Extensions to the SOLPS edge plasma simulation code to include additional surface interaction possibilities

D P Coster, X Bonnin*, M Warrier**,

Max Planck Institute for Plasma Physics,
EURATOM Association, Garching, Germany

** Formerly: Max Planck Institute for Plasma Physics, EURATOM Association, Greifswald, Germany*
Presently: Chargé de Recherche, Laboratoire d'Ingénierie des Matériaux et Hautes Pressions, CNRS
*** Formerly: Max Planck Institute for Plasma Physics, EURATOM Association, Greifswald, Germany,*
Presently: Institute for Plasma Research, BHAT, Gandhinagar, Gujarat, India

March, 2005
Oak Ridge

Overview

- What is SOLPS?
- What is used in SOLPS at the moment?
- What simple extensions have already been used?
- What is the present development strategy?
- What should be possible in the longer term?
- What is needed?
- Summary

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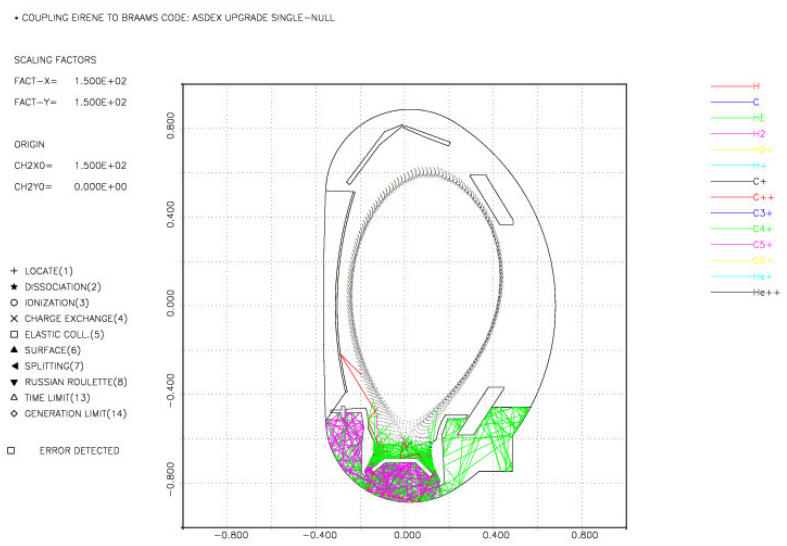
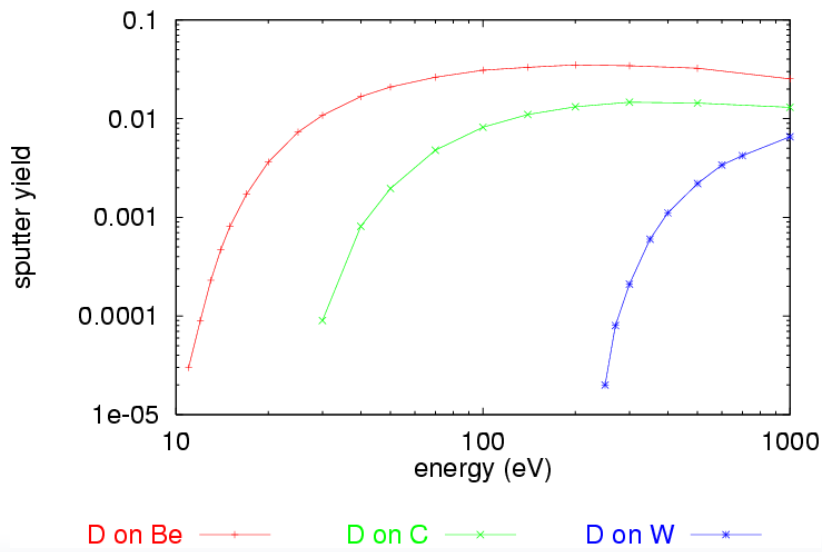
Model for the edge plasma of a tokamak

- plasma
  - 2d
  - fluid
  - multi-species
- neutrals
  - 2d or 3d
  - kinetic model or fluid model
- material surfaces
  - plasma streams towards
    - recycling
    - sputtering
    - erosion/deposition
  - source of neutrals for the plasma





Models for the edge plasma

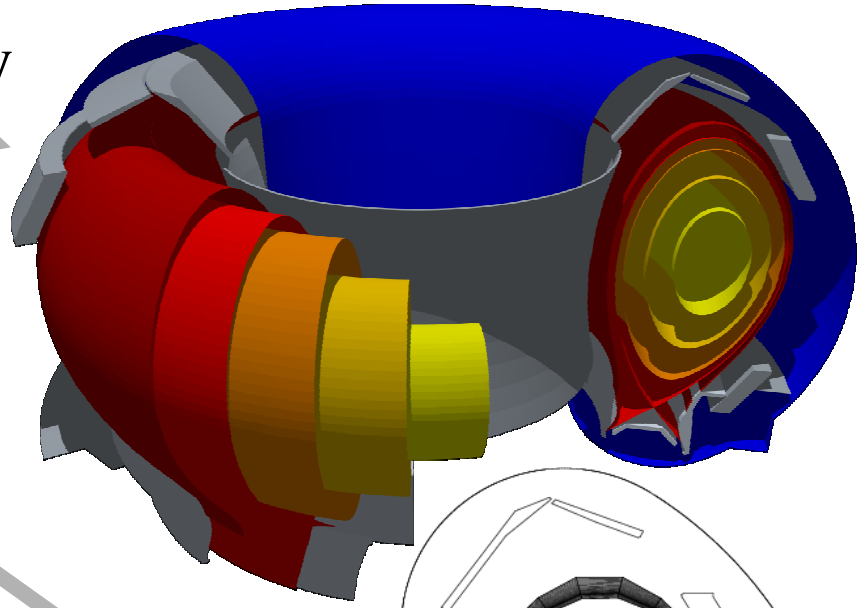
Hierarchy of models

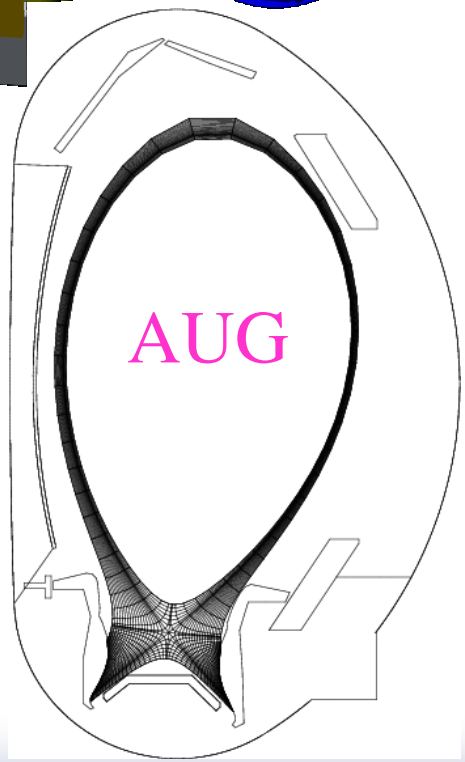
- in dimensionality
  - "two point" models (upstream versus downstream)
  - 1d
    - specialist studies
    - kinetic models (often 1-space, 2 or 3-velocity)
  - 2d
    - current "work horses"
    - one dimension along the field line (parallel), the other "radial"
  - 3d
    - specialist studies
    - stellarators
    - in development
- in physics included
  - impurities?
  - atomic physics
  - self consistency
- in "cost" of running

	DIVIMP	**ERO-JET**	**ASCOT**
Majority or impurity	Impurity	Impurity	Majority
2d or 3d	2d	3d	3d
Drifts	No	Partial (ExB)	Yes
Methane physics	???	Yes	N/A
Computational expense	Small	Large	2 days (2-6 hours elapsed)

Plasma model for the tokamak edge

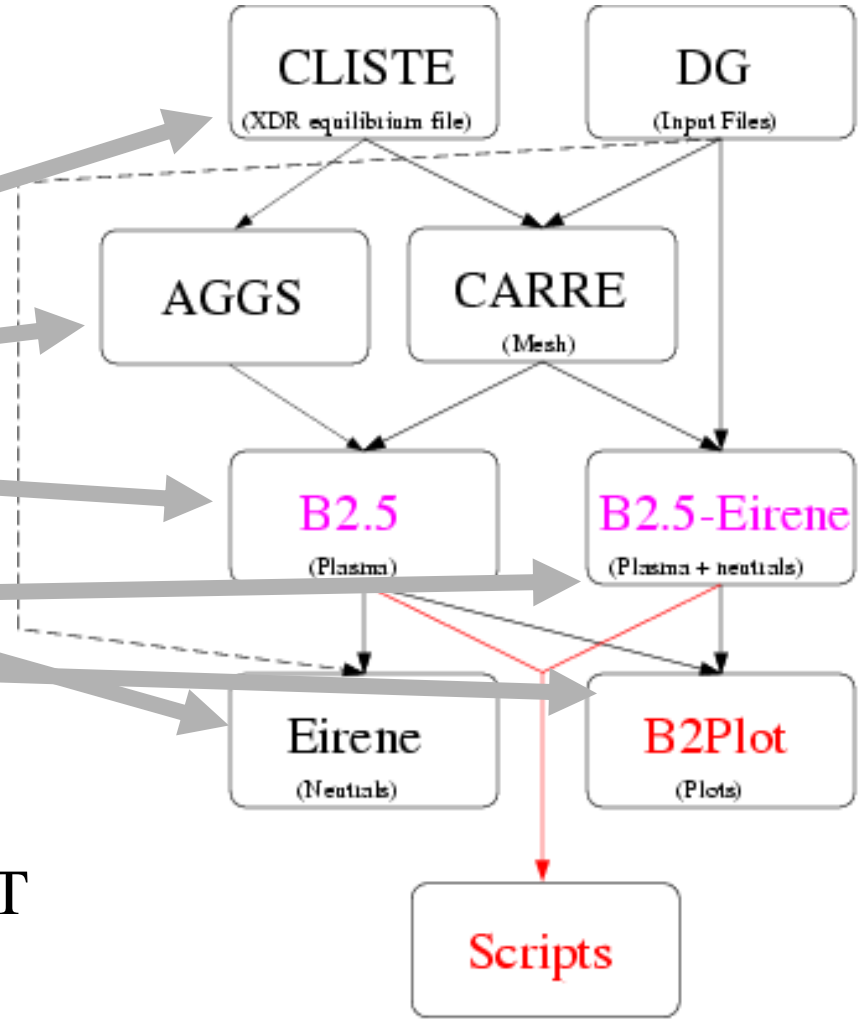
- Tokamak has toroidal symmetry
  - usually use 2d approach
- Edge plasma usually collisional
  - fluid approach
    - with kinetic corrections
      - much “cheaper” than kinetic approach!
- Conservation equations
  - density of each charge state
  - parallel momentum of each charge state
  - electron energy
  - ion energy
  - charge





SOLPS: Scrape-Off Layer Plasma Simulation

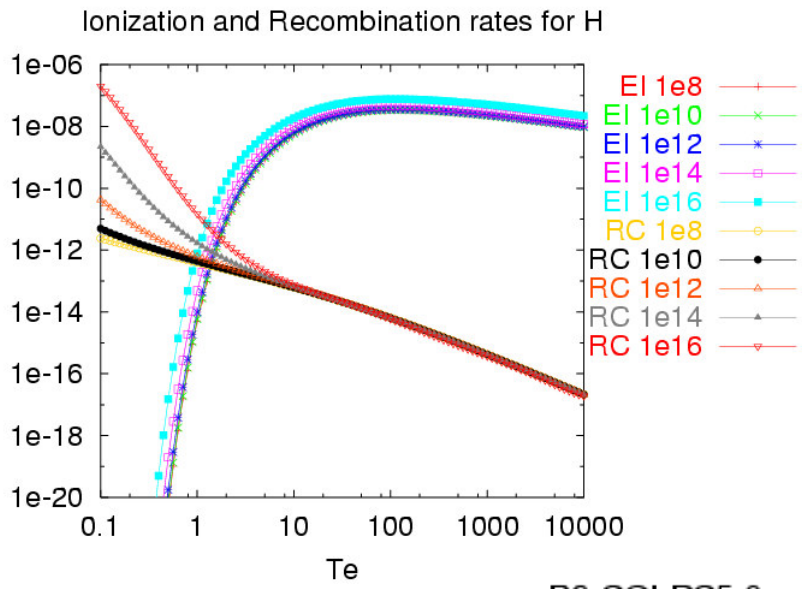
- One of the standard edge codes
  - (others include UEDGE from Livermore, EDGE2D-NIMBUS from JET)
- Suite of codes
  - Equilibrium → Grid
  - Plasma code
  - Neutrals code
  - Plasma+Neutrals Code
  - Diagnostics Code
- Developed over the last 15 years
- Used on existing machines (AUG, JET, CMOD, JT60-U, TCV, MAST ...)
- For design studies (ITER, SST, HT7U, ...)

