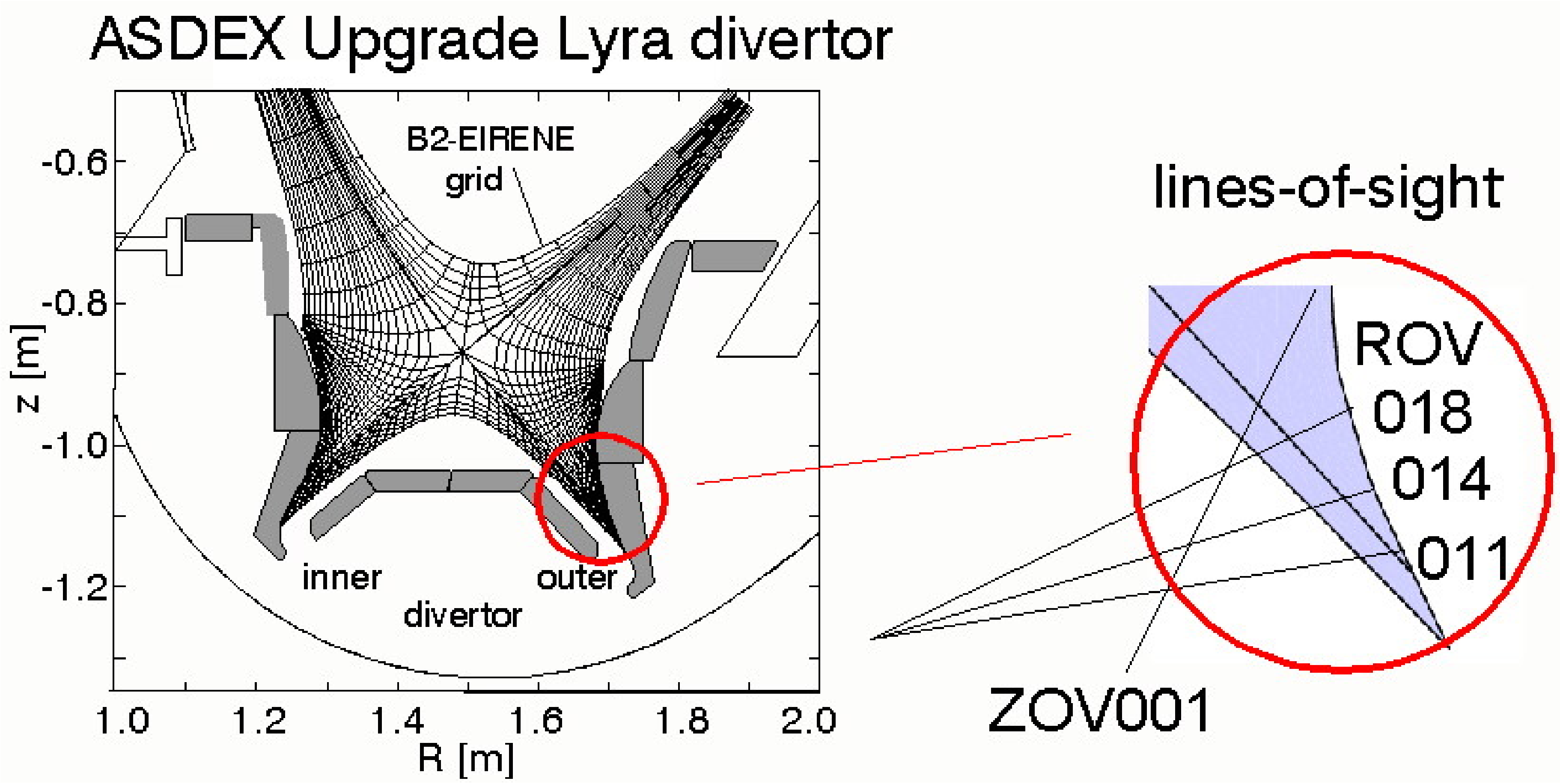


Fz-Juelich		R A P S


EIRENE Graphics: ASDEX-U (ref. 5c)
Y
X
-45.0
-90.0
.0
Fz-Juelich
Molecule density (cm**-3) log
R A P S
1.000E+01 1.057E+01 1.114E+01 1.171E+01 1.229E+01 1.286E+01 1.343E+01 1.400E+01


