Max-Planck-Institut fur Plasmaphysik, EURATOM Assoziation

Integrated modelling of the edge plasma and plasma facing components

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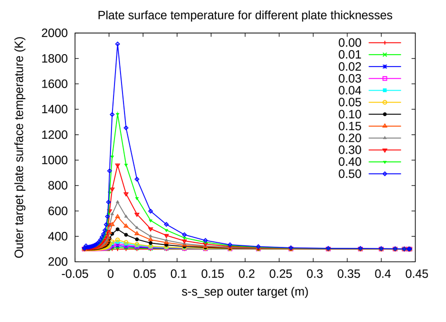
Introduction

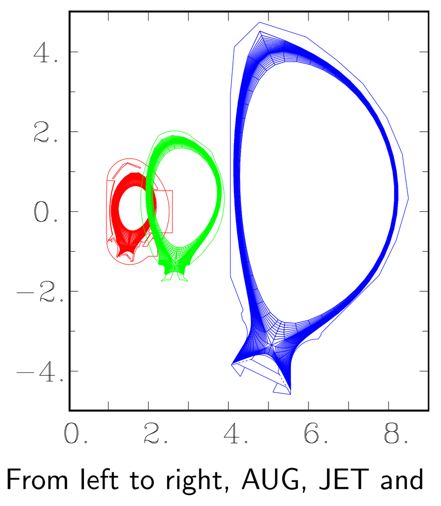
- Modelling of the interaction between the edge plasma and plasma facing components (PFCs) has tended to place more emphasis on either the plasma or the PFCs
  - Either the PFCs are essentially assumed not to change with time and the plasma evolution is studied
  - Or the plasma is assumed to remain static and the detailed interaction of the plasma and the PFCs are examined, with no back-reaction on the plasma taken into consideration

- B2 component of the SOLPS package of codes [Schneider *et al.*, 2006](and references therein) has been recently extended [Coster *et al.*, 2005, Warrier *et al.*, 2003, Coster *et al.*, 2006] to include
  - a treatment for thermal fluxes in the wall components
  - improved treatment of chemical and other sputtering processes
  - ability to model mixed-materials



Output from the "steady-state" (time-independent) thermal model for the plate for various (artificial) thicknesses (in meters) of the outer target plate of AUG exposed to an Ohmic plasma. The backplate temperature was assumed to be 300K.

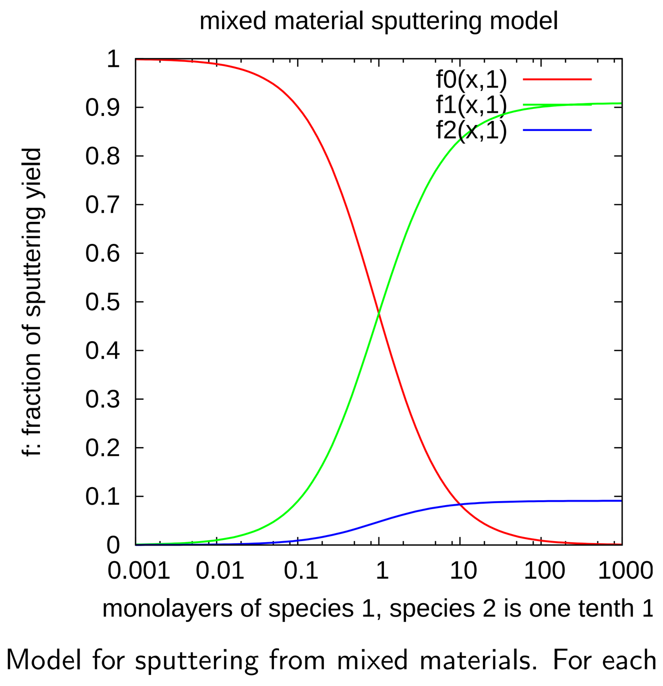
- mixed materials models applied to AUG, JET & ITER
- scenarios examined
  - single C species, base and deposited C
  - two isotopes of C
    - wall and targets made from different isotopes
    - wall and targets from one isotope, gas puff from another
  - Be and C
    - wall from Be, targets from C
    - Be walls and targets, C gas puff



From left to right, AUG, JET and ITER.

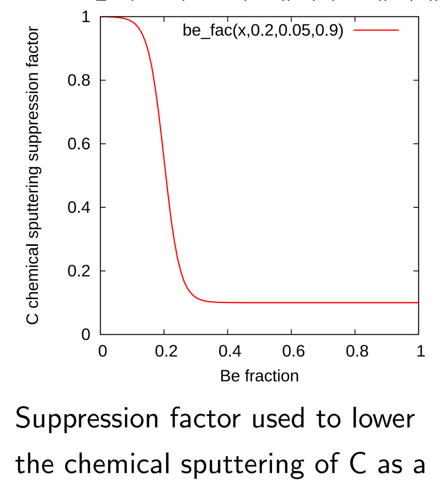
Mixed-material surface physics

- deposited material is tracked by the code, and a 0D time-dependent problem is solved at each position where the plasma interacts with a surface (as described in [Coster *et al.*, 2006])
- layer thickness is tracked, together with its composition (fraction of Be, C, *etc.*)
- then used to determine the fraction of sputtered material arising from the layer (Be, C, *etc.*) and from the base material (Be or C)
- model multiplies the rate from the basic sputtering processes (ignoring the presence of the mixed materials) by a factor giving the fractional presence of the individual materials in the mix



Model for sputtering from mixed materials. For each deposited species, i, the number of mono-layers, l_i, is calculated. Then the fraction of deposited material exposed for sputtering is $f_i = \frac{l_i^\beta}{\alpha + \sum_i l_i^\beta}$. The contribution from the base material is then $f_0 = 1 - \sum_i f_i$. α is taken as 1 for these cases and reflects how quickly the base material disappears from the calculation. β reflects how quickly deposited material hides the base material; here values of 1 have been used. For the graph species two has one tenth the mono-layers of species one.