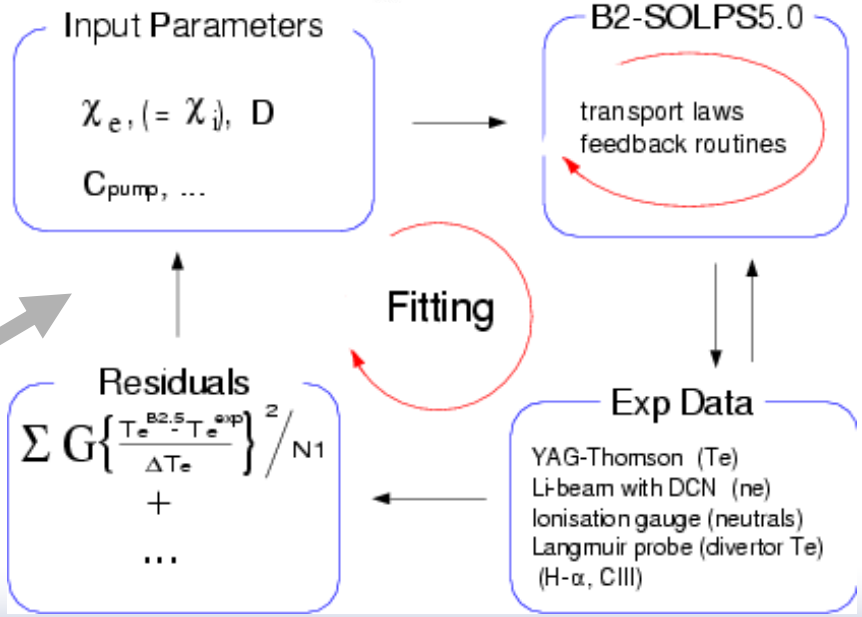


SOLPS 5.0

Plasma model, II

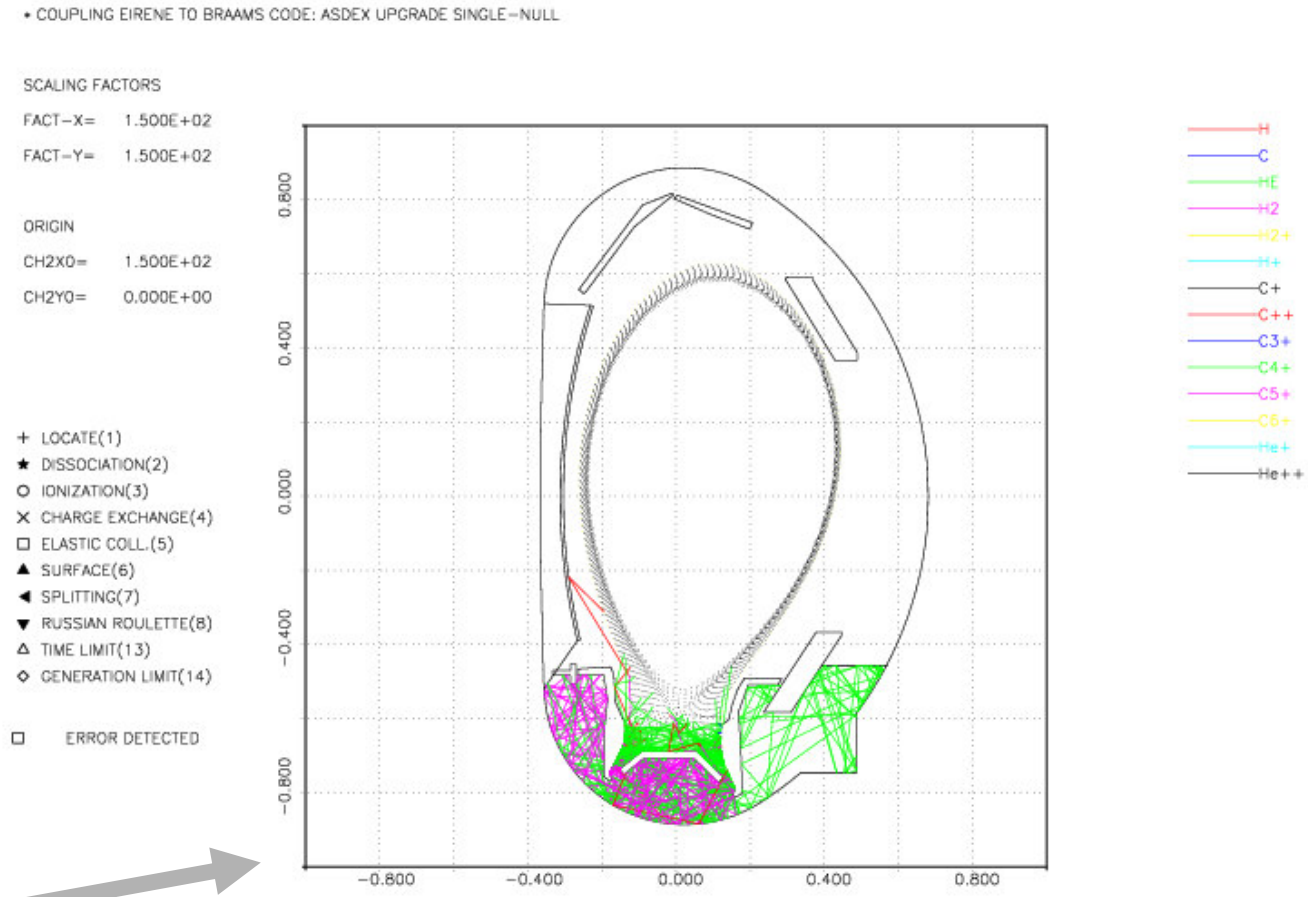
- Processes included
  - ionisation
  - charge exchange
  - recombination
  - radiation
  - ...
- Transport
  - (mostly) classical along field lines
  - anomalous + classical perpendicular to field lines
    - major uncertainty are the anomalous perpendicular transport coefficients to be used
      - automatically fitted to experiment
      - coupling to turbulence codes





Neutral model

- Plasma recombines to form neutrals
  - at surfaces [interaction with solids/or liquids]
  - in the volume
- Neutrals act as sources of particles, momentum and energy for the plasma
- Neutrals also interact with material surfaces
- Neutrals can be described by one of (or combination of)
  - fluid model
  - kinetic model



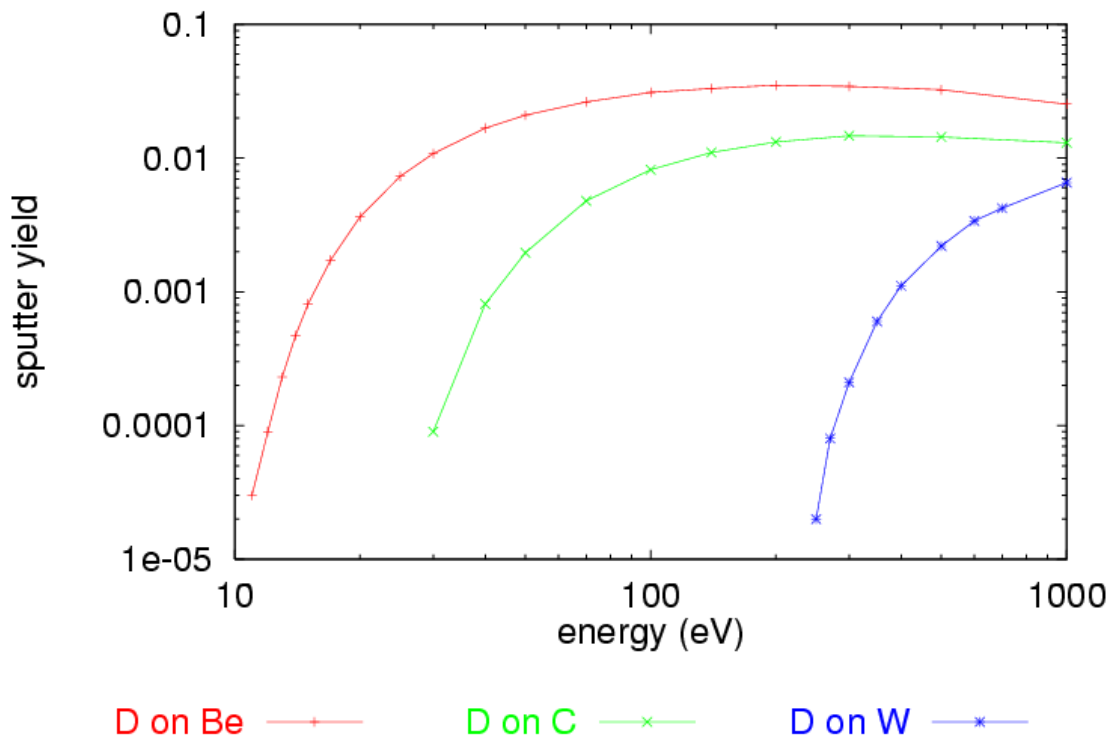
Neutral model, fluid or kinetic?

	Fluid	**Kinetic**
Dimensionality	2D	2D or 3D
Speed	Fast	Slower
Accuracy	Satisfactory upstream	Good everywhere
Ease of including details of structures	Difficult	Relatively easy
Ease of including atomic/surface physics effects	Moderate	Relatively easy for most, more difficult for others
Convergence	No new complications	Monte-Carlo noise

Ultimately a choice between speed and accuracy

Surface models

- Need the surface model to provide
  - recycling/reflection coefficients (particles and energy)
    - fixed
    - TRIM
  - sputtering coefficients
    - physical
      - TRIM
    - chemical
      - fixed yield
      - Roth
      - ...



  - any additional sources of particles or energy
    - sublimation
    - ...

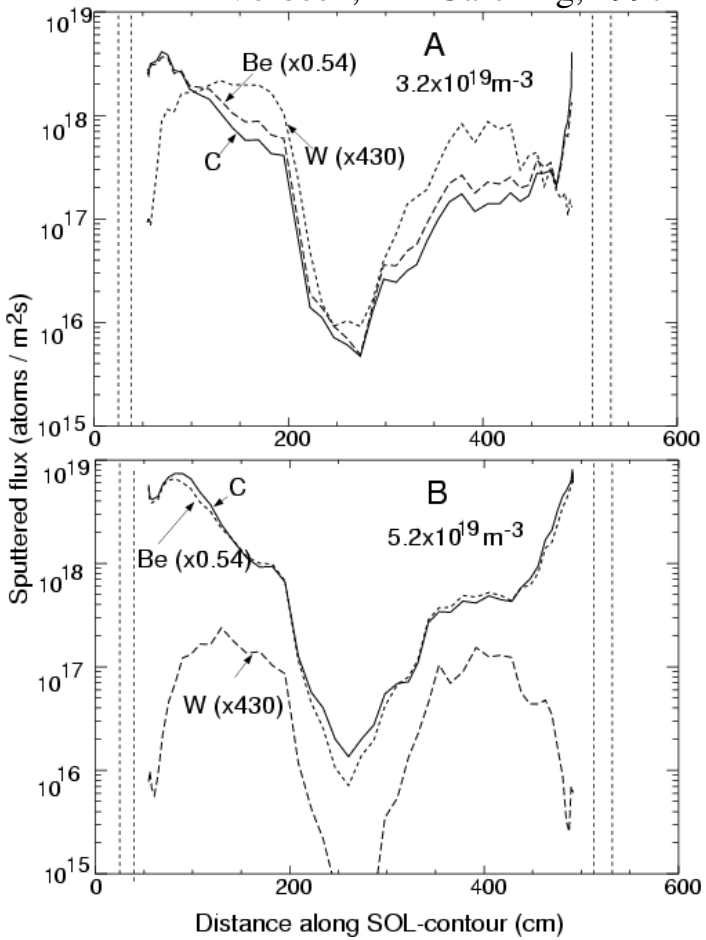
Surface models, II

- In typical runs today, we often assume
  - carbon arising from sputtering does so as C^0
    - can use CH_4
    - higher hydrocarbons are also important
  - carbon neutrals or ions leaving the plasma "stick"
    - i.e. zero recycling
- To do better, we need
  - better idea of what mix of hydrocarbons comes off the surface
  - to improve the hydrocarbon model in the codes
    - in development at the moment (Reiter …)
  - better idea of sticking/recycling/re-erosion properties for the various hydrocarbons
    - currently in development in a specialised code (ERO, Kirschner …)
- Details of the processes are often first looked at by more specialised codes, then later incorporated (if necessary) in "work horse" codes (*e.g.* ERO-JET, Jülich)

What can the SOLPS output be used for?

- Provides a plasma background for more specialised codes
  - EIRENE (Reiter, Jülich)
    - to look at charge exchange erosion
    - opacity effects (photon transport)
    - pumping
    - diagnostic interpretation
  - DIVIMP (Stangeby, Toronto)
    - to look at tungsten erosion and deposition
    - direct simulation of some diagnostics
  - ERO-JET (Kirschner, Jülich)
    - to try and understand erosion/re-deposition
    - role of hydrocarbons
  - ASCOT (Sipila, HUT)
    - L-H transitions
    - ion orbit power loss to targets
  - ...

Verbeek, IPP-Garching, 1997



- **But all this is predicated on the SOLPS output being a good match to the experiment**

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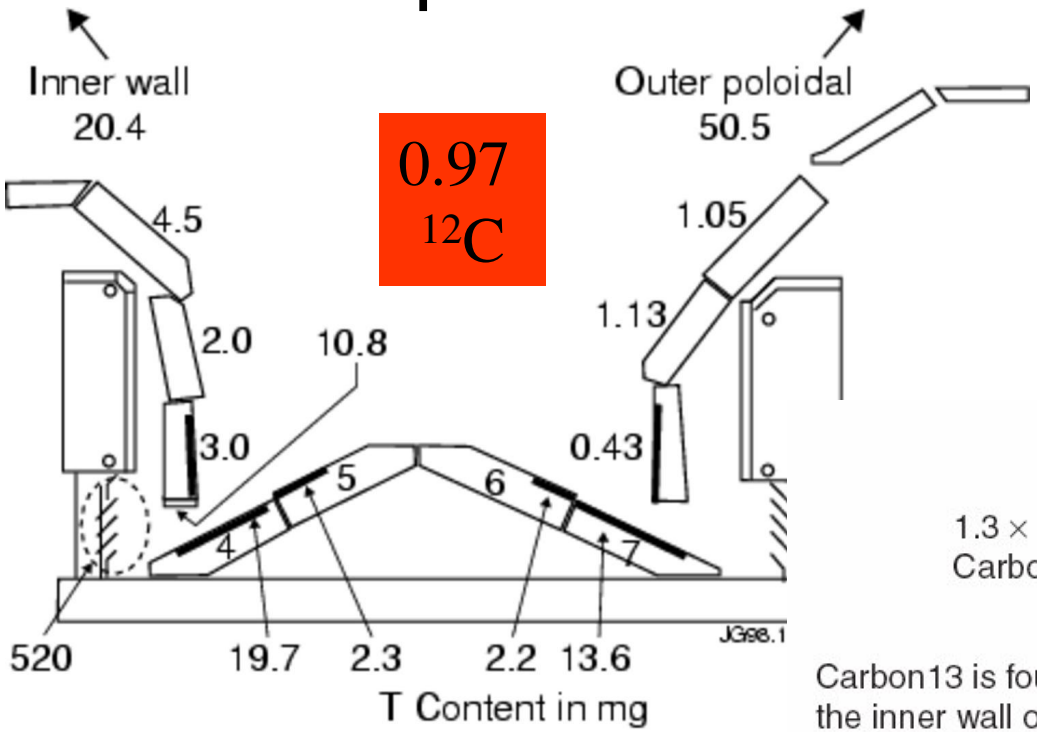
SOLPS impurity modelling