EIRENE Graphics: ASDEX-U (ref. 5c)
Y
X
-45.0
-90.0
.0
Fz-Juelich
Atom density (cm**-3) log
R A P S
1.000E+01
1.057E+01
1.114E+01
1.171E+01
1.229E+01
1.286E+01
1.343E+01
1.400E+01

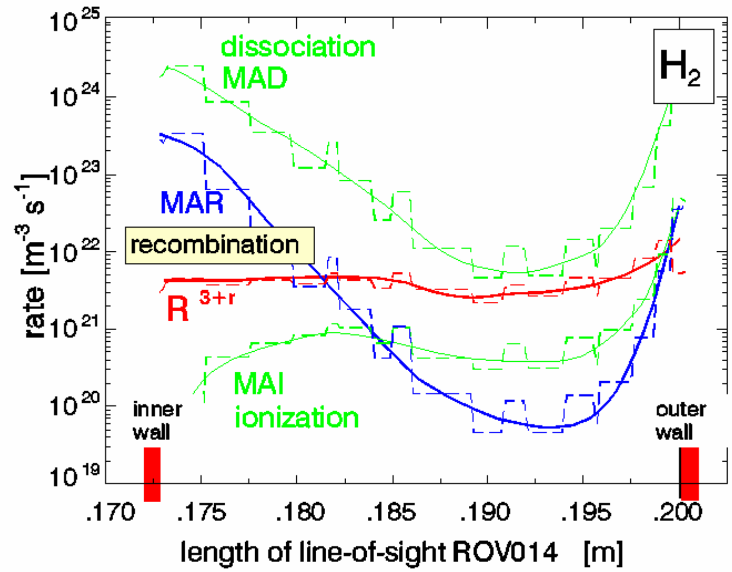
Molecular spectroscopy to verify or disproof model predictions



Radiation in divertor plasmas
Molecular Assisted Recombination (MAR)

$H_2(v) + e \Rightarrow H + H^-$ dissociative attachment
$H + H^+ \Rightarrow H + H^*$ mutual neutralisation
or
$H_2(v) + H^+ \Rightarrow H + H_2^+$ ion conversion ⇚ dominant channel
$H_2^+ + e \Rightarrow H + H^*$ dissociative recombination

⇛ combination of spectroscopy, CR-model and B2-EIRENE:



D_2?

molecules contribute near the surfaces to plasma recombination

- dependence of $H_2(v)$ on wall material and temperature
- recombination of atoms at surfaces and reflection coefficients

Self sustained neutral cushion?
B2-EIRENE simulation: MAR or MAD?

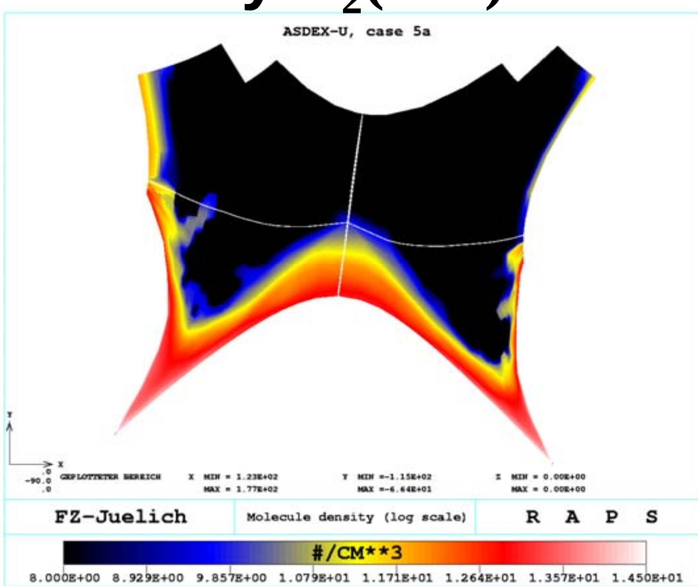
$P + H_2(v) \rightarrow H + H_2^+$, $e + H_2^+ \rightarrow H + H^* \rightarrow H + H$ (MAR)

$P + H_2(v) \rightarrow H + H_2^+$, $e + H_2^+ \rightarrow H + H^* \rightarrow H + H^+ + e$ (MAD)

