Atomic Data in ITER Edge Modelling

A.S. Kukushkin[1], H.D. Pacher[2],
D. Reiter[3], V.Kotov[3]

[1] ITER Organization, Cadarache, France
[2] INRS EMT, Varennes, Canada
[3] FZ Jülich, Jülich, Germany

ADAS Workshop, Ringberg, October 2007

Introduction

ITER: modelling is the way of extrapolation from present experiments

A&M&S data necessary to model the plasma and wall interaction

data on surface interaction equally important!

Composition of the ITER plasma:

fusion reactions	➔	D, T, He
mixed materials on PFCs	➔	Be, C, W
impurity seeding for core control	➔	Ne, Ar
diagnostics	➔	Li, …
off-normal events	➔	O, Fe, Cu, …

Plasma conditions

Core: fully ionized (but NBI, pellets?), T ~ 0.2 – 20 keV, n ~ 10^{20} m^{-3}

Edge: many neutrals, T ~ 0.1 – 200 eV, n ~ 10^{18} – 10^{21} m^{-3}

ITER Modelling

Edge plasma outside the separatrix (B2-Eirene):

- essentially 2D
- “dirty” plasma (neutrals, impurities, wall interactions)
- multi-fluid model for ions & electrons
  - → a separate fluid for each charge state
- Monte-Carlo model for neutrals
  - → geometry detail, full set of reactions
  - → neutral-neutral collisions included
  - → radiation transport can be included

Core plasma inside the separatrix (ASTRA):

- 1D transport across 2D flux surfaces
- No wall interactions, simplified neutral model
- Focus on the transport detail (transport barrier, pedestal, etc.)
- Edge properties and limitations via effective boundary conditions (parameterized B2-Eirene results)

This presentation: mostly edge

Fuel: D & T, Atoms and Molecules

Atoms: c-x, excitation, ionization, recombination well known (?)

3-body recombination and multi-step ionization important

neutral-neutral collisions: important in ITER, gas-like behaviour

radiation (Lyman series) transport: affects plasma parameters,
less important for engineering data
(power loading, pumping)

Molecules: more complex physics, large variety of reactions

elastic collisions with ions (energy transfer to targets – strong effect)

➔ importance of vibrational excitation (affect dissociation rate)

Vibrational excitation of DT? Of T_2?

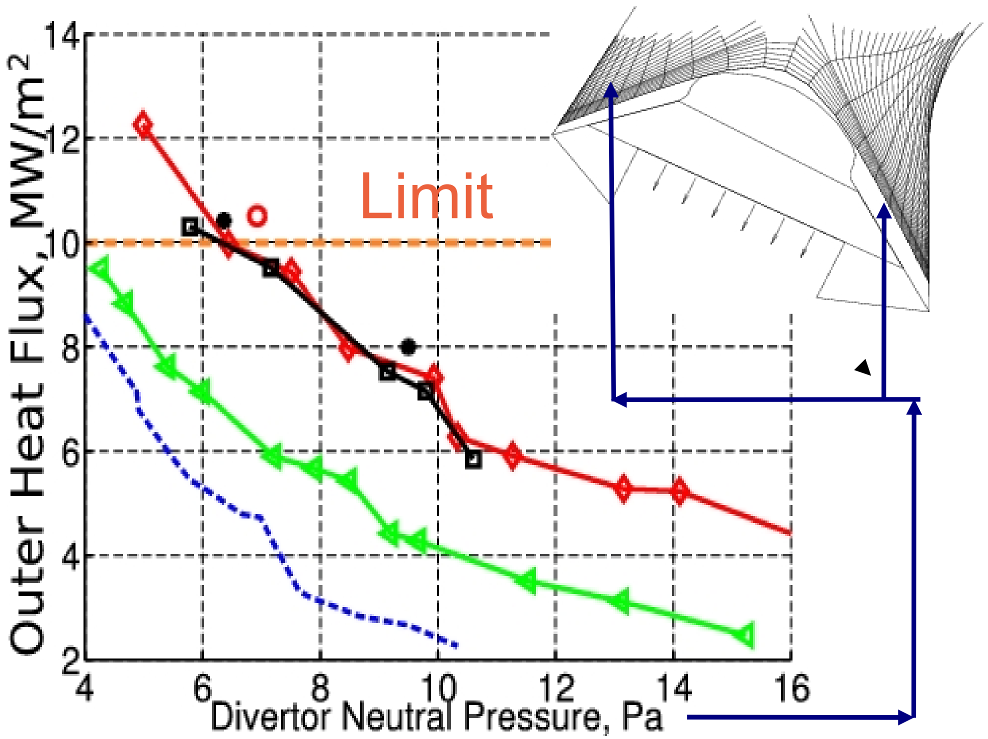
Excitation of dissociation products? – important (MAR story)