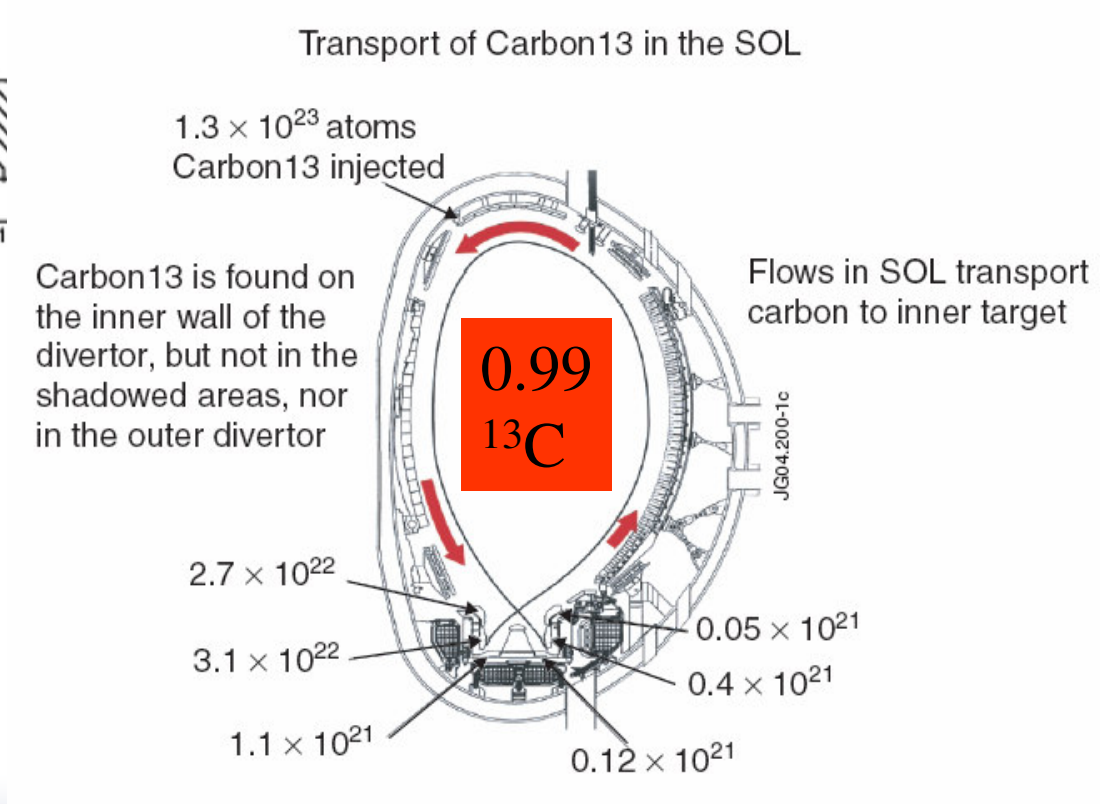
- D+^{12}C+^{13}C+He SOLPS (B2-EIRENE) modelling for JET
- Attempt to explain C asymmetry
- The following don't work
  - Transport ballooning
  - Position of gas puffs
  - Drifts
- Need more

Experimental data: C asymmetry



Coad, JNM 2001

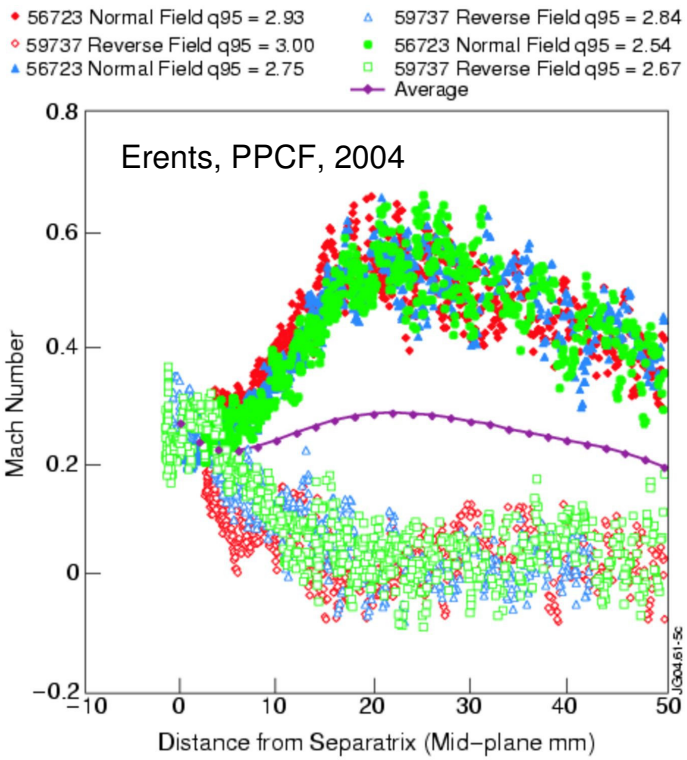
^{13}C gas puff

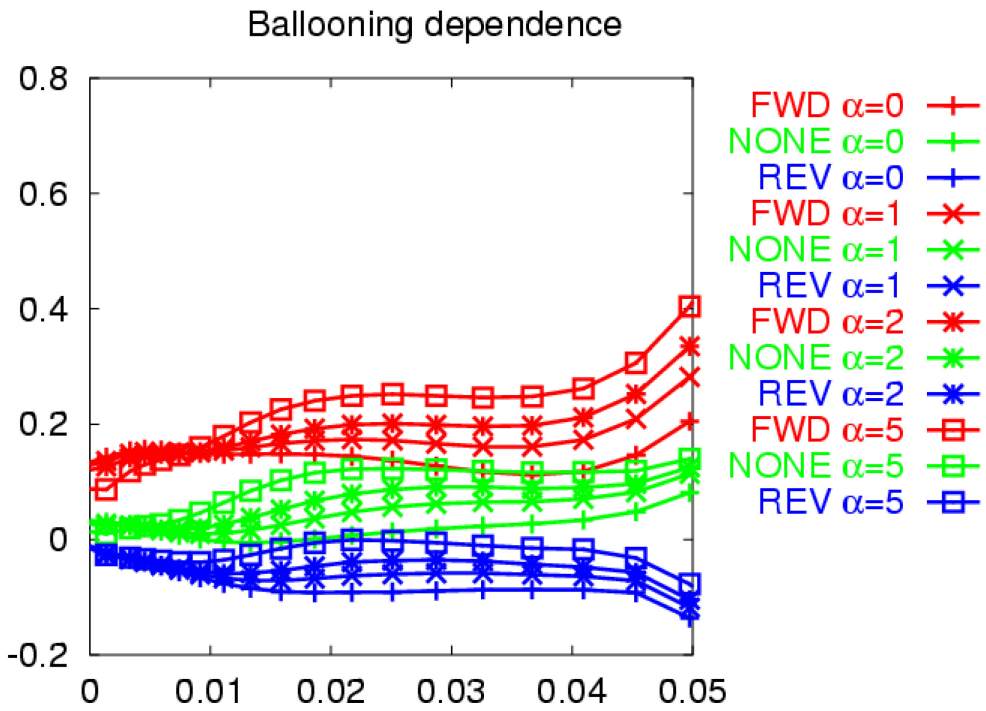


Strachan, EPS, 2004

Using T as a marker for C migration

Mach number comparisons, II

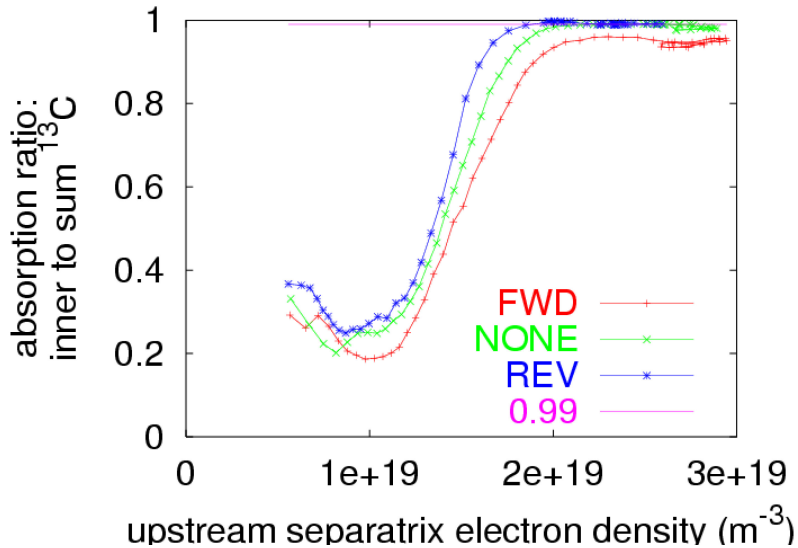


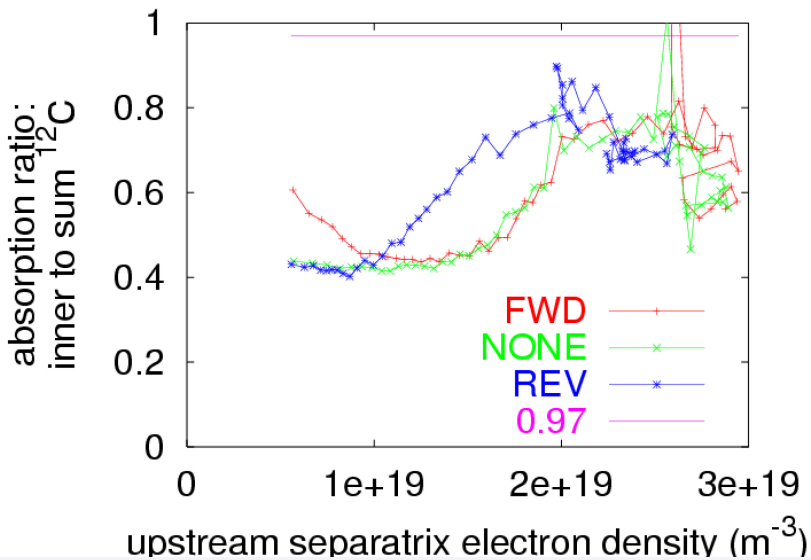


- Experiment vs SOLPS (drifts + ballooning)
- Match (reasonably) drifts
- But, still don't reproduce experimental C asymmetries

^{13}C asymmetry strongly affected

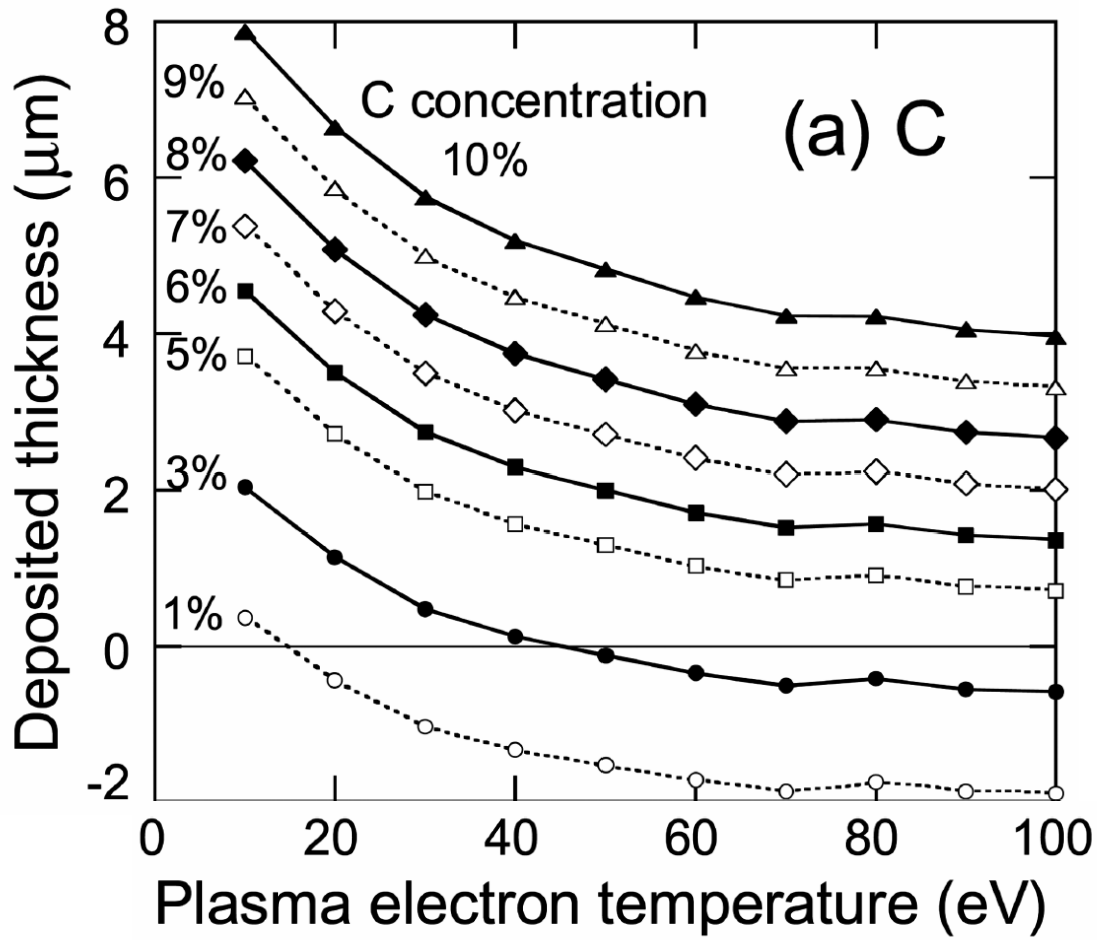
- With increasing density, the ^{13}C asymmetry is strongly affected, with most of the ^{13}C appearing at the inner target
- The ^{12}C asymmetry increases somewhat, though not to "experimental" levels





Introduce a new recycling model

- Nothing we have done seems to have been able to raise the intrinsic C (^{12}C) asymmetry to the experimental levels
- Introduce a new recycling model to SOLPS
  - usually we assume C does not recycle
  - change so that above a critical temperature, C is assumed to recycle
  - motivated by --->



"Deposited thickness of C exposed to a plasma containing D^+ ions and different amounts of C^{4+} ions as a function of the plasma temperature. The plasma ion fluence is 1 x 10^{21} cm^{-2}. The thickness is calculated [...] on the basis of [physical] sputtering yields and reflection coefficients of the pure C [...] materials. Negative values in the ordinate represent net erosion." [Ohya et al, Physica Scripta Vol 111, 138-144, 2004: fig. 1]

Results of the new model:

	^{12}C			^{13}C		
drifts	fwd	no	rev	fwd	no	rev
Crec=0	0.62	0.46	0.40	0.30	0.35	0.37
C13rec=1	0.58	0.45	0.47	—	—	—
C13rec=10eV	0.62	0.47	0.41	0.53	0.45	0.44
Crec=10eV	0.95	0.57	0.45	0.64	0.45	0.38
C13rec=5eV	0.63	0.46	0.45	0.64	0.50	0.34
Crec=5eV	1.14	0.85	0.48	0.81	0.54	0.41

Table 2: Fraction of the C absorbed at the inner target (incoming-outgoing) to that absorbed at both targets for various assumptions about C recycling. Based on T analysis, the ^{12}C asymmetry is approximately 0.97 and from the ^{13}C gas puff experiment, the ^{13}C asymmetry is approximately 0.99.