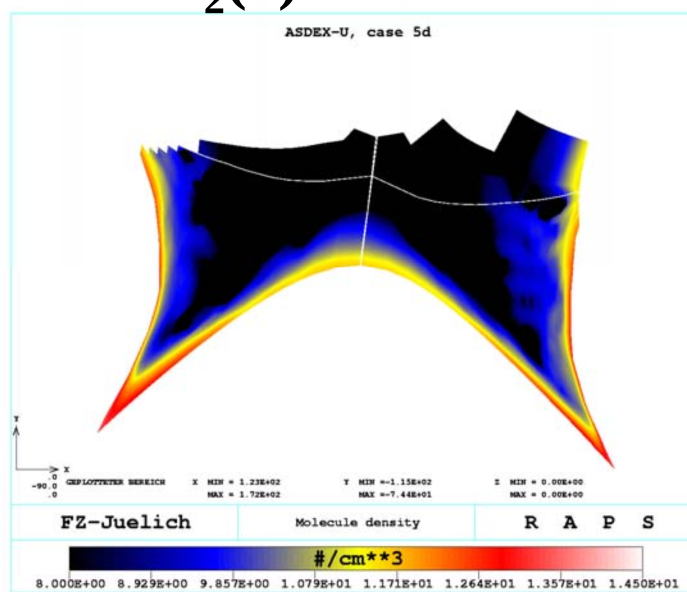
H_2 density field in Divertor:

Neutral gas “cushion” is strongly reduced by H_2 + p ion conversion

only $H_2(v=0)$



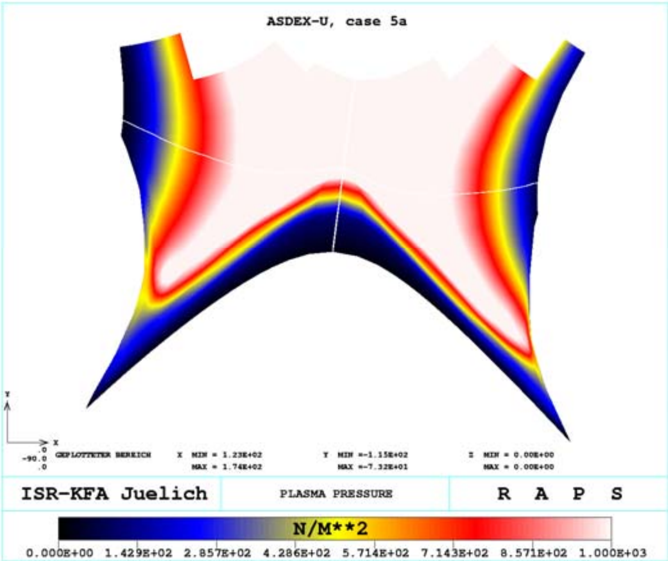
$H_2(v)$ included

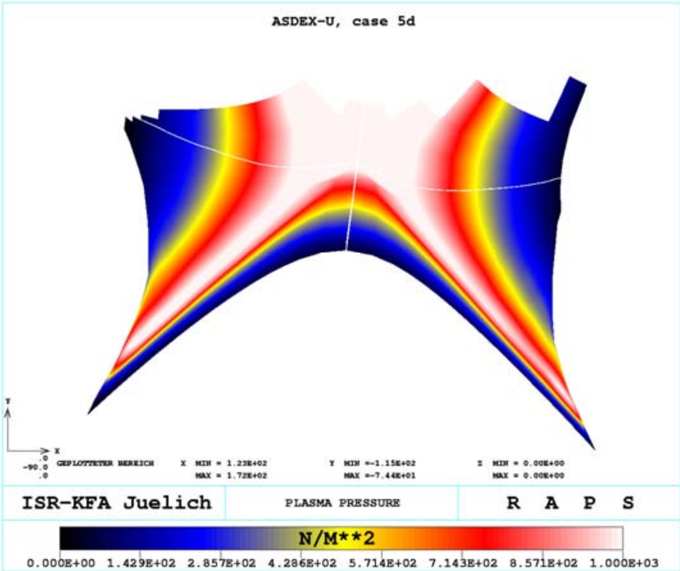


Self sustained neutral cushion?
B2-EIRENE simulation: MAR or MAD?