Rotational excitation – energy transport? Effect on cross-sections?

Excitation of atoms and molecules reflected and desorbed from walls?

-- could be important; no data available?

An example of the effect of gas dynamics on ITER divertor performance



►Peak power loading: one of the critical parameters of the design

--- previous, linear ITER model

— ... + Neutral-Neutral Collisions (NNC)

— ... + Detailed Molecular Kinetics

— ... + Radiation Opacity

►Strong effect of Neutral-Neutral collisions (blue vs. green)!

See: Kukushkin A., et. al, Nucl. Fusion, **45**, 608 (2005)

D.Reiter, Kotov V., et. al, J. Nucl. Mat., **363-365**, 649 (2007)

Sensitivity to Target Shape: Geometry Variation

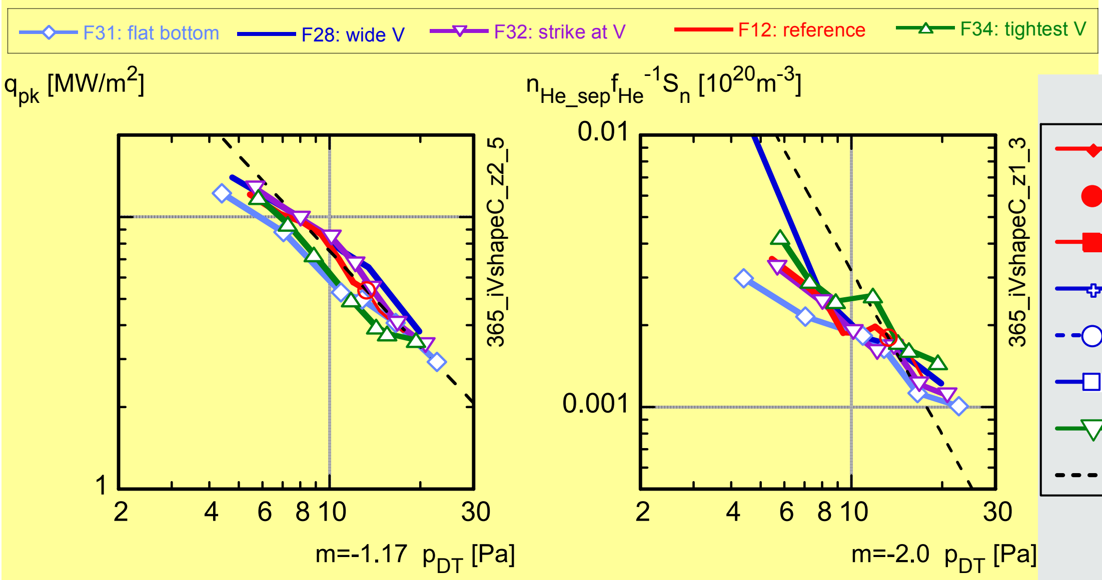
Density scans for 5 bottom shapes, different “V”