- For the first time we have been able to see in SOLPS simulations the sorts of asymmetry seen in experiment
- [Previous EDGE2D-NIMBUS studies had
  - added an artificial flow
  - added a (partly) artificial force
  - implemented a giant convective cell]

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Recent Inclusions in the SOLPS Code

- Need to distinguish between Eirene and B2
  - Eirene (most not yet implemented in the standard SOLPS version)
    - Position of C sputtering at MCW (Kukushkin)
    - Switch from Be surface to C based on deposition (Kukushkin)
    - Better hydrocarbon atomic physics (Janev, Reiter, …)
    - Neutral-neutral collisions (Reiter …)
    - Photon transport (Reiter, Wiesen, …)

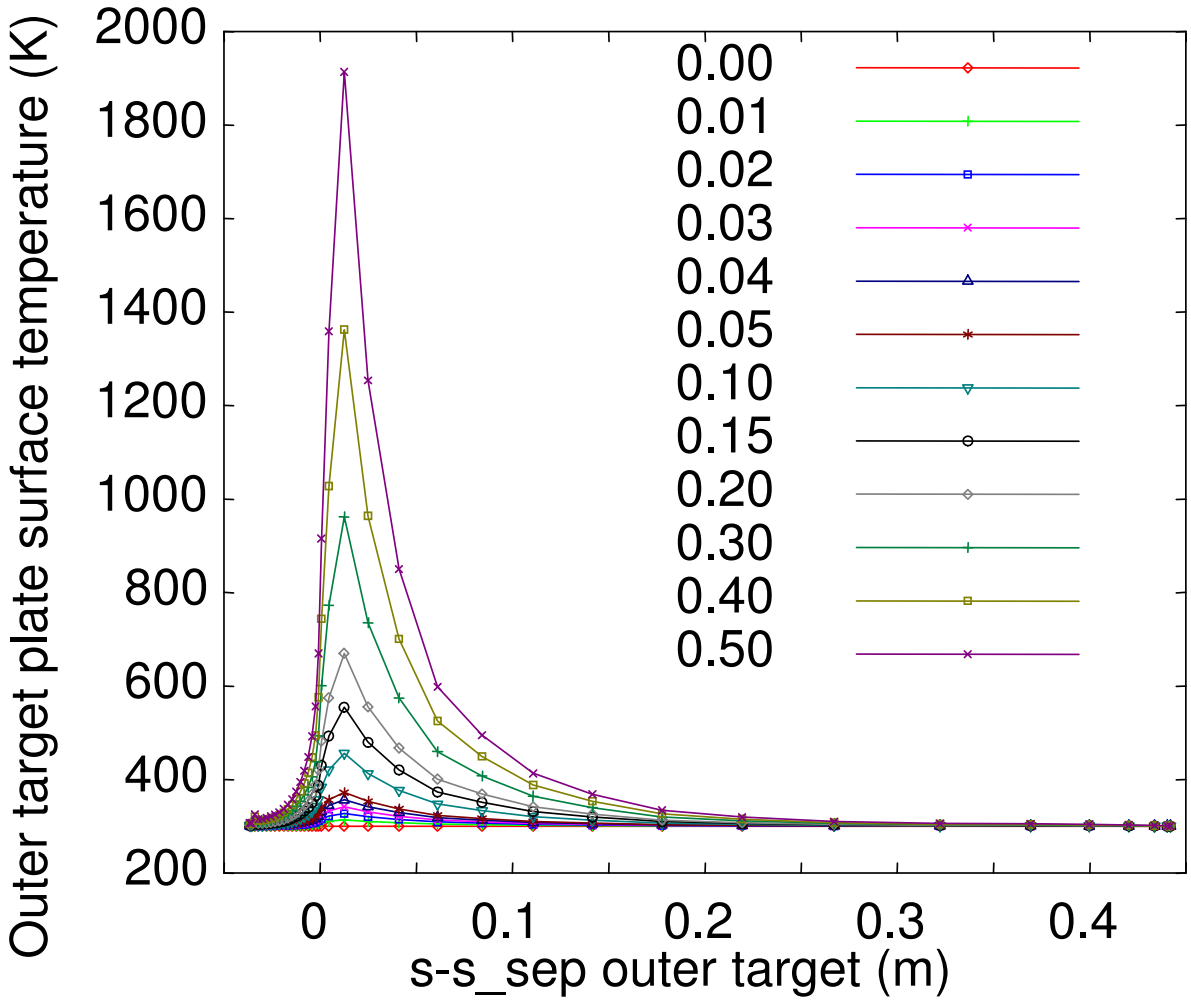
Recent Inclusions in the SOLPS Code

- Need to distinguish between Eirene and B2
  - B2
    - Roth chemical sputtering model (Warrier, Bonnin)
    - RES (Warrier, Bonnin)
    - Backscattering (Warrier, Bonnin)
    - Plate heat transport model
      - 1d in the plate, time-independent
      - 1d in the plate, time dependent
    - Thermal evaporation
    - Mixed materials
      - Brand new
      - In development

Plate thermal models

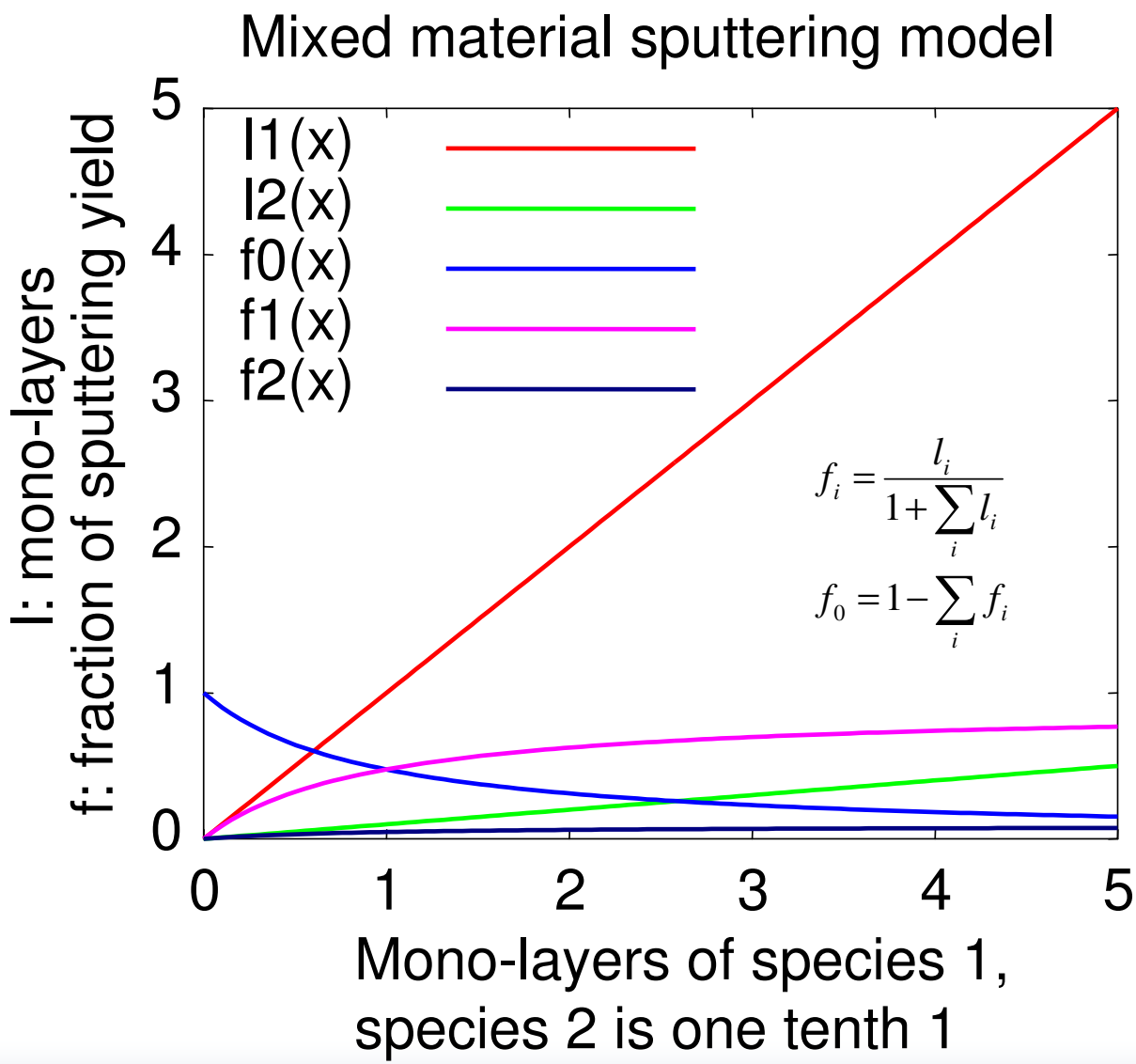
- Thermal models for each surface element:
  - –Specified temperature
  - –1d-space, time-independent (steady-state)
  - –1d-space, time-dependent (ELMs, short pulse tokamaks)
    - •Linear spacing
    - •Logarithmic spacing (in development)
  - –2d-space, time dependent (slot available, not coded)

Plate surface temperature for different plate thicknesses



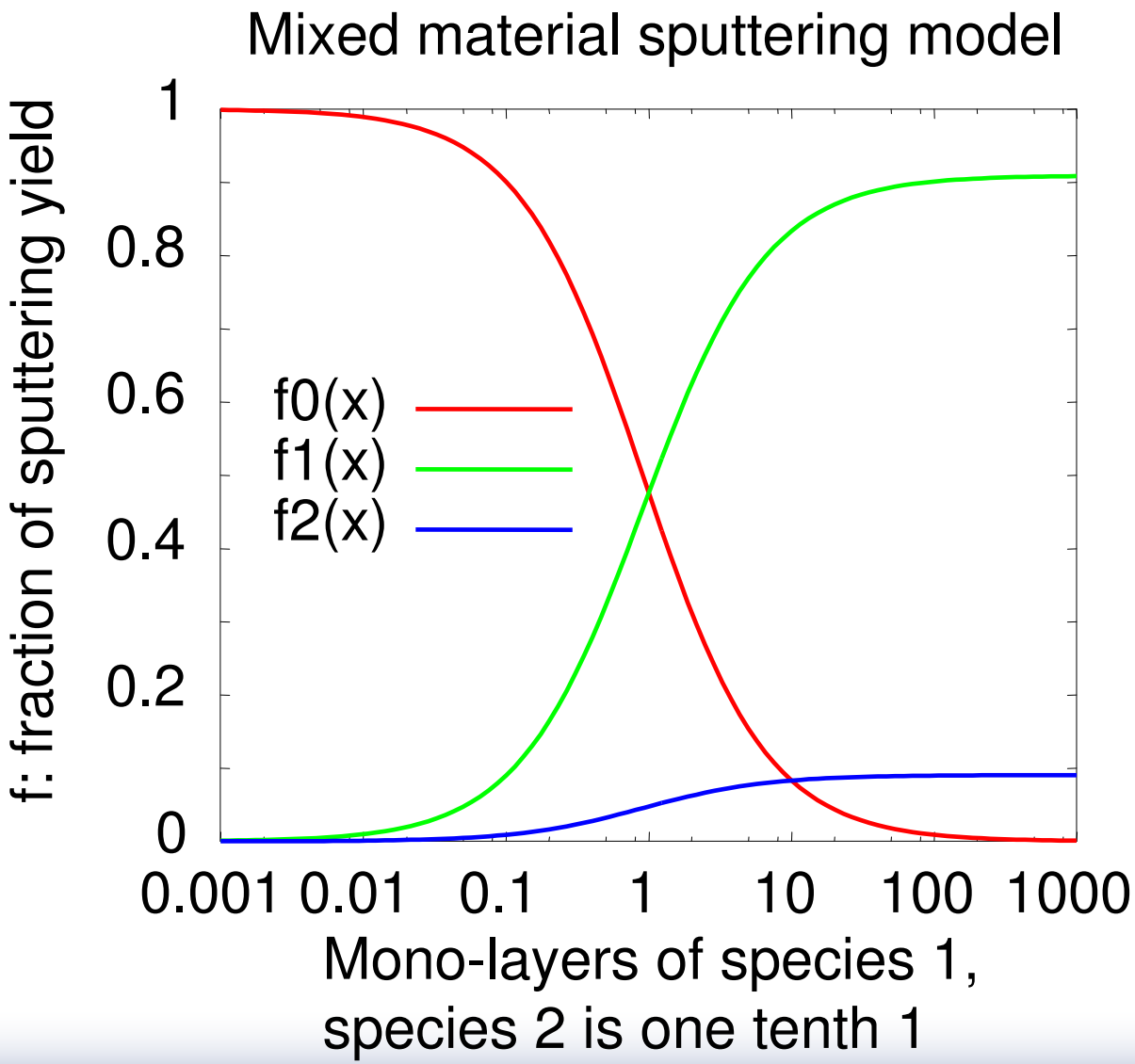
Started mixed materials

- Started implementation of a mixed materials model into B2
  - 0d for each surface element
  - Time dependent
  - Sputter fraction dependent on the number of deposited mono-layers
  - To do better we need input from the PSI community!



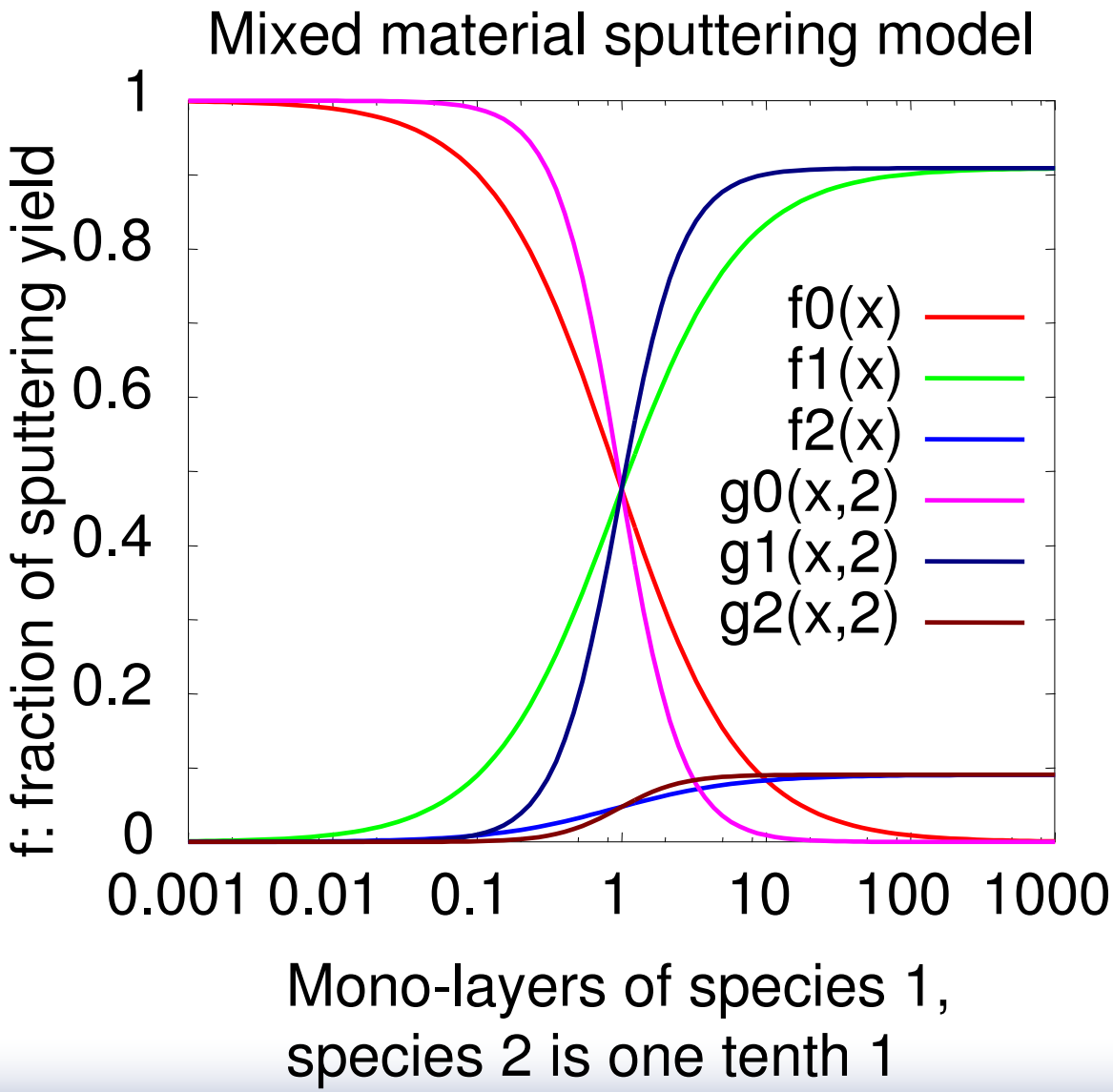
Sputter fraction determined by deposited layers