Pressure drop at inner target disappears:
re-attachment due to MAD

$H_2(v=0)$	$H_2(v)$

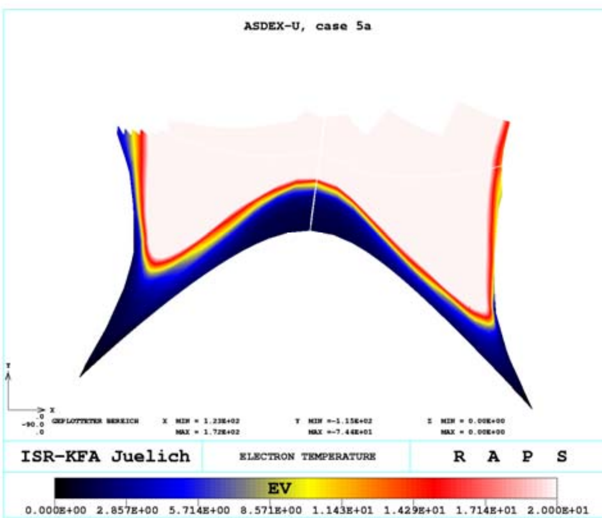




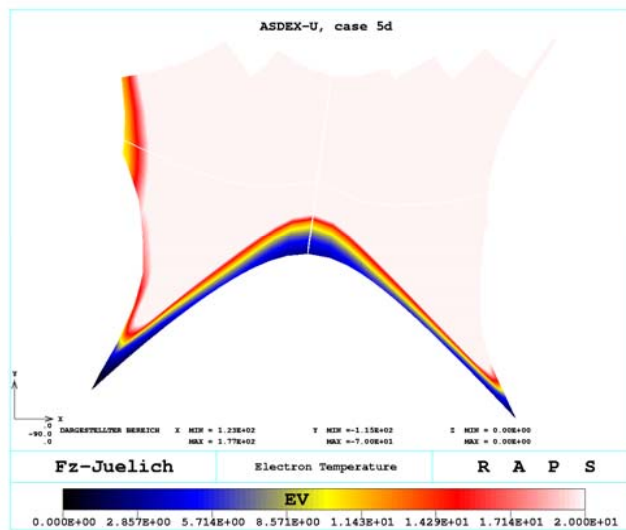
Self sustained neutral cushion?
B2-EIRENE simulation: MAR or MAD?