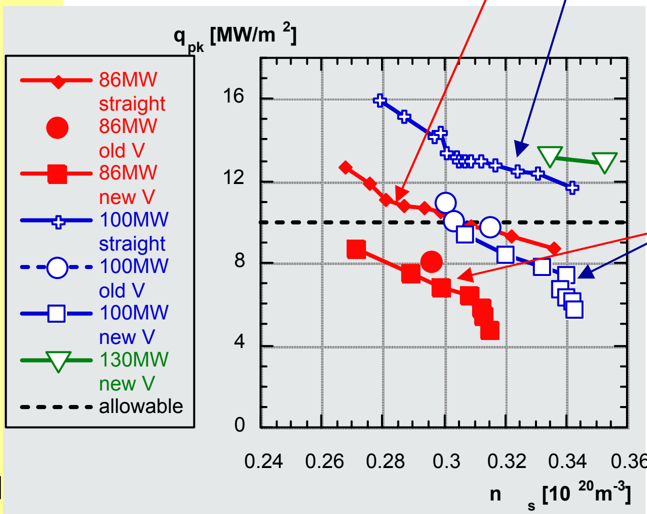
Weak variation in target loading, fuelling and pumping conditions with non-linear neutral transport

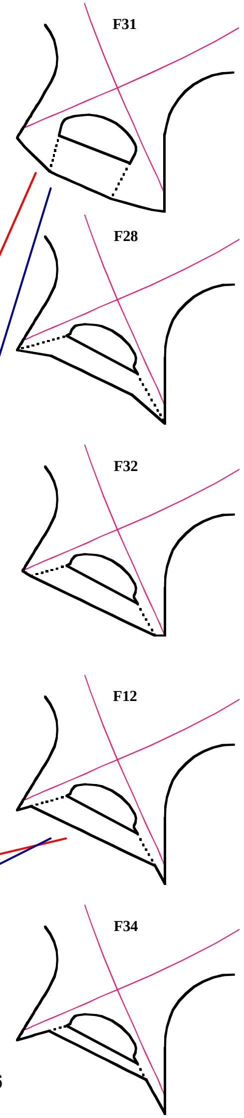
➔It is less important to maintain a closed V-shape near strike point than previous linear neutral transport model predicted

Linear model: neutrals fly freely outside the plasma in PFR. Wall geometry important for transport, neutral pressure not.

Non-linear model: short mean-free-path, neutrals do not “feel” solid structures. Neutral pressure determines the transport.







MAR Story – ITER Modelling

Molecular package

Effective rates (excitation) introduced for:

$e + D_2 \Rightarrow 2D + e$

$e + D_2 \Rightarrow D + D^+ + 2e$

$e + D_2 \Rightarrow D_2^+ + 2e$

$e + D_2^+ \Rightarrow 2D$

$e + D_2^+ \Rightarrow D + D^+ + e$

$e + D_2^+ \Rightarrow 2D^+ + 2e$

Added:
ion conversion

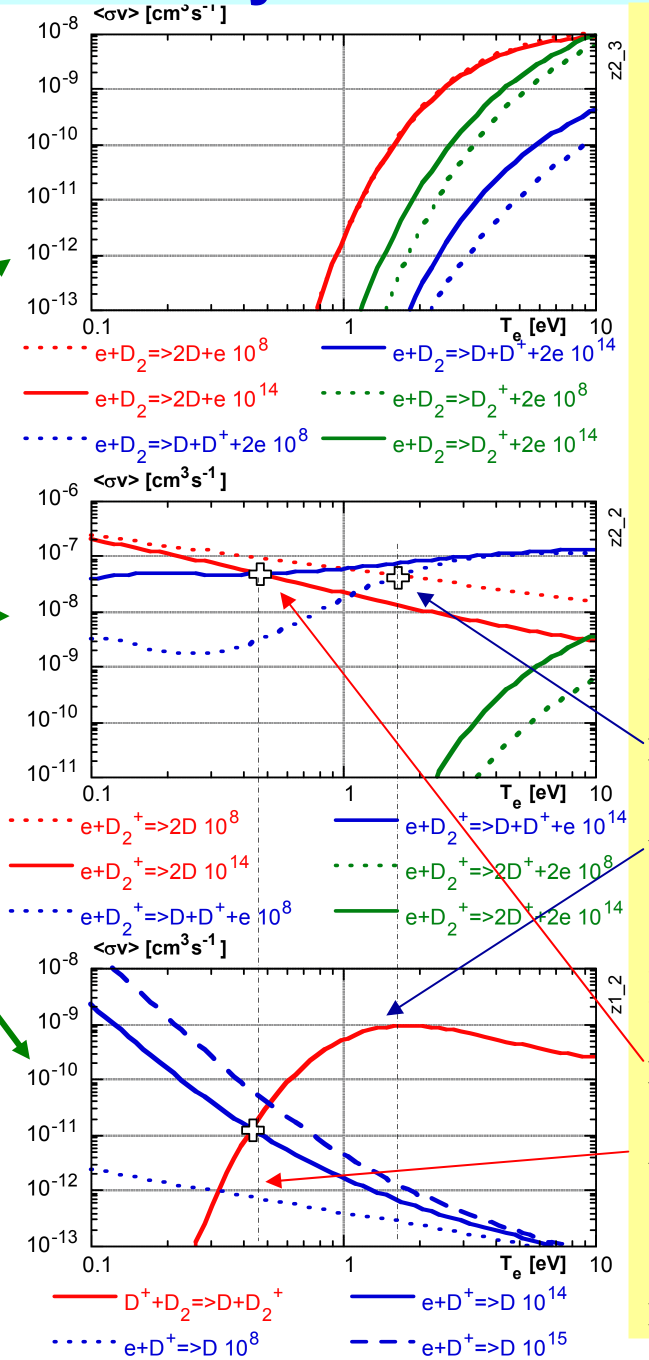
$D^+ + D_2 \Rightarrow D + D_2^+$

and elastic collisions

$D^+ + D_2 \Rightarrow D^+ + D_2$

Low T_e: $n_m/n_e < 1$, 3-body recombination is strong

High ion conversion: low rate of D_2^+ decay into 2D



MAR idea:

$D^+ + D_2 \Rightarrow D + D_2^+$

$e + D_2^+ \Rightarrow 2D$

$D^+ + D_2 + e \Rightarrow 3D$

(equiv. recombination)

Can be spoiled by D^+ production from D_2^+

No excitation (dotted lines):

recombination prevails below 2 eV

ion conversion high, > 3-body rec.

➔ strong effect

Excitation allowed for (solid):

recombination below 0.5 eV

ion conversion low

➔ no effect at high density

$n < 10^{20}\ m^{-3}$: effect on diagnostics?

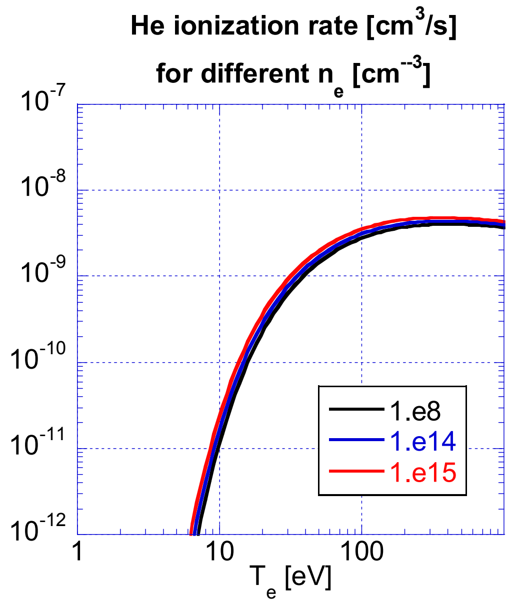
Reaction Product: He

Recycling impurity ➔ neutrals important

Ionization, excitation, recombination well known (?)