- Model gives a transition from pure base material erosion to pure deposited material erosion in the range from ≈ 0.01 to 100 mono-layers



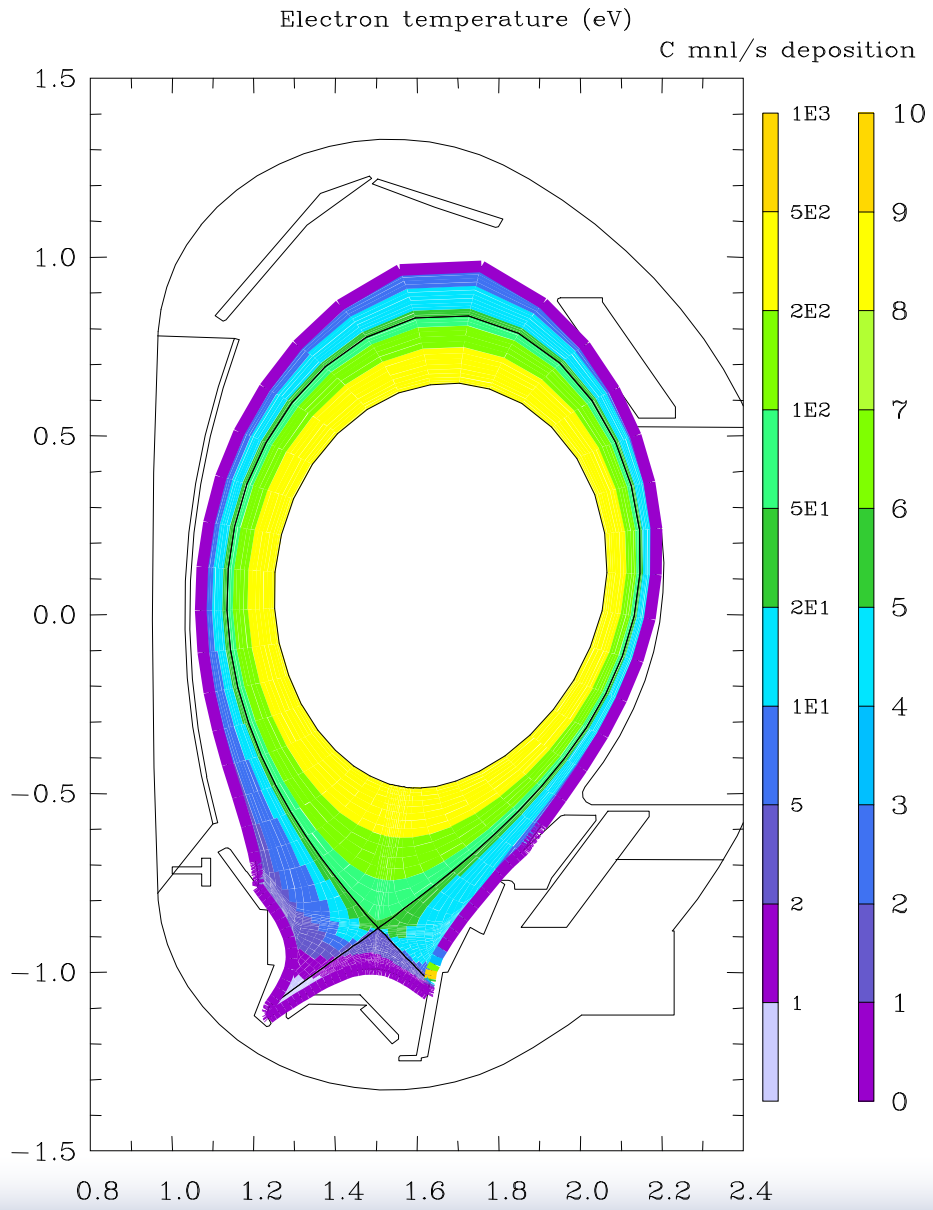
Model very simple!

- Can make the transition "faster" by raising **x**, the mono-layer fraction, to a power, **n** (here 2)
- **n** could be chosen by comparison to sputter modelling
- Or the entire simple model could be replaced



Applying the model to a C case

- Here we have plotted
  - Te on the plasma grid in
  - C deposition rate in mono-layers per second
- Strongest erosion at the outer target
- Ohmic standard shot, 18737
  - Perhaps not the most relevant of conditions



Geometry and coordinates

We will be plotting time traces later at positions "55" and "112"

Targets:

Outer **T**op

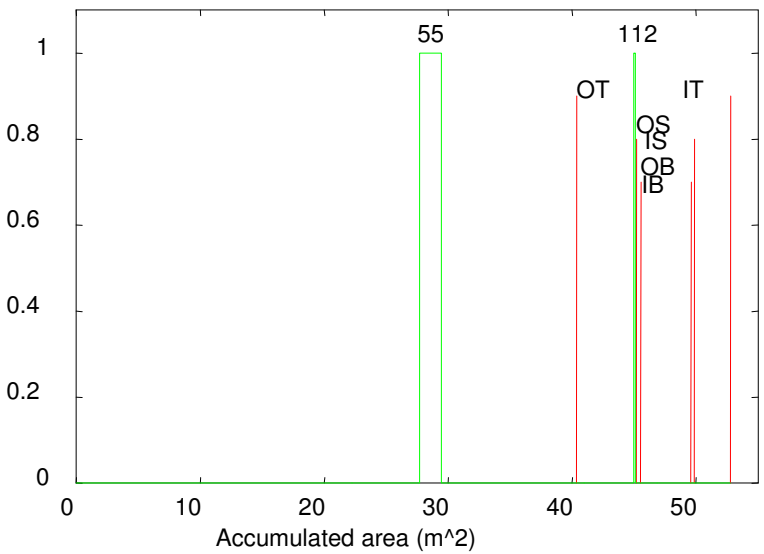
Outer **S**ep.

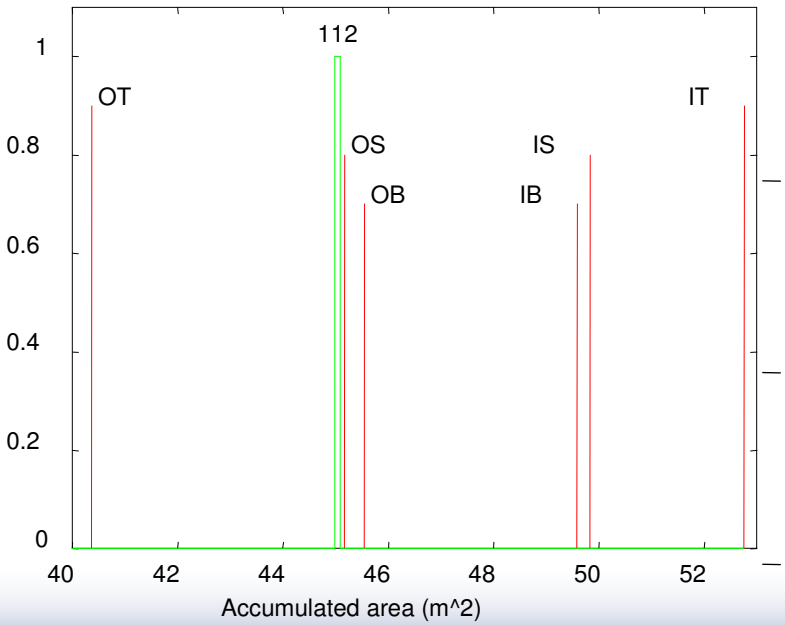
Outer **B**ot.

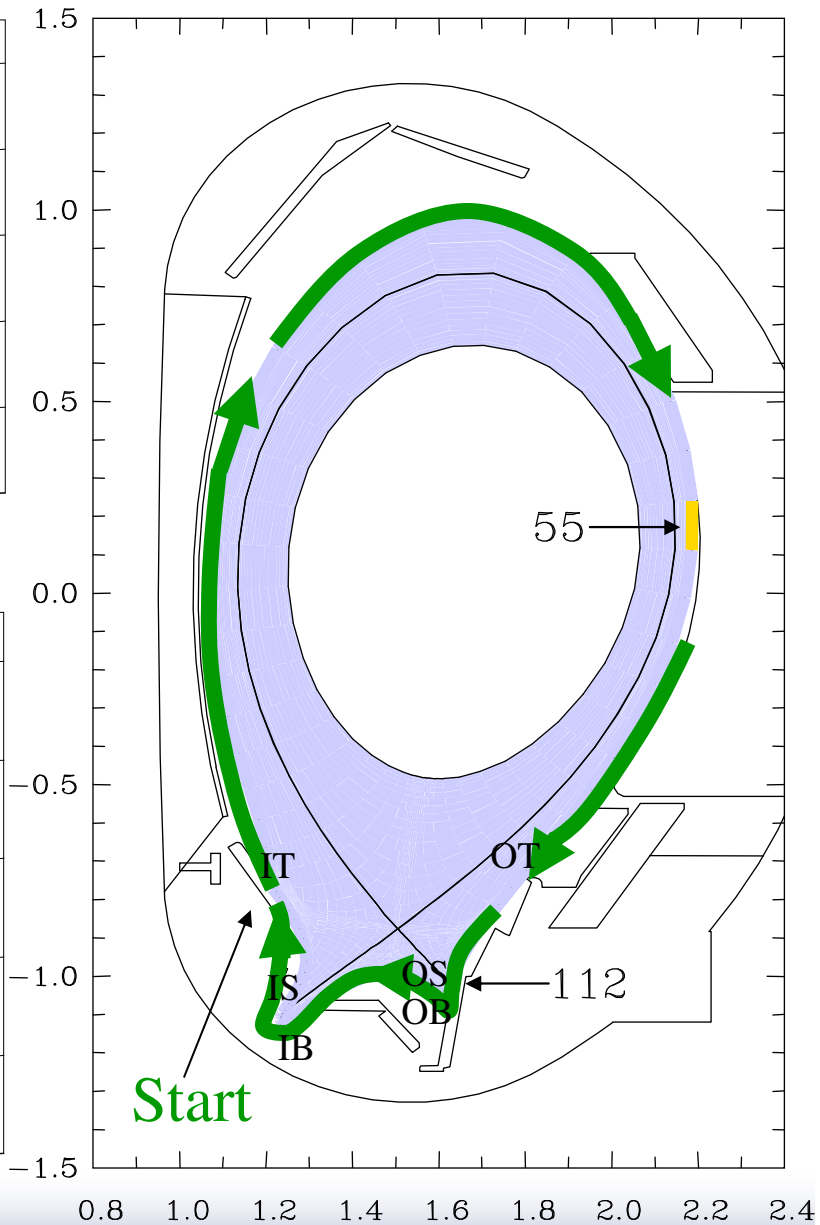
Inner **B**ot.

Inner **S**ep.

Inner **T**op







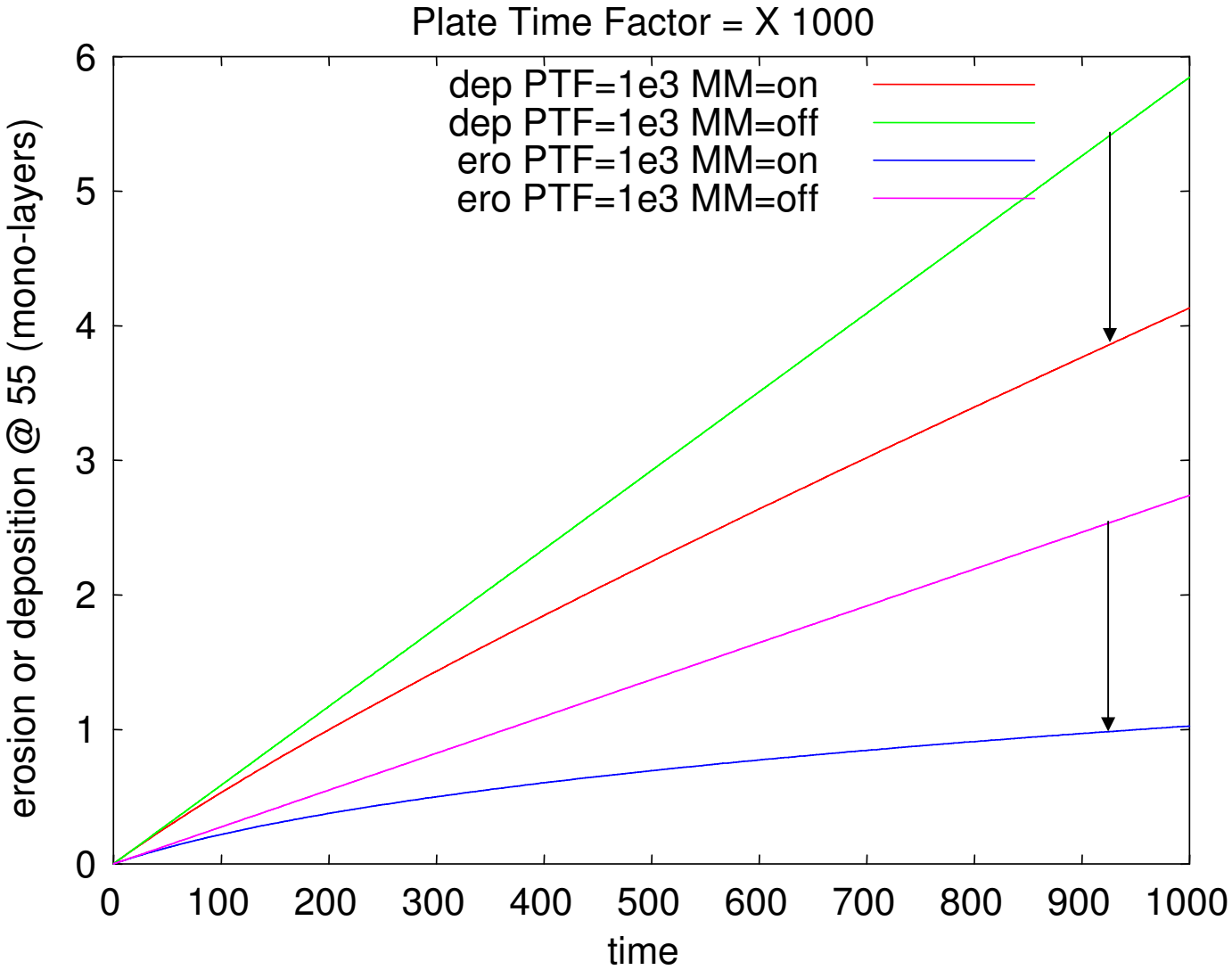
Mixed materials, D+C+He

- Comparing mixed materials model off with on
- Why mixed materials?
  - Base C
  - Deposited C
  - Both can be eroded
- Targets: C
- Walls: C
- AUG standard Ohmic shot (18737)
- Plasma conditions unaffected because base C == deposited C (assumption)