Electron temperature field in Divertor

$H_2(v=0)$



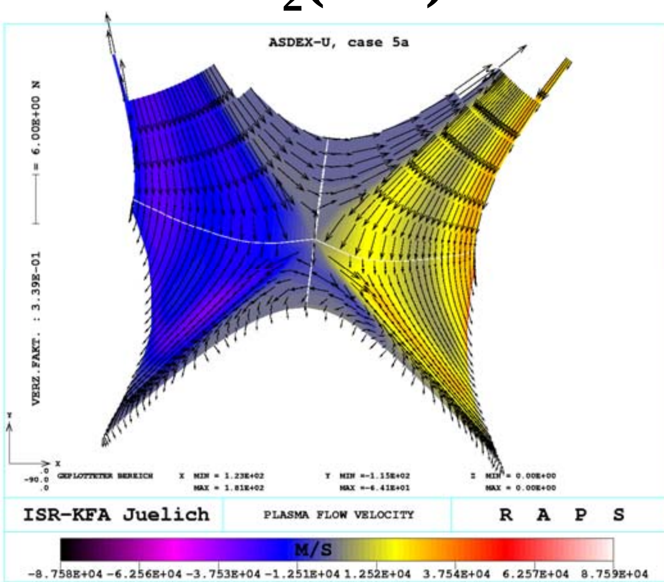
$H_2(v)$



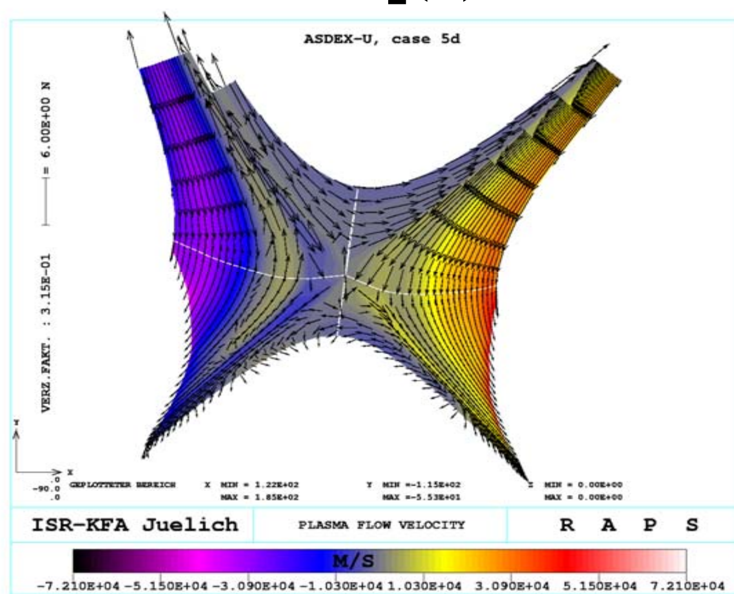
Self sustained neutral cushion?
B2-EIRENE simulation: MAR or MAD?

Changed flow pattern: flow reversal (right)
(dominant force (friction) changes sign

$H_2(v=0)$



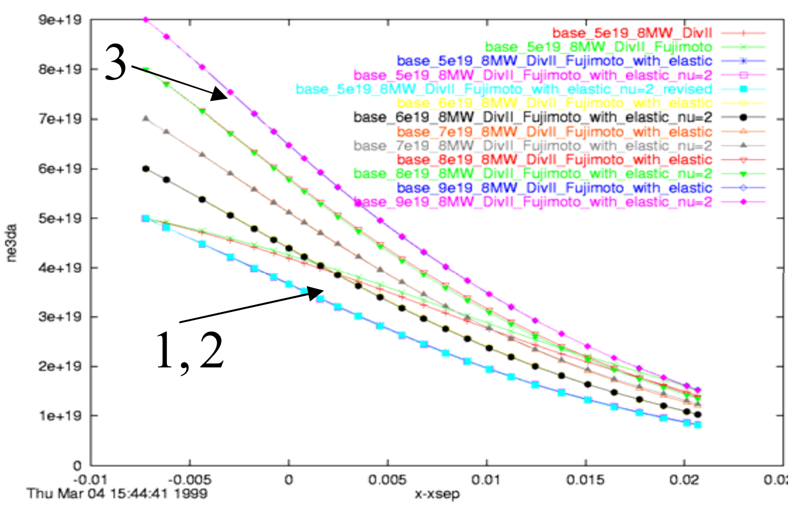
$H_2(v)$



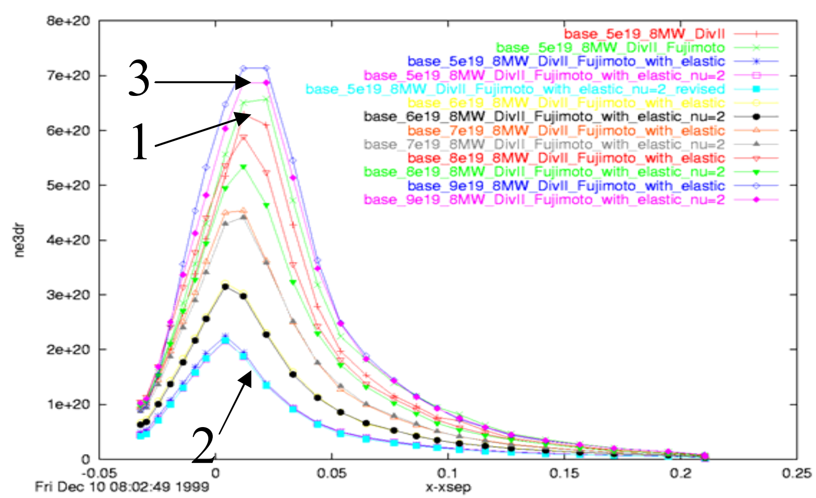
The detached divertor state due to plasma chemistry is a very robust finding from plasma codes. However: Molecule chemistry can change the overall divertor state drastically

The initial detached state (1) (no mol. vibr. chemistry) can be recovered from (2) (with mol.vibr.) by either:

- increasing the upstream density (3) or
- assuming different (anomalous) cross field transport



Outer midplane density profile



Outer target density profile

CONCLUSIONS

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.

- The role of vibrationally excited molecules on overall Divertor dynamics seems accepted.

- The relative role of surface processes (vs. volume processes) to establish this vibrational excitation seems less clear.