- further augmented by allowing for an enhancement factor for the chemical erosion of deposited C, and/or for a suppression of chemical erosion dependent on the local concentration of Be
- $f_{Be}(x, a, b, c) = 1 - \frac{c}{2}(\tanh(\frac{x-a}{b}) - \tanh(\frac{-a}{b}))$
- $a = 0.2$, $b = 0.05$ and $c = 0.9$
- chosen to give a maximum suppression of 90% with a transition at about 20% Be fraction



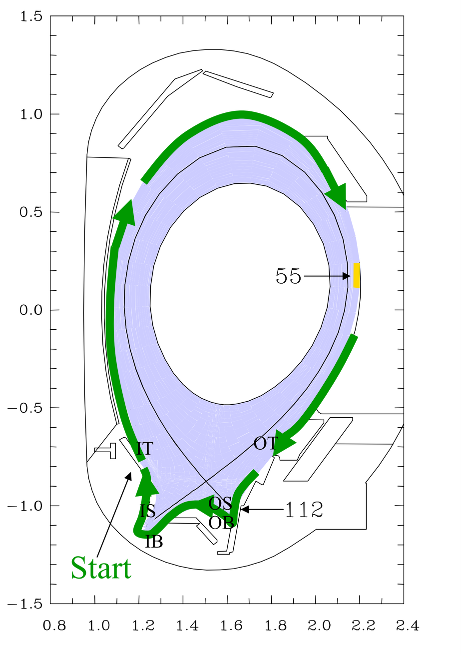
Suppression factor used to lower the chemical sputtering of C as a function of the Be fraction.

Results

- two coordinates used for the surfaces
  - linear counting of surfaces starting from the intersection of the outer SOL with the inner target
  - accumulated area of these surfaces

	AUG		JET		ITER	
	pos	A.A.	pos	A.A.	pos	A.A.
SOL 1	1	0.00	1	0.00	1	0.00
SOL 2	96	40.32	96	135.09	74	695.33
OUTER 2	97	40.36	97	135.29	75	697.46
OUTER 1	132	45.51	120	141.10	102	725.25
PF 2	133	45.55	121	141.18	103	725.68
PF 1	180	49.55	168	149.40	126	787.34
INNER 1	181	49.58	169	149.47	127	787.63
INNER 2	216	52.73	192	154.85	154	805.11

A.A. = Accumulated area



Convention for "surface" coordinates.

C

- simplest variant is to use only one species of C, but to track the deposited C and allow it to be eroded
- provides a strong test of the coding since — if the deposited C is assumed to erode like the original C — then the plasma result should be unchanged
- verified (see [Coster *et al.*, 2006]).

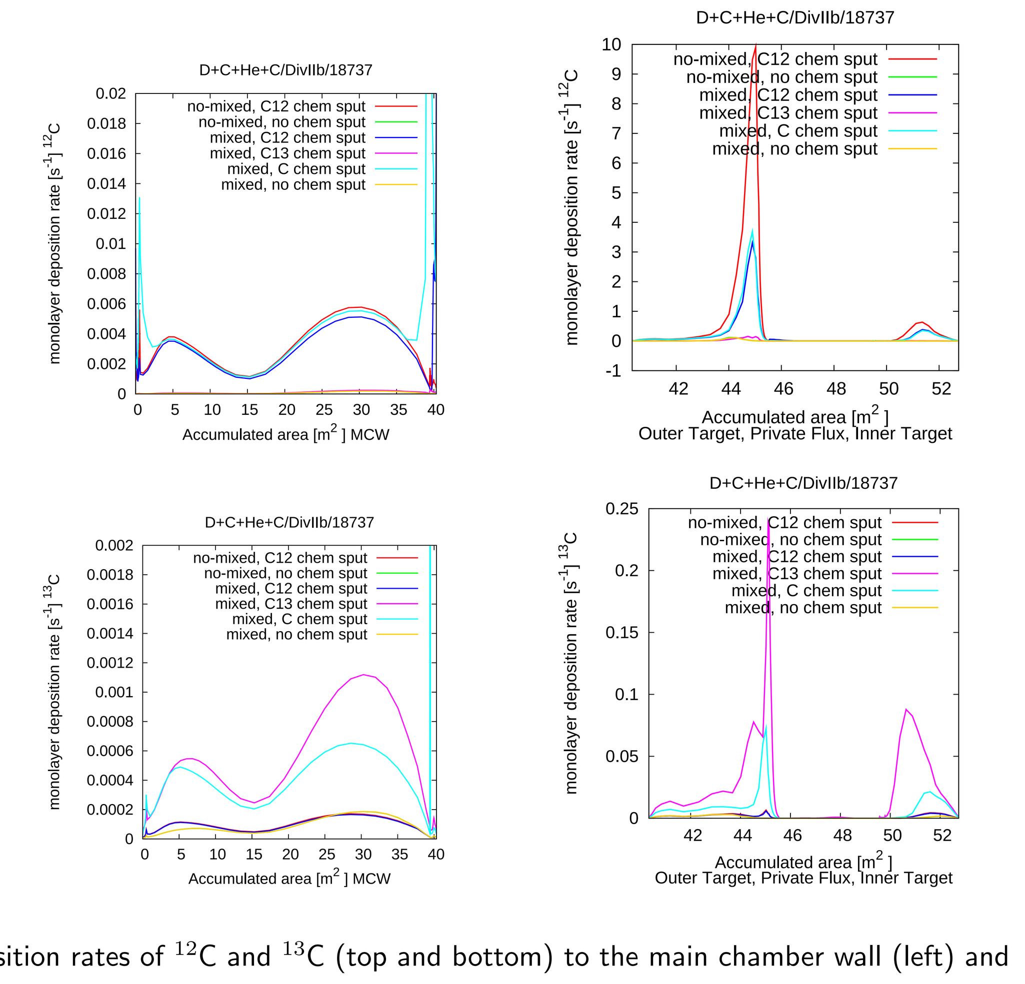
C-C

- next, more complicated variant, is to to distinguish two species of C
  - can be used to distinguish in the plasma eroded from various surfaces by, say, making the target from ^{12}C and the walls from ^{13}C
  - explore ^{13}C gas puffs in a ^{12}C machine — closer to the experiment

^{12}C targets, ^{13}C walls

AUG

- simulation based on an AUG Ohmic pulse for ^{12}C targets and ^{13}C walls
  - with and without mixed materials modelling
  - with no, only ^{12}C, only ^{13}C and both ^{12}C and ^{13}C chemical sputtering