Mixed materials, D+C+He

Surface 55

- Smaller base material erosion when switching on Mixed Materials Model

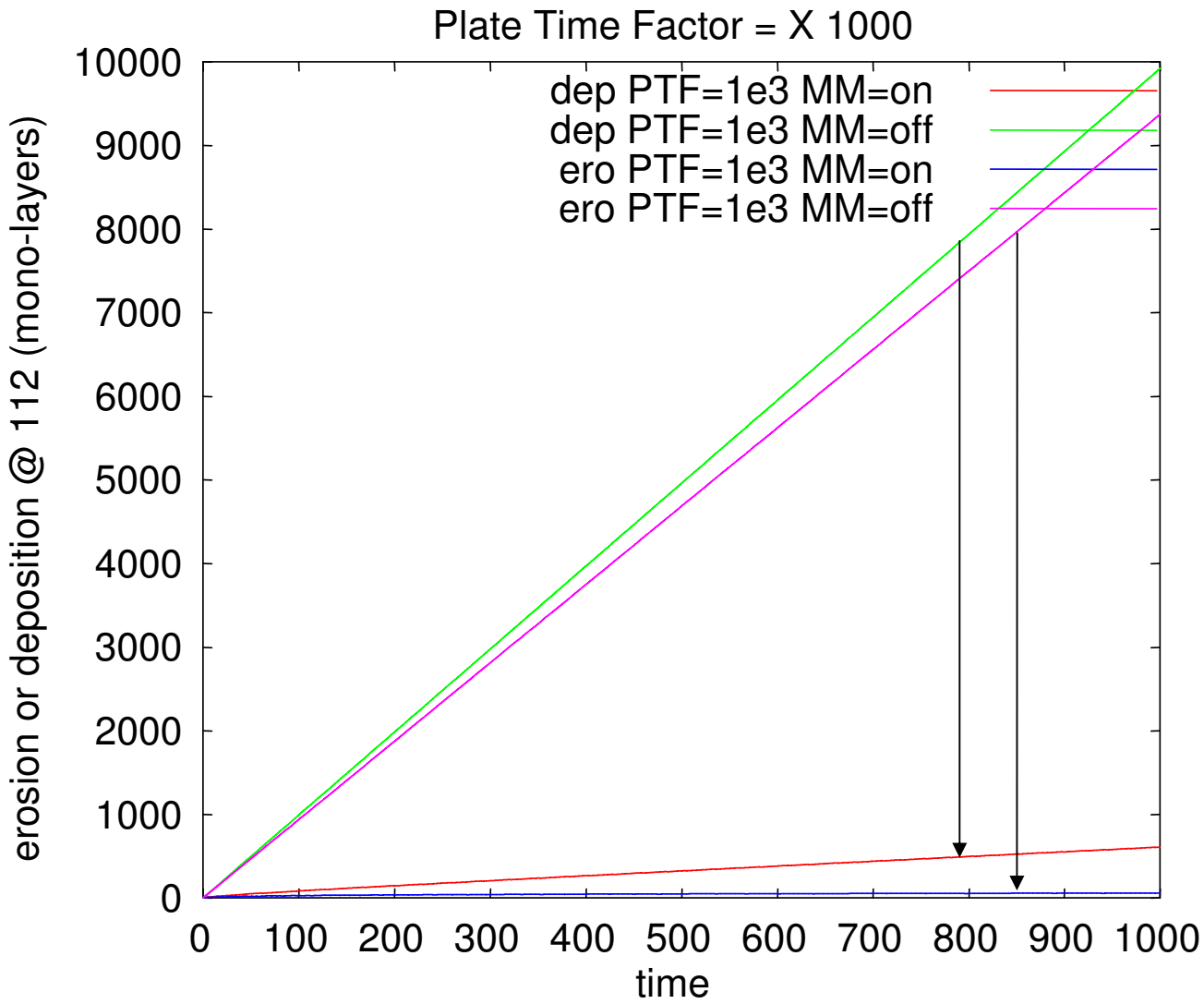


Mixed materials, D+C+He

Surface 112

- Substantial drops in erosion and deposition when Mixed Material Model switched on

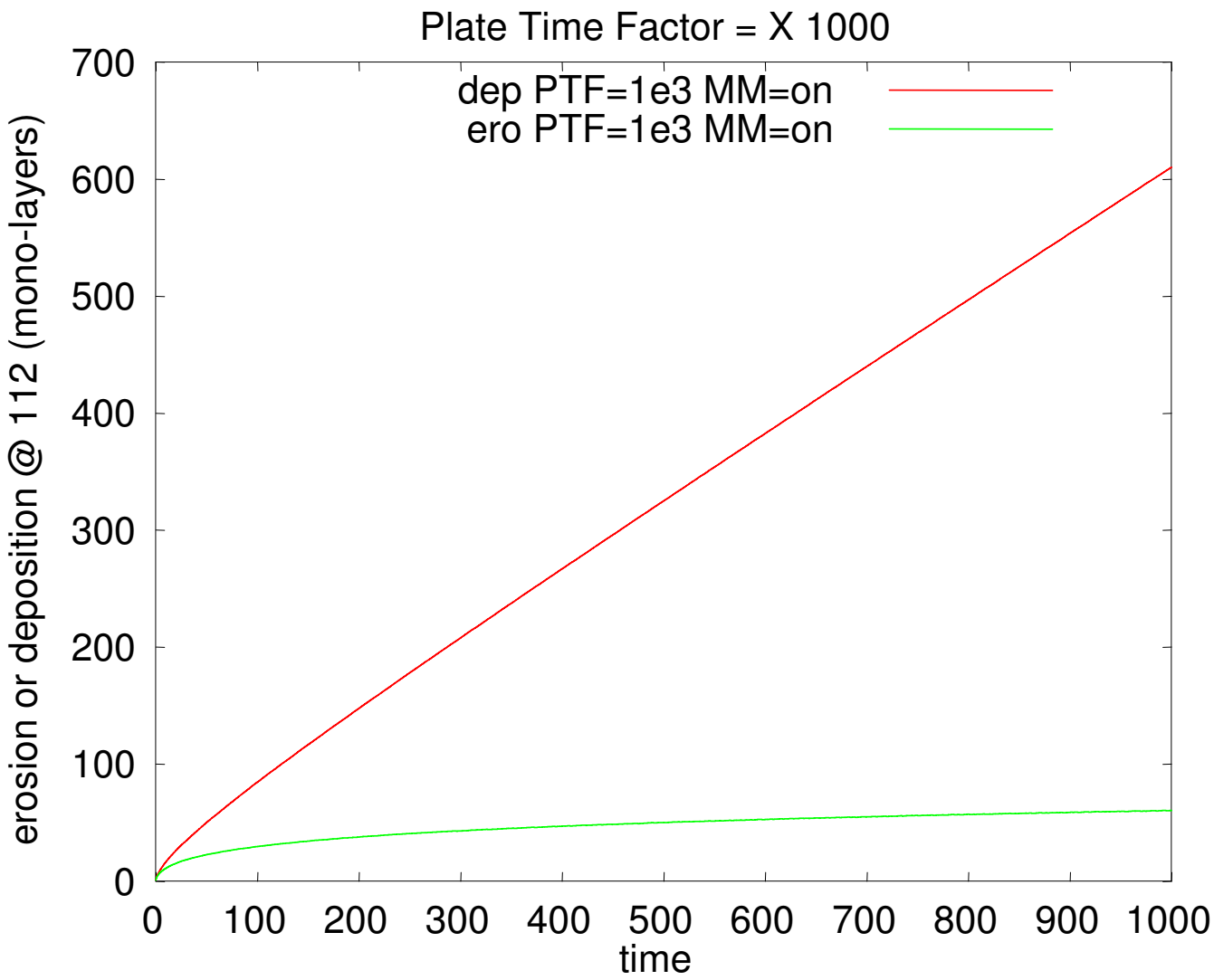
- Much larger erosion and deposition at this surface than at 55 (fluxes much higher)



Mixed materials, D+C+He

Looking just at the mixed materials case for 112

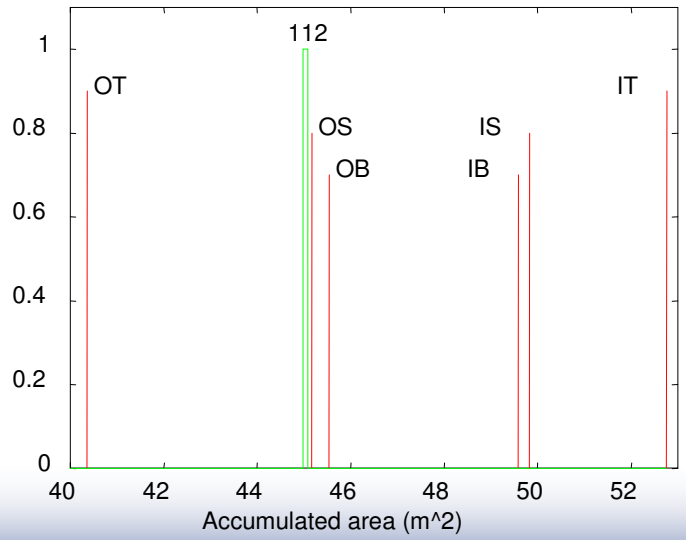
- Base material erosion essentially switched off
- Would occur earlier if model were "sharpened"

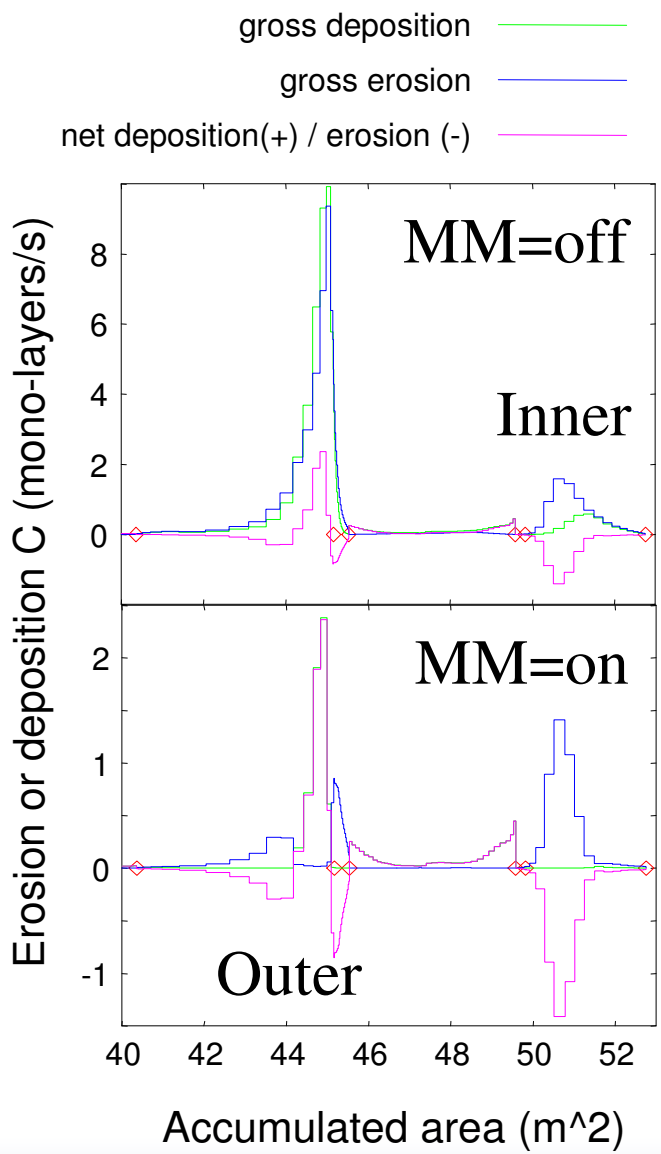


Mixed materials, D+C+He

Pattern of erosion and deposition

- For Mixed Materials Model off
  - Peak gross of 10 mono-layers/s
- For Mixed Materials Model on
  - Peak gross of 2.5 mono-layers/s
- Plasma conditions unchanged