Multi-step processes unimportant:

1st excited level close to ionisation



Elastic collisions with D, T ions

– important, drastically improve He removal

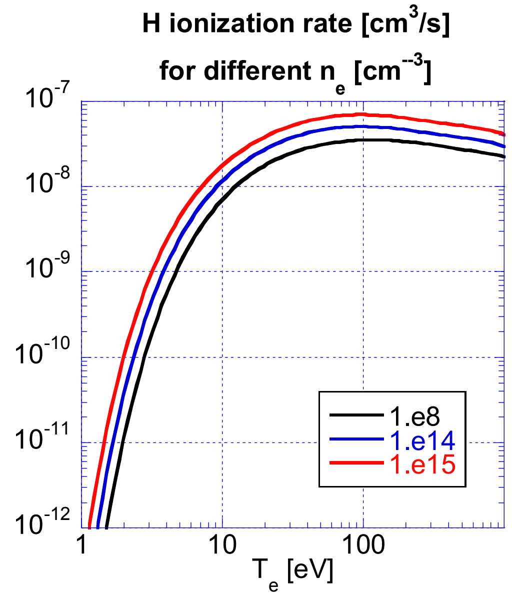
Resonance charge exchange

– unimportant, too little He in the plasma (?)

Charge exchange with D, T ions:

from available data, the cross-sections low; accuracy?

Importance of meta-stable states?

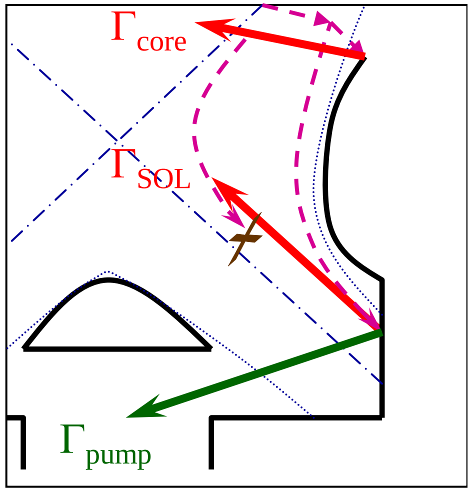


Elastic Collisions He + D$^+$

Core: He-He collisions negligible ➔ transport ~ linear

➔ $n_{He} = n_{He}^{c} + n_{He}^{e} + n_{He}^{n}$

(fusion/ core transport + separatrix He^{++} + influx He^0)



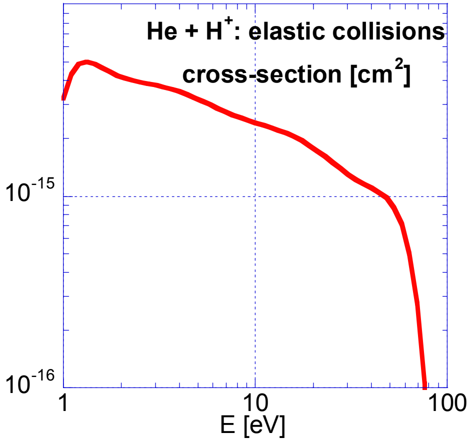
Edge: thermal force ➔ He neutralisation in outer SOL