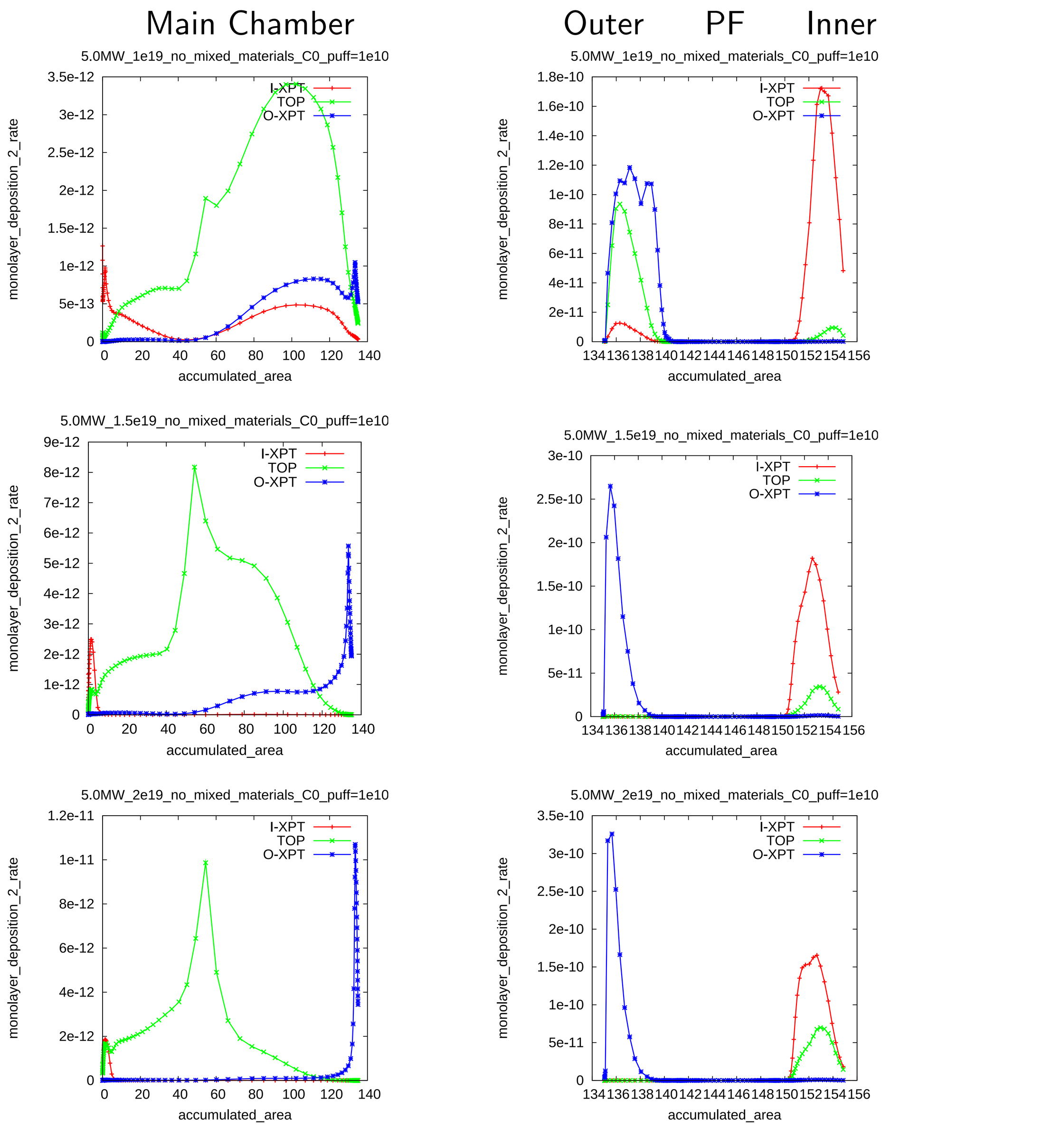
Deposition rates of ^{12}C and ^{13}C (top and bottom) to the main chamber wall (left) and targets (right) for an AUG simulation with varying sputtering models. (In the right panel, the outer target is to the left, the private flux in the middle and the inner target on the right.)

C walls, C gas puff

JET

- As seen previously in simulations of ^{13}C gas puff on JET [Coster *et al.*, 2005]
  - strong dependence on density is seen in the deposition patterns at the targets
- gas puff simulations with
  - 3 gas-puff positions
  - 3 densities
- examine deposition along main chamber wall and along targets

- at the lowest density, injection at the top of the machine arrives predominantly at the outer target
- at the highest density it arrives predominantly at the inner target
- note also the increased localisation near the injection point of the redeposition at higher densities
- Mixed materials model switched off
- Small, non perturbative gas-puffs



Deposition rates to the main chamber wall (left) and targets (right) of ^{13}C arising from a ^{13}C gas puff at three different densities (separatrix electron densities of 1×10^{19}, 1.5×10^{19} and $2 \times 10^{19} m^{-3}$, top to bottom) for JET simulation with gas inlets close to the inner X-point, the top of the machine, and the outer X-point. (In the right panel, the outer target is to the left, the private flux in the middle and the inner target on the right.)

C-Be

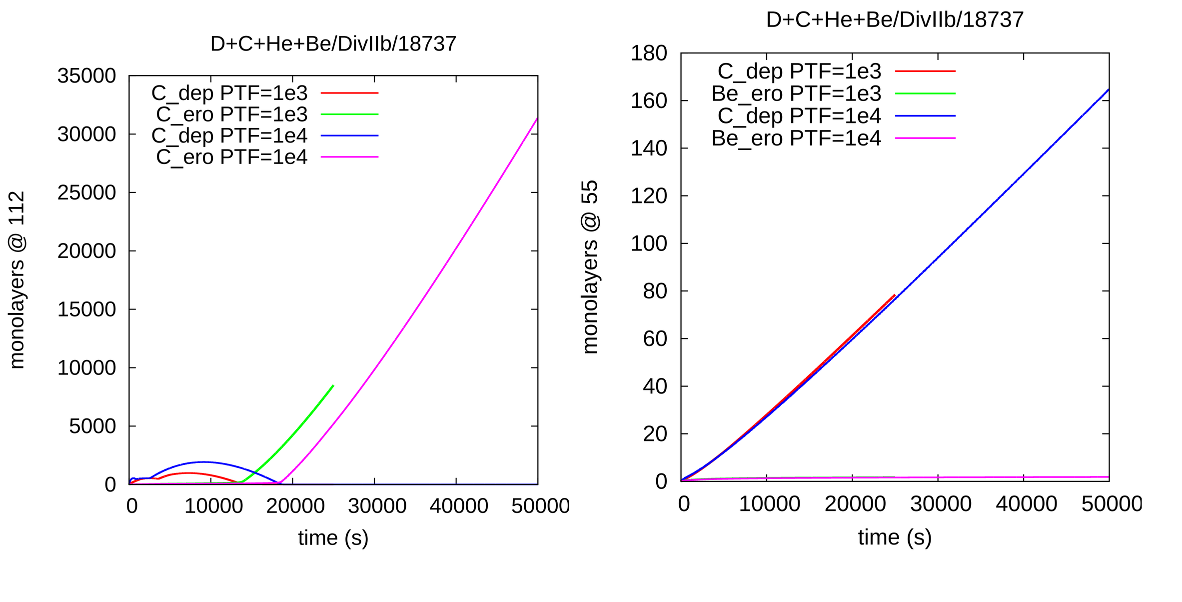
- ITER design currently foresees a mix of 3 materials to be used
  - C targets
  - W baffles
  - Be walls
- at the moment, modelling with SOLPS of W is problematic
  - too many charge states
  - forthcoming development of a bundled charge state model
- can simulate some of the effects by limiting the calculations to Be and C