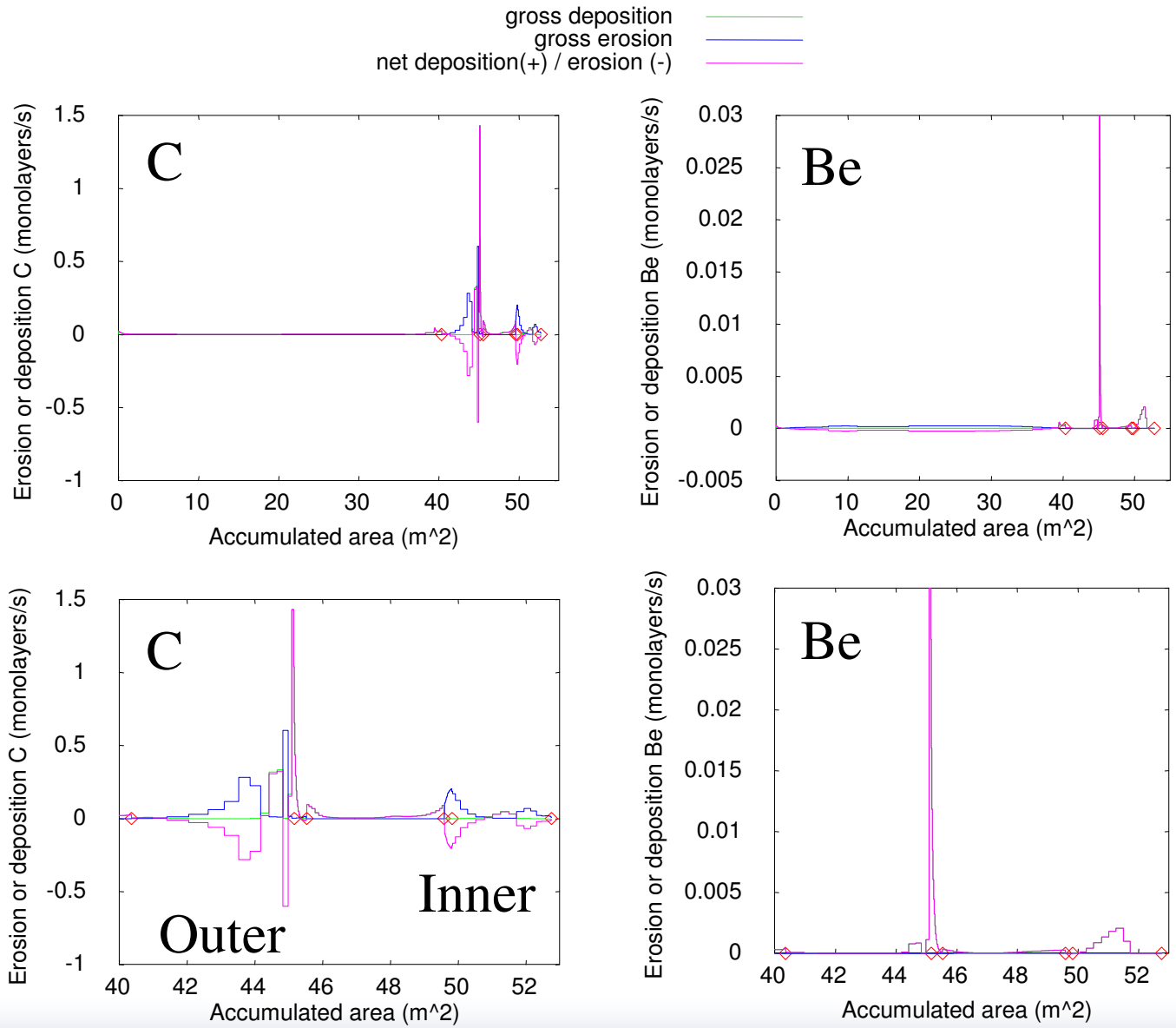


Mixed materials, D+C+He+Be

Targets: C

Walls: Be

Be erosion (from the walls) is much lower than C



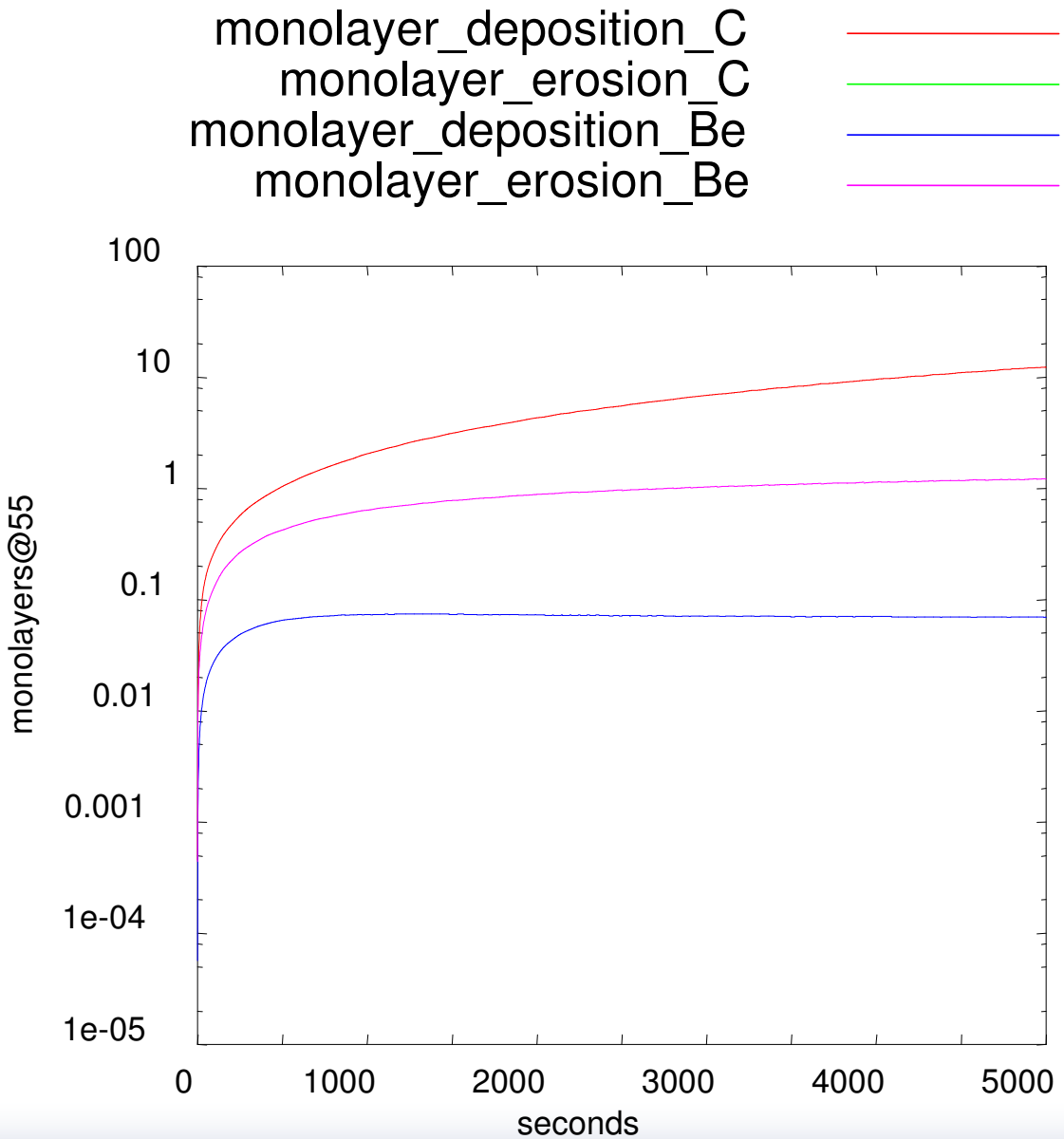
Mixed materials, D+C+He+Be

Targets: C

Walls: Be

Analysis at 55 (near the outer mid-plane)

- C continues to be deposited
- Be deposition stops

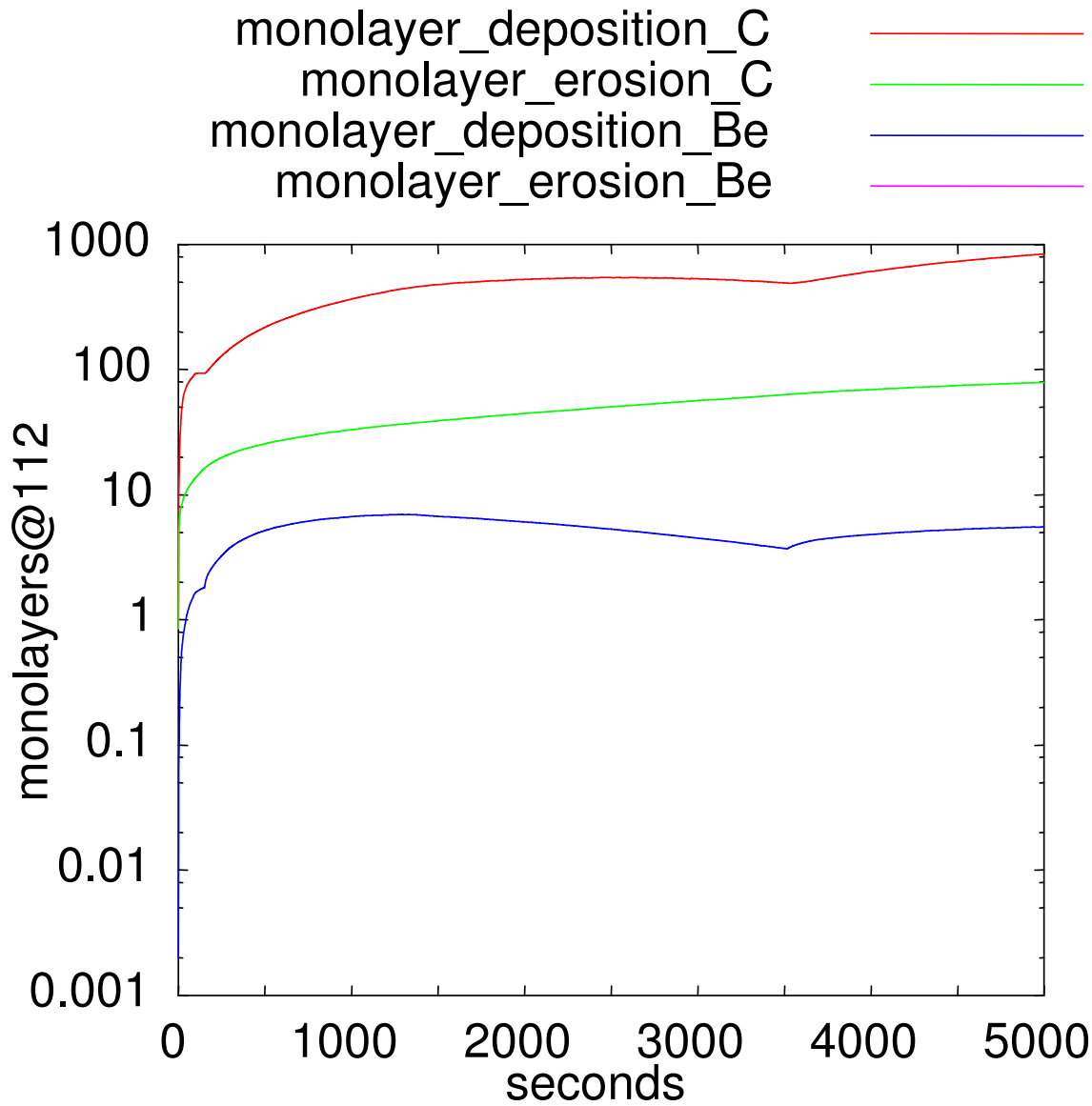


Mixed materials, D+C+He+Be

Targets: C

Walls: Be

Analysis at 112 (near the outer target separatrix)



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In the longer term

- Isotope exchange

- Thermal desorption of hydrocarbons deposited between ELMs by the ELM event
  - By direct fluxes
  - Increase of target temperature

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- What is used in SOLPS at the moment?
- What simple extensions have already been used?
- What is the present development strategy?
- What should be possible in the longer term?
- What is needed?
- Summary

What is needed (I)?

- Mixed material model could be used to look at wall retention, isotope exchange
  - Needs physics input
- Changes also need to be incorporated into Eirene
  - What species come back?
    - Get the hydrocarbon updates into the SOLPS Eirene
- Temperatures at the targets go down to < 0.1 eV
  - Need to extend the TRIM tables down in energy
    - Molecular Dynamics?
    - (Also need Be onto C, C onto Be, etc.)

What is needed (II)?

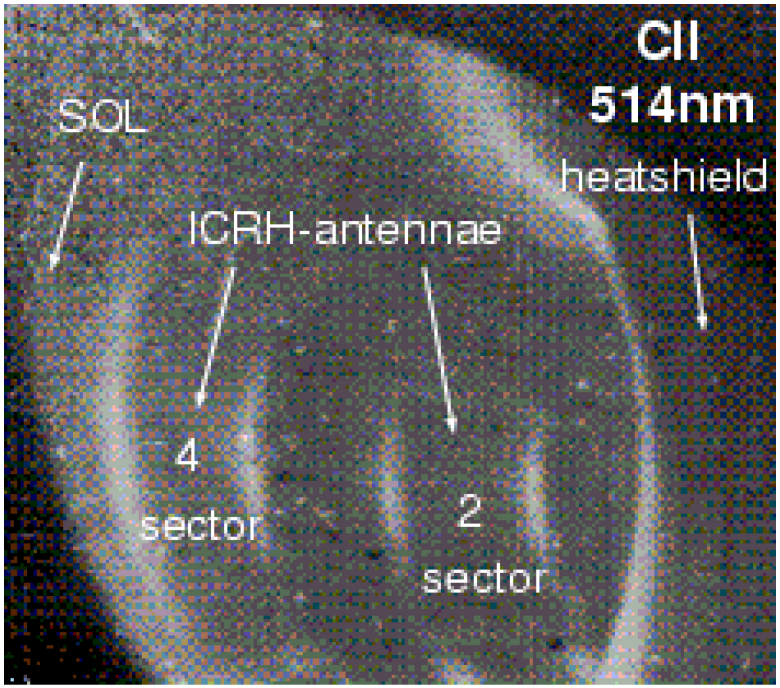
- Need to improve the very simple model for mixed materials that has been implemented
  - Physical sputtering from W/Be/C mixture on W, Be or C
  - Chemical sputtering of C from W/Be/C mixture
  - What are the properties of these mixed materials?
    - Heat transport coefficients
    - Thermal evaporation
    - …
- Need W data
  - ADAS format by preference

Summary

- Hierarchy of models for edge plasma modelling available
  - SOLPS, UEDGE or EDGE2D-NIMBUS type codes attempt to calculate a self-consistent solution
  - Other models have more detailed PWI models
    - Need to transfer physics back to the self-consistent codes if large effects are seen
- On-going development in SOLPS
  - Plasma (drifts)
  - Neutrals (neutral-neutral collisions, photon transport, hydrocarbons)
  - Plasma Wall Interaction
    - More processes
    - Mixed materials

Assumptions/Limitations – 2D Transport

- Transport codes
  - No 1st principles treatment of radial transport
    - Radial and poloidal dependence of transport coefficients
    - Non-diffusive nature (+ pinches)
  - Parallel transport on a better footing (except for kinetic effects)
- 2D
  - Ignore 3D effects
    - Erents arguments wrt Mach probe
    - Localised recycling, sources etc.