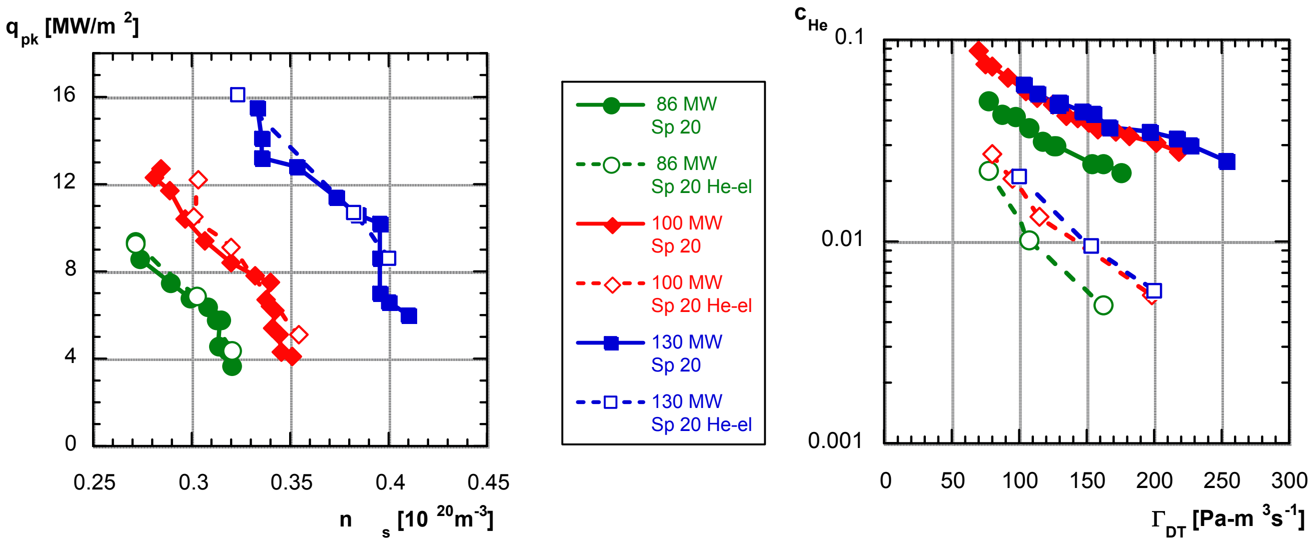
He^0 fluxes: competition between Γ_{pump} and $\Gamma_{core} + \Gamma_{SOL}$

Elastic collisions heat He up ➔ Γ's increase

EC on: q_{pk} the same, c_{He} down

Γ_{pump} wins – drop of the cross-section above 50 eV?





Surface Materials: Be

Physical sputtering: rates known (?)

No molecules ➔ no chemical erosion (despite carbides?)

Ionization, recombination: data exist; accuracy?

Excitation, multi-step ionization?

Elastic collisions with D, T ions?

Surface chemistry (Be-C, Be-W, Be-H)

Limited experience in ITER modelling so far

Surface Materials: C

Hydrocarbons ➔ chemical erosion a major source

Physical sputtering: rates known (?)

Atoms:

- Ionization, recombination: data exist; accuracy?
- Excitation, multi-step ionization?
- Elastic collisions with D, T ions?

Ions:

- Ionization, recombination, excitation well known?
- Charge exchange with D, T unimportant?

Hydrocarbons:

- May determine T accumulation in the machine
- Extremely complex system, isotope effects?
- Needs thorough bookkeeping
- No experience in ITER modelling so far

C: Deposition and Re-Erosion (DRE model)

C deposition: danger of T co-deposition

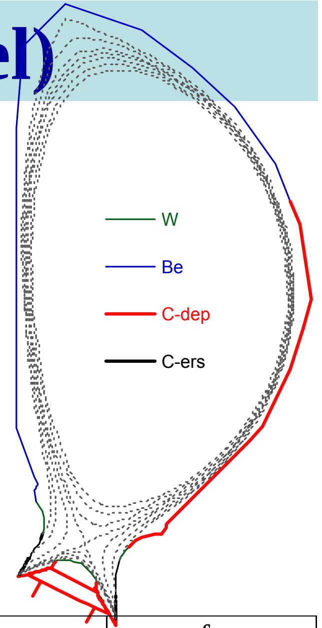
Re-erosion of deposits affects both surface and plasma properties