- Again, a number of scenarios can be explored
  - Be walls with a C target
  - C walls and a Be target
  - Be walls and target with a C gas puff

Be walls, C target

AUG

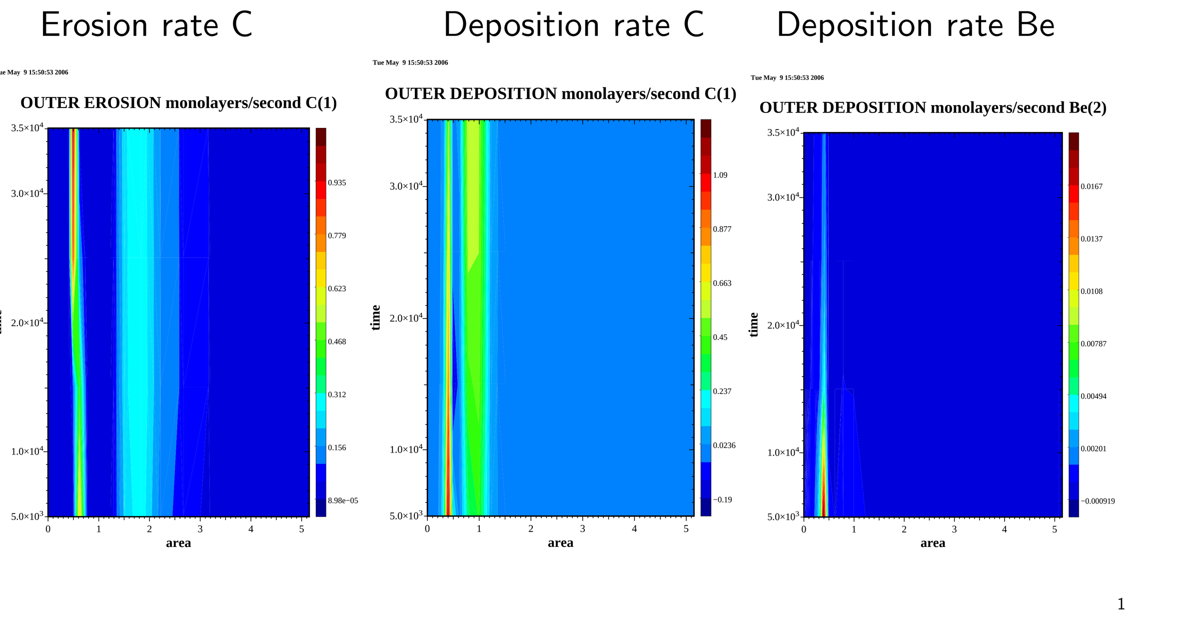
- simulations with Be walls and C targets for AUG
  - new, very long, time-scales were sometimes observed
  - fortunately effects seem localised



Deposition and erosion rates of C and Be for (left) a surface at the outer target and (right) the outer-midplane. The PTF factor is the relative enhancement factor used to advance time for the surface model with respect to the time-step used for the plasma.

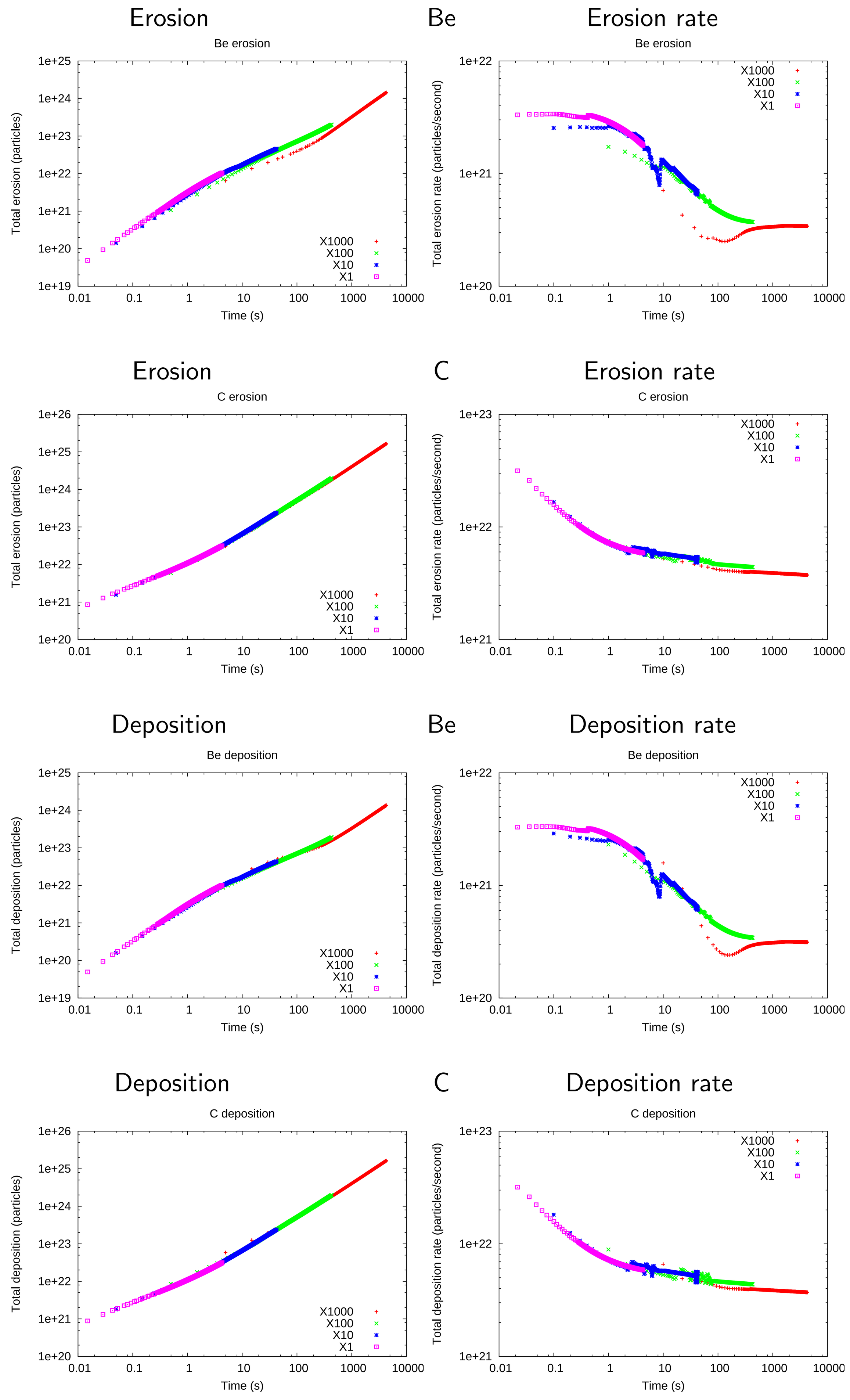
Looking at the outer target:

Erosion rate C | Deposition rate C | Deposition rate Be



ITER

Simulations have also been performed for an ITER with Be walls and C targets:

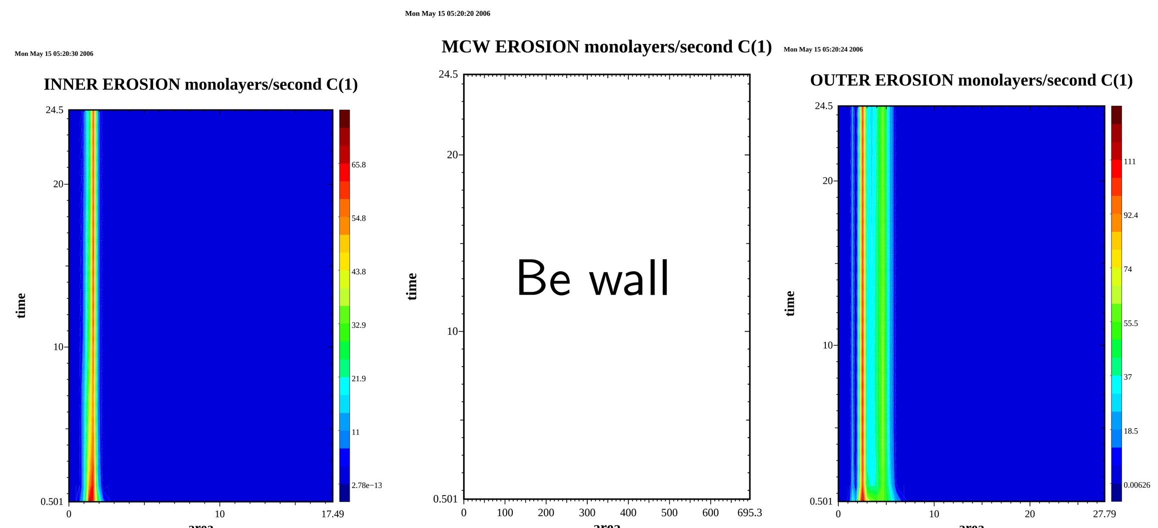


Left: Total deposition and erosion for Be and C for an ITER simulation. Right: corresponding rates. The X multipliers are the time enhancement factors used for the surfaces with respect to the basic plasma time-step.

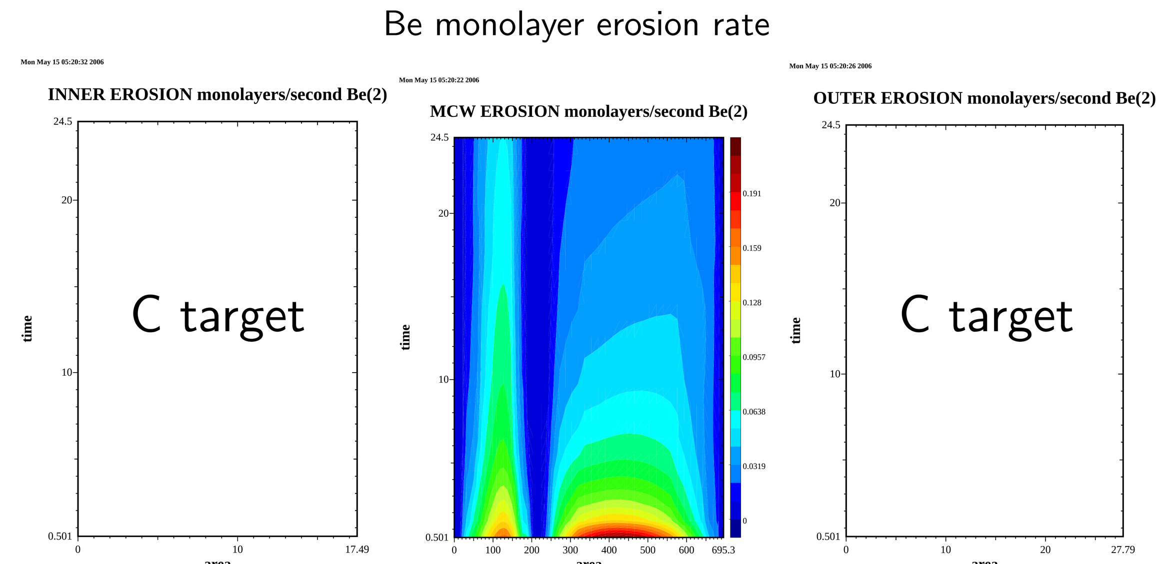
Instead of looking at the integrated quantities, we can look at the distribution:

Inner Target Main Chamber Wall Outer Target

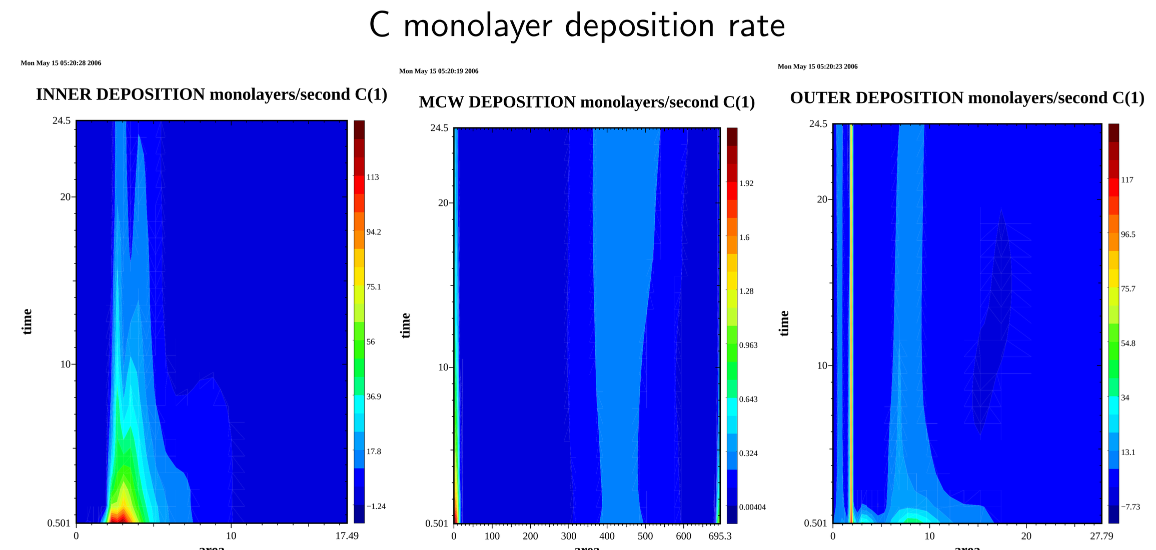
C monolayer erosion rate



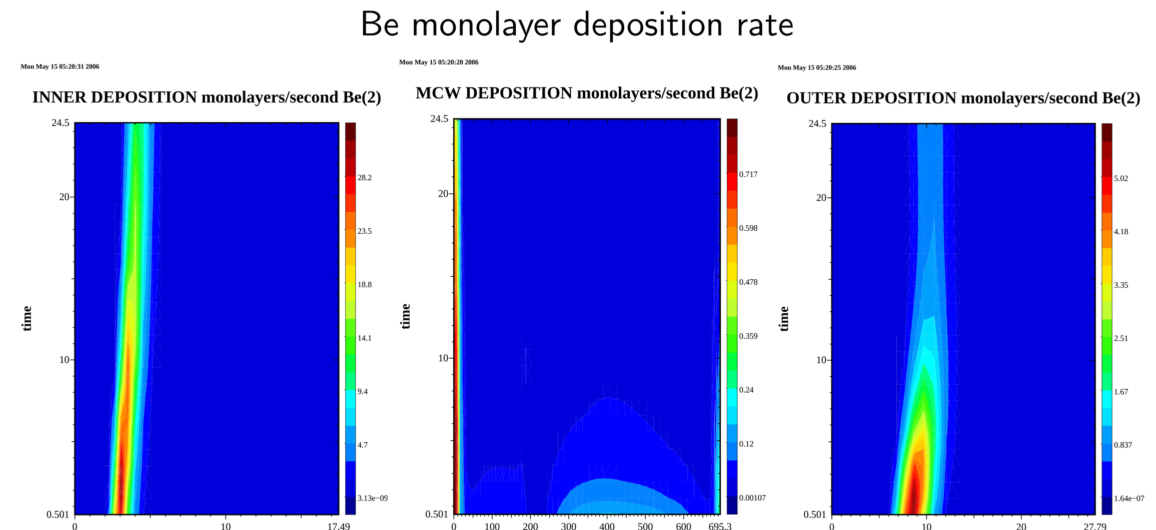
Be monolayer erosion rate



C monolayer deposition rate



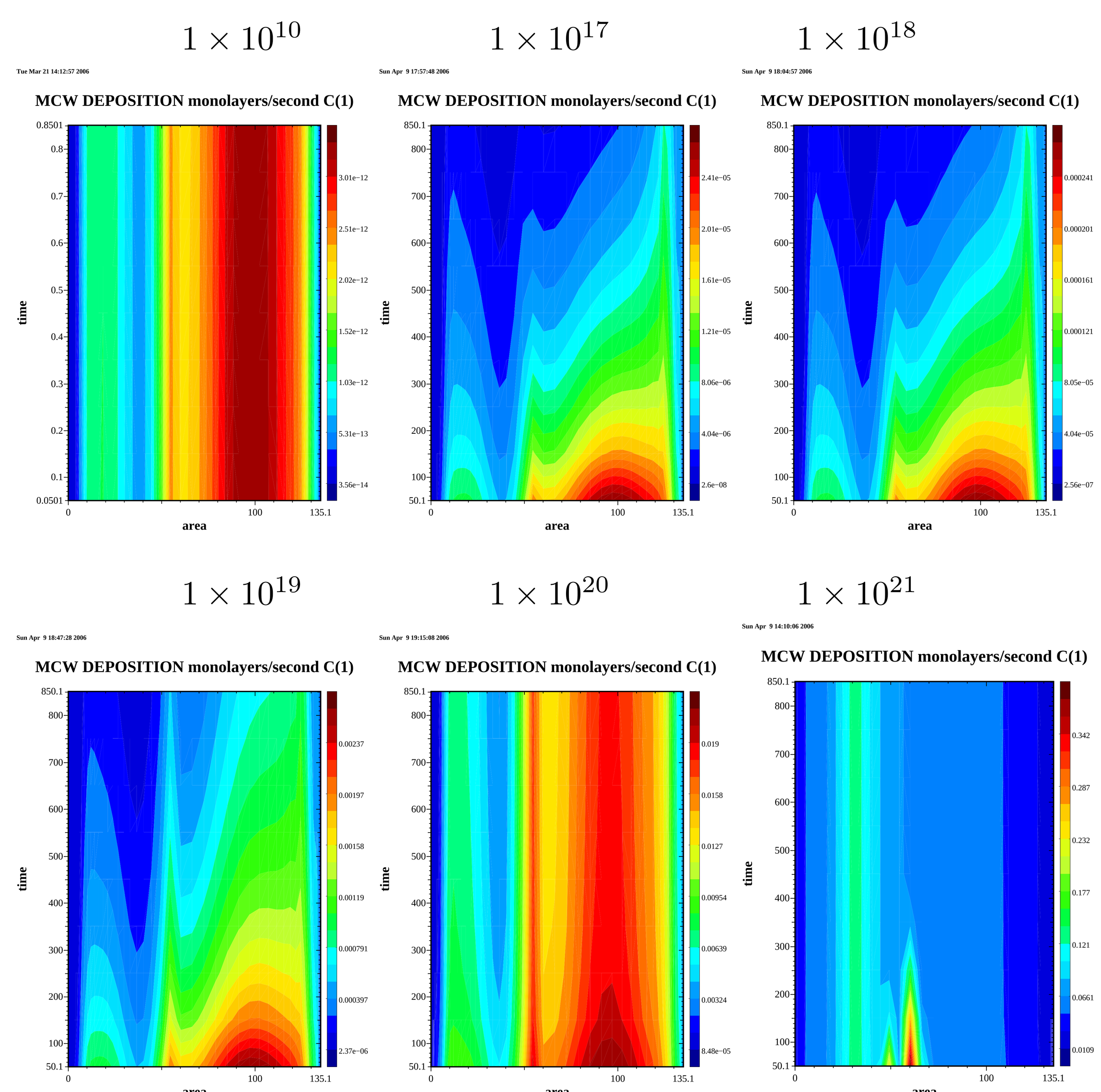
Be monolayer deposition rate



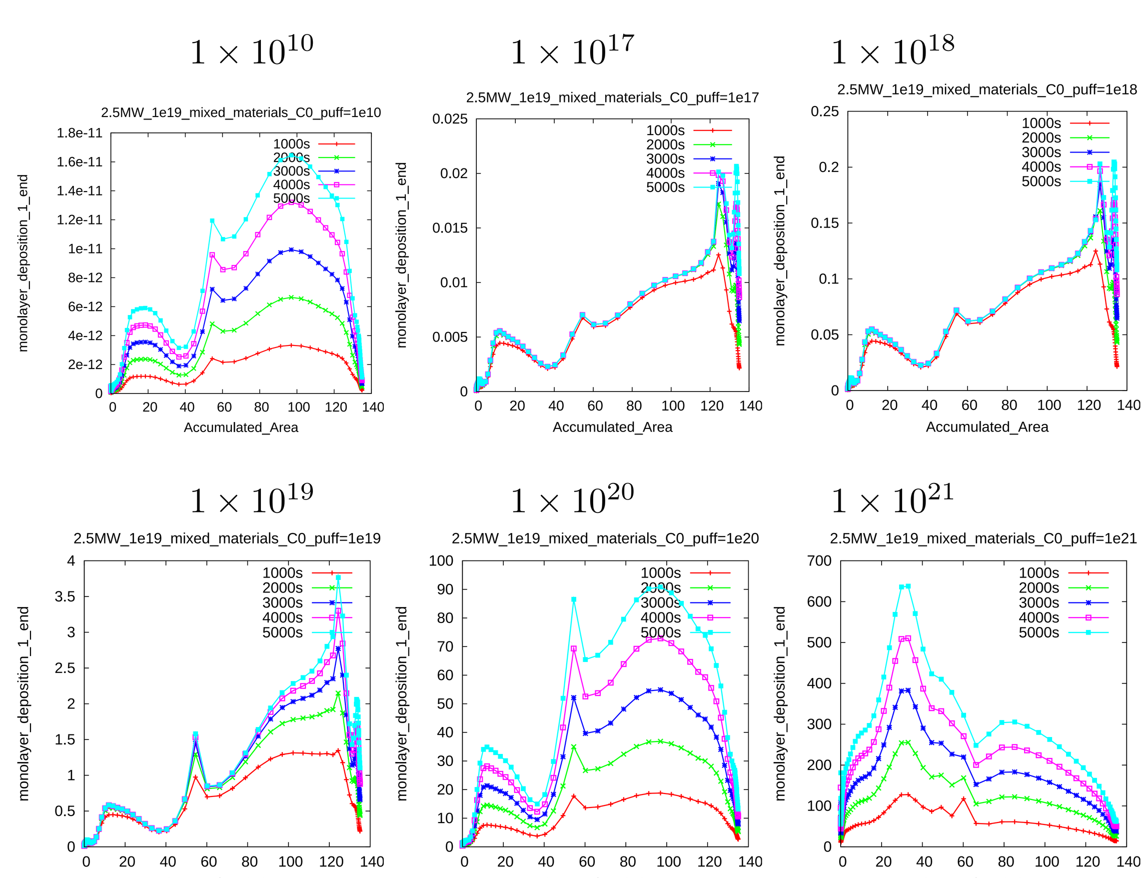
Be walls and target, C gas puff

JET

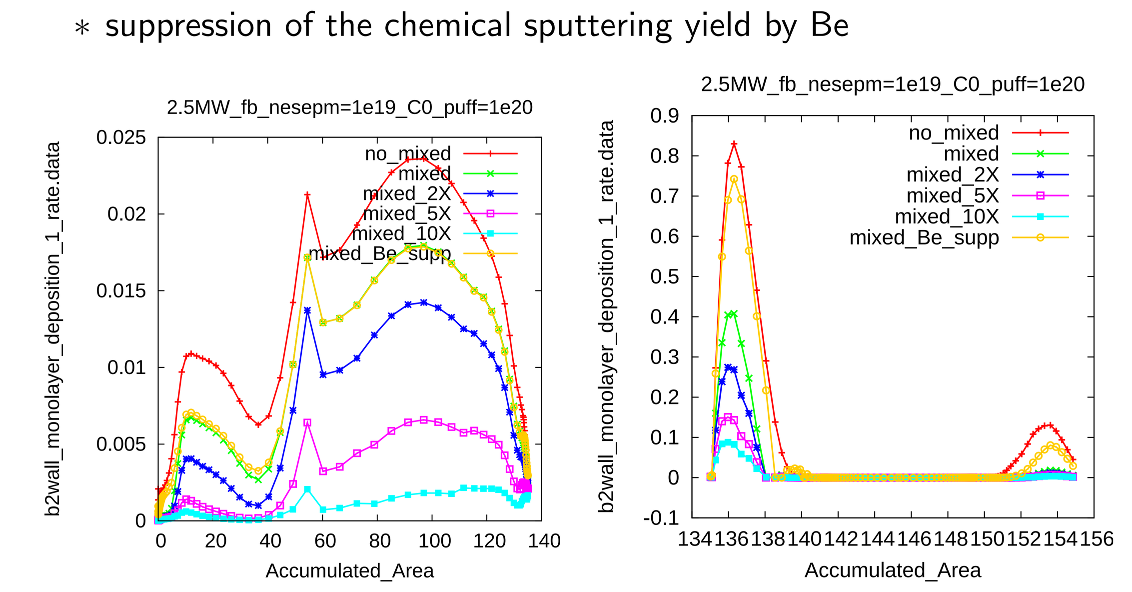
- strong dependence of the main chamber C deposition on the on the C puff rate