Model: compare deposition and would-be erosion rates of C

deposition-dominated: normal C surface

erosion-dominated: original metal, but no C absorption

iterate until converges → BC consistent with the solution



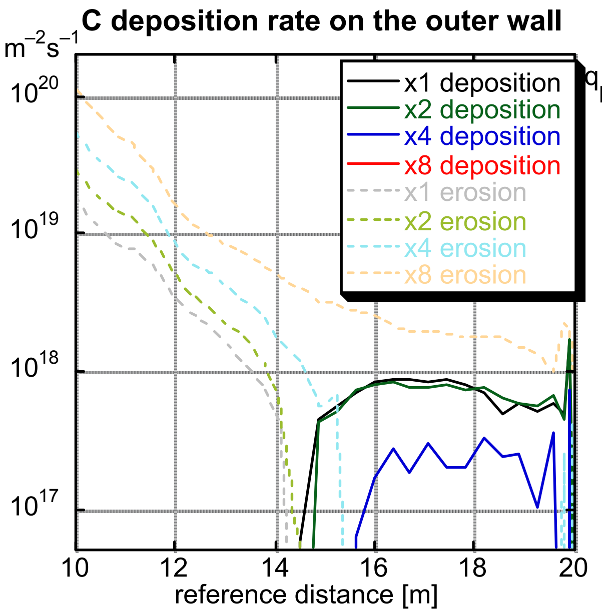
wall factor	f_w
C0 (full)	0.84
C1-Yx1	1
C1-Yx2	0.83
C1-Yx4	0.71
C1-Yx8	0.71

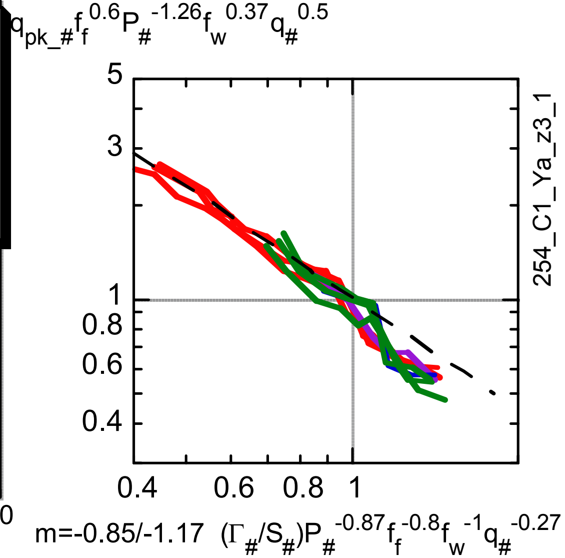
Const Y_{ch} → ∃ C deposition in the main chamber

Y_{ch}×8 for deposits →no C deposition (flux dependence?)

Full C wall closer to DRE than metal wall

(different scaling for metal!)





Surface Materials: W

Physical sputtering: rates known (?)

No molecules ➔ no chemical erosion (despite carbides?)

Ionization, recombination: no full data set; accuracy?

Excitation, multi-step ionization?

Elastic collisions with D, T ions?

– probably unimportant, atomic mass too large

Too many charge states, usual multi-fluid approach inefficient

➔“bundle” certain charge states together for transport

➔ technology of effective rates is needed

Surface properties: hydrogen uptake, interaction with Be, C?

Limited experience in ITER modelling so far
(DIVIMP – test particle approximation)

Seeded Impurities: Ne, Ar(, Kr, Xe)

Atomic species, no chemistry
Ne, Ar very probable candidates for core plasma control;
Kr, Xe might cause problems with transmutations, although radiate better

Ne: ionisation, recombination data exist for all charge states; accuracy?
    detailed excitation data? multi-step ionization?
    elastic collisions with D, T ions – some data exist; accuracy?

Ar: the same state as for Ne, probably less reliable?

Data for the core conditions equally important

Conclusions

Edge modelling is now an essential part of the ITER project

- design analysis
- development of the operation strategy

It relies strongly on the A&M&S data supplied by the community

- the results depend on the consistency and accuracy of the data (MAR, molecule collisions/excitation, deposition/re-erosion, …)

Most important groups of species:

- Fuel (D, T, D_2, T_2, DT): data for the edge (A&M) and beam (A). *Isotope effects in molecules!*
- Ash (He): data for the edge
- Wall produced, light (Be, C): data for the edge. *Hydrocarbons!*
- Wall produced, heavy (W): data for the edge & core. *Bundling!*
- Seeded (Ne, Ar): data for the edge and core
- Structural materials (Fe, Cu, …): data for the edge and core to study effect of off-normal events

Data on surface interactions equally important for all groups