- rate is approximately constant for the lowest gas puff rate (corresponding to a linearly growing layer)
- rate tapers off for the intermediate gas puff rates



- examine the effect of differing sputtering models
- compare
  - no-mixed-materials model
  - mixed-materials model
    - ∗ deposited C with same properties as base C
    - ∗ 2 × enhancement of the chemical sputtering yield of deposited carbon
    - ∗ 5 × enhancement of the chemical sputtering yield of deposited carbon
    - ∗ 10 × enhancement of the chemical sputtering yield of deposited carbon
    - ∗ suppression of the chemical sputtering yield by Be



Monolayer deposition rates of the puffed C to the main chamber wall (left) and targets (right) with varying mixed materials models applied to JET. (In the right panel, the outer target is to the left, the private flux in the middle and the inner target on the right.)

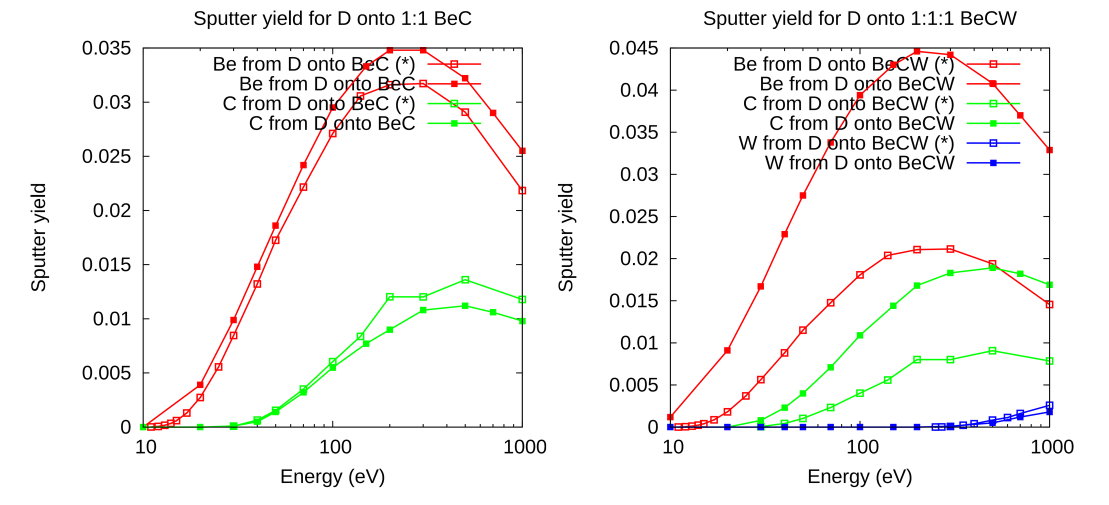
- highest net deposition in the main chamber for
  - model without re-erosion ("no-mixed")
  - Be suppressed erosion
  - "standard" model
  - 2 × enhancement factor for erosion of re-deposited C
  - 5 × enhancement factor for erosion of re-deposited C
  - 10 × enhancement factor for erosion of re-deposited C

Summary

- mixed material model has been implemented in the B2 part of SOLPS
  - tracks
    - ∗ erosion of base material
    - ∗ deposited material
    - ∗ re-erosion of deposited material
  - simple model for sputtering based on scaling the sputtering from "pure" (single species) surfaces by the local concentration
  - can have enhanced chemical erosion of deposited C
  - can have C chemical erosion decreased in the presence of Be
- simulations have been performed for
  - AUG, JET, ITER
  - different C walls; C walls and C gas puff ; C targets and Be walls; Be walls and targets and C gas puffs
- find:
  - new time-scales are introduced
  - whether ^{13}C injected at the top of a JET simulation ends up at the inner or outer target depends strongly on the density
  - in the ITER simulation, the net C deposition rate starts at around 2×10^{23} C atoms per second, but as deposited areas build up, this drops to around 3×10^{21} after 70 minutes discharge time.
- *Caveats:*
  - no drifts
  - no Monte-Carlo neutrals
  - walls at plasma boundary
  - models still need to be improved

Outlook

- planned to improve the somewhat *ad hoc* mixed-materials sputtering models used by use of 3d data sets based on TRIM calculations (angle, incoming particle energy, fraction of (say) C in Be/C layer)
  - comparing with recent TRIM simulations for 1:1 BeC and 1:1:1 BeCW
    - ∗ likely effect small differences between present model for BeC
    - ∗ larger differences for BeCW
      - · the presence of the heavier element enhancing the erosion of Be & C
- also need surface and bulk properties
  - melting temperature
  - vapour pressure
  - emissivity
  - heat capacity
  - thermal conductivity
  - ...



Left: Physical sputtering yields of Be and C produced by D bombardment of a 1:1 mixture of Be and C. The lines labelled with (*) indicates that the single species TRIM data [Eckstein, 1998] were used, and scaled by the relative fraction of the Be or C in the mixture ($\frac{1}{2}$ in this case). Right: Physical sputtering yields of Be, C and W produced by D bombardment of a 1:1:1 mixture of Be, C and W. The lines labelled with (*) indicates that the single species TRIM data [Eckstein, 1998] were used, and scaled by the relative fraction of the Be, C or W in the mixture ($\frac{1}{3}$ in this case).

- in the near future, the ADAS project [ADAS,] is planning to release a bundled charge model for W
  - should soon be possible to extend the C-Be calculations to C-W, Be-W and to C-Be-W
- mixed-materials modifications should also be included in the Eirene part of SOLPS as well

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