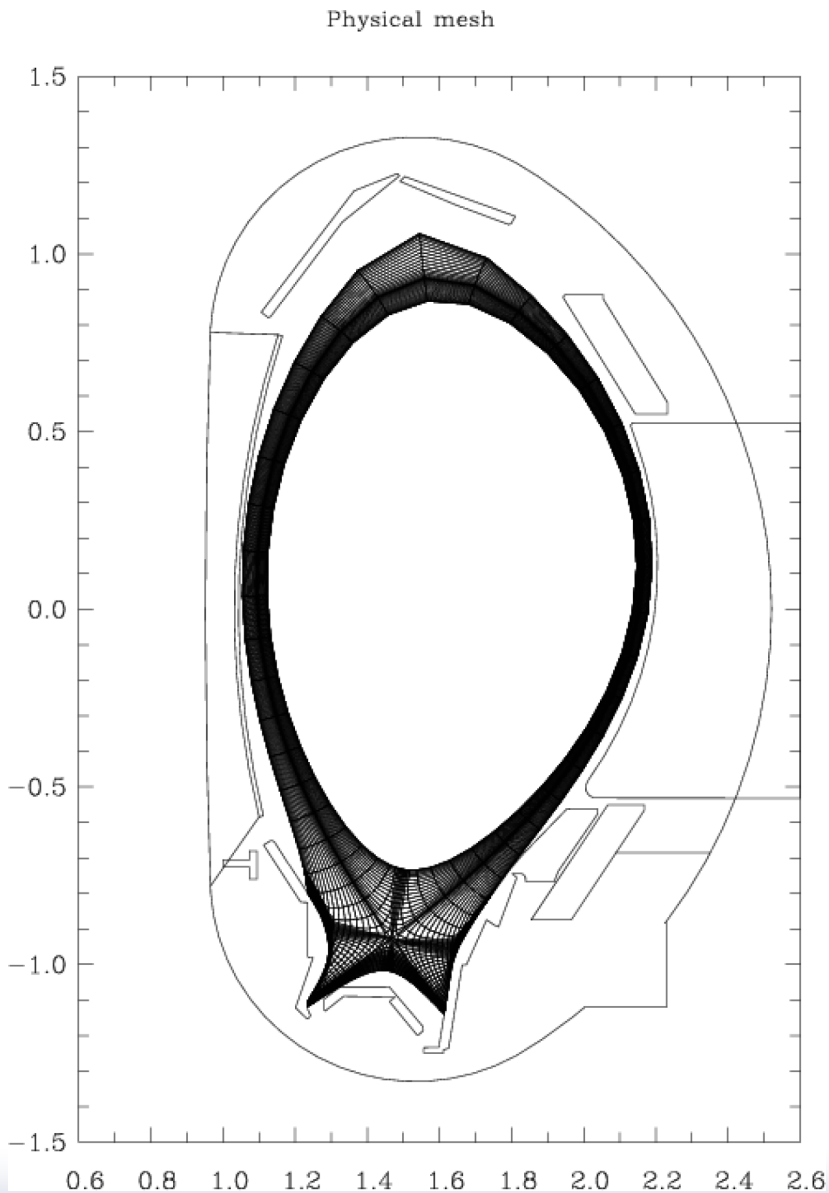


Th. Pütterich

D. P. Coster, X. Bonnin, "ITPA Modeling Assumptions and Limitations", DIV/SOL November 2004

Assumptions/Limitations – Limited Domain

- Solution domain somewhat limited
  - Doesn't extend all the way to the vacuum vessel
  - What are the appropriate boundary conditions there?
  - Implications for
    - heat/particle loads in main vessel
    - Sources of impurities



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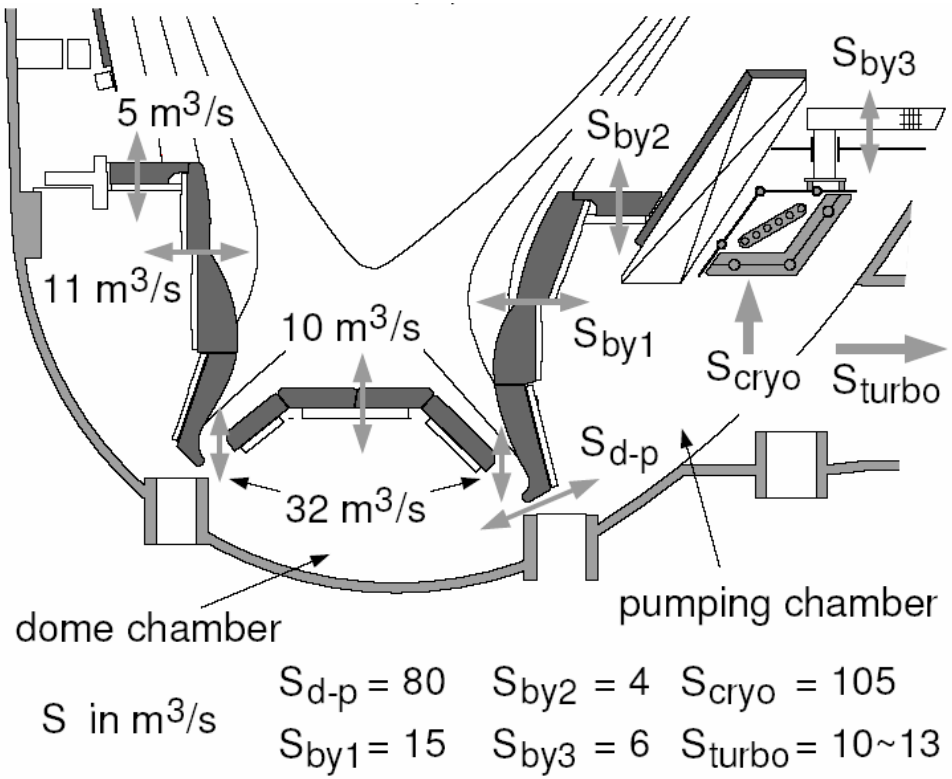
Assumptions/Limitations, Neutrals

- Neutral treatment
  - Kinetic: coupling to a Monte-Carlo code
    - More accurate, slower
    - Monte-Carlp Noise
  - Fluid: usually not full Navier-Stokes
    - Not as accurate
      - Own temperature?
  - Still discussion of role of physics
    - He elastic collisions
    - Hydrocarbon break up chains
    - Vibrational excitations
  - Often details of bypasses, wall out-gassing neglected
  - Neutral-neutral collisions and opticall thick regions



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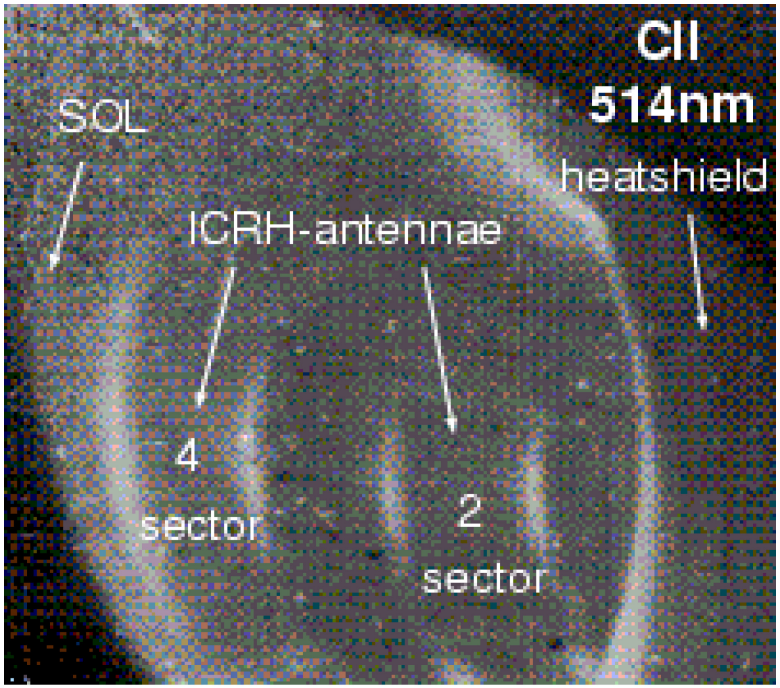
Assumptions/Limitations, Impurities

- Impurities
  - Intrinsically produced
    - Somewhat simplified erosion/deposition models
  - Plasma solution domain usually doesn't extend to vacuum vessel
    - Problem with main chamber sources
  - PSI models usually too simple
    - Usually not affected by the plasma in the simulations
      - Heating
      - Out-gassing/absorption
      - Isotope exchange
      - ELM target cooling with Ar at inner target
      - Hydrocarbon chemistry including T co-deposition
    - How can we improve them?

D. P. Coster, X. Bonnin, "ITPA Modeling Assumptions and Limitations", DIV/SOL November 2004



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Assumptions/Limitations, Drifts

- Drifts
  - Still not complete agreement on the equations to be implemented
  - Not nearly as robust as the non-drift versions
    - Often have additional time-step limitations
    - Sometimes have problems with extending to far into the core
    - Sometimes have problems with reduces solution domain in terms of plasma parameters

D. P. Coster, X. Bonnin, "ITPA Modeling Assumptions and Limitations", DIV/SOL November 2004

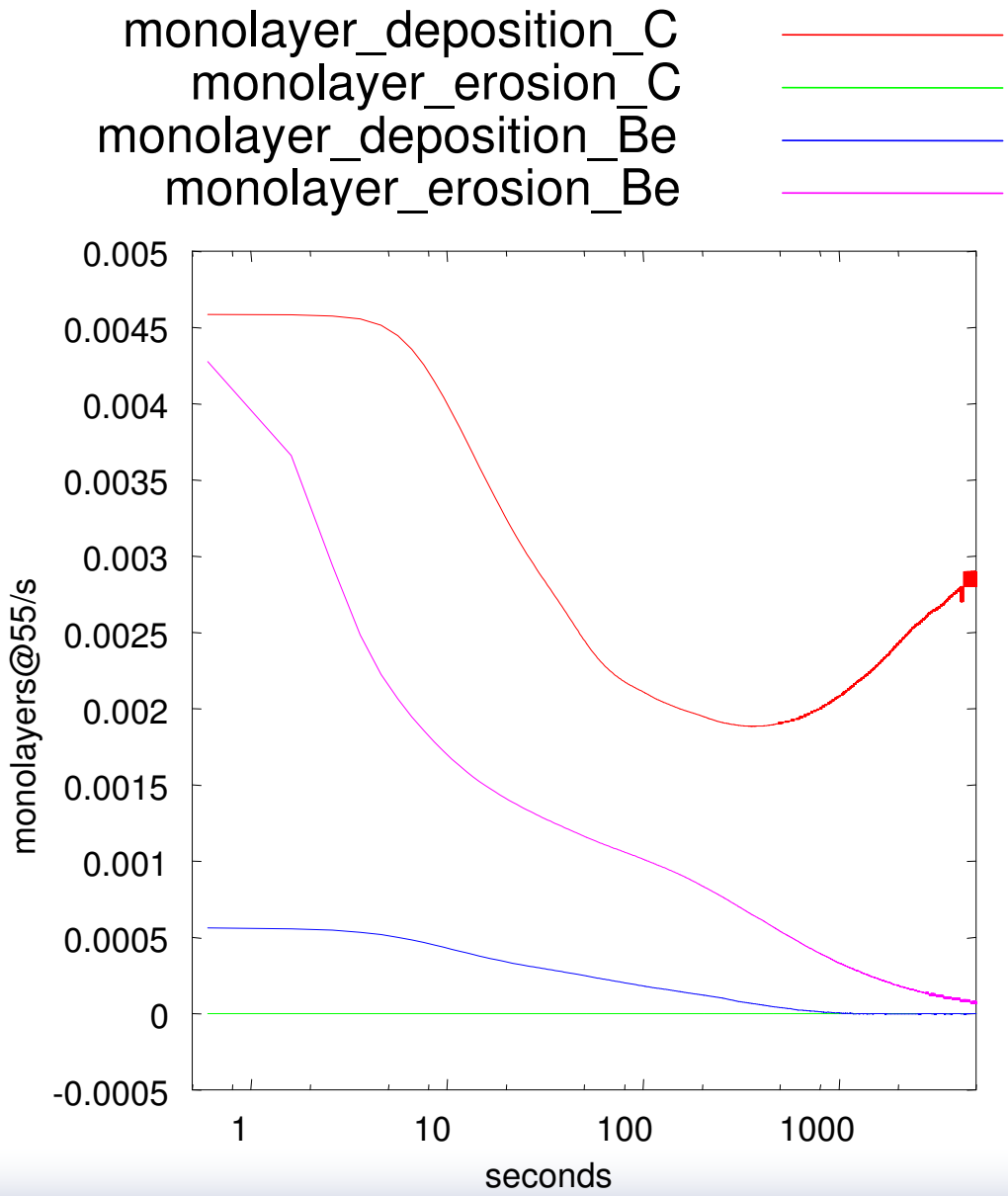
Mixed materials, D+C+He+Be

Targets: C

Walls: Be

Analysis at 55 (near the outer mid-plane)

- C continues to be deposited
- Be deposition stops

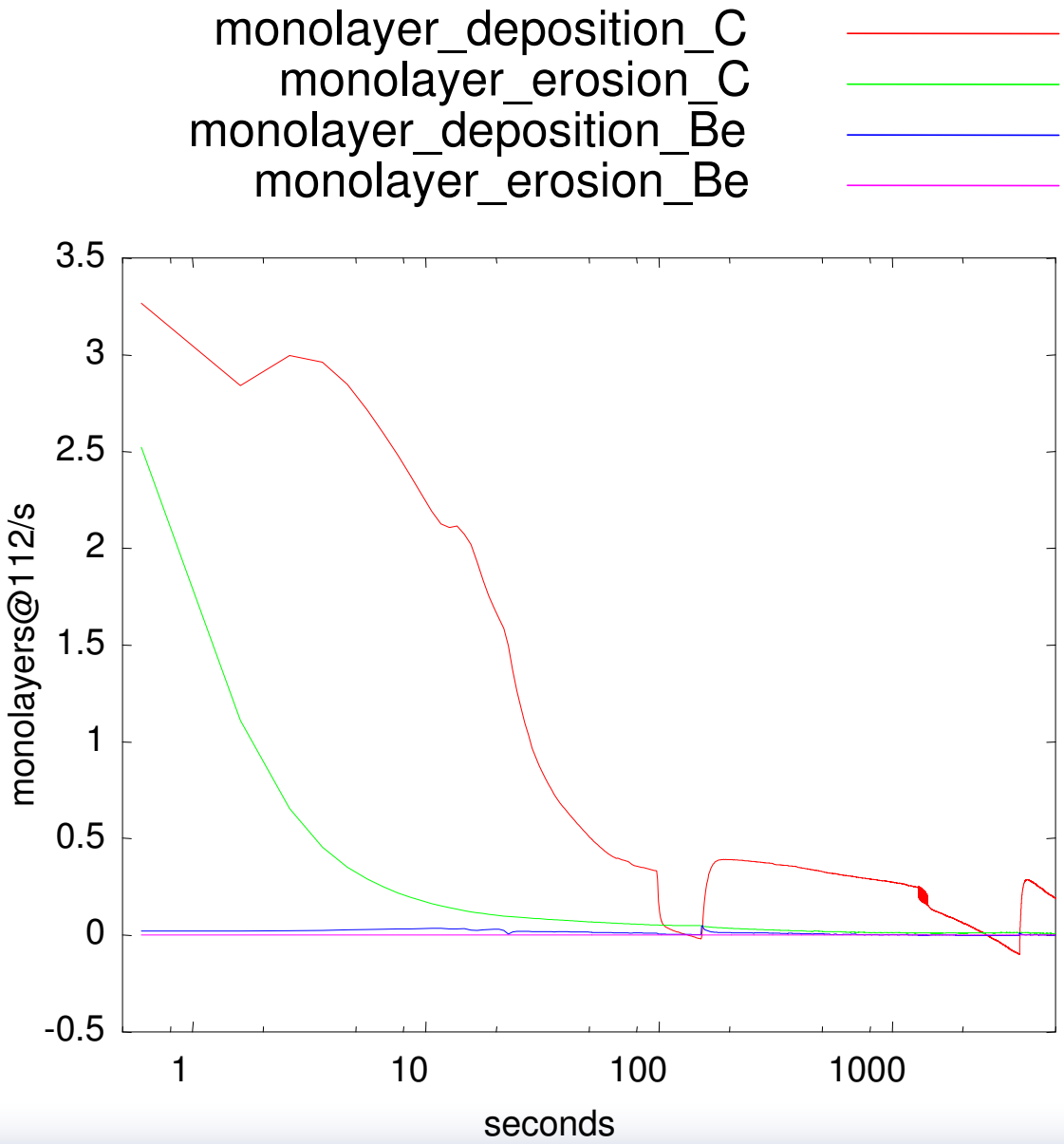


Mixed materials, D+C+He+Be

Targets: C

Walls: Be

Analysis at 112 (near the outer target separatrix)



Mixed materials, D+C+He+Be

Targets: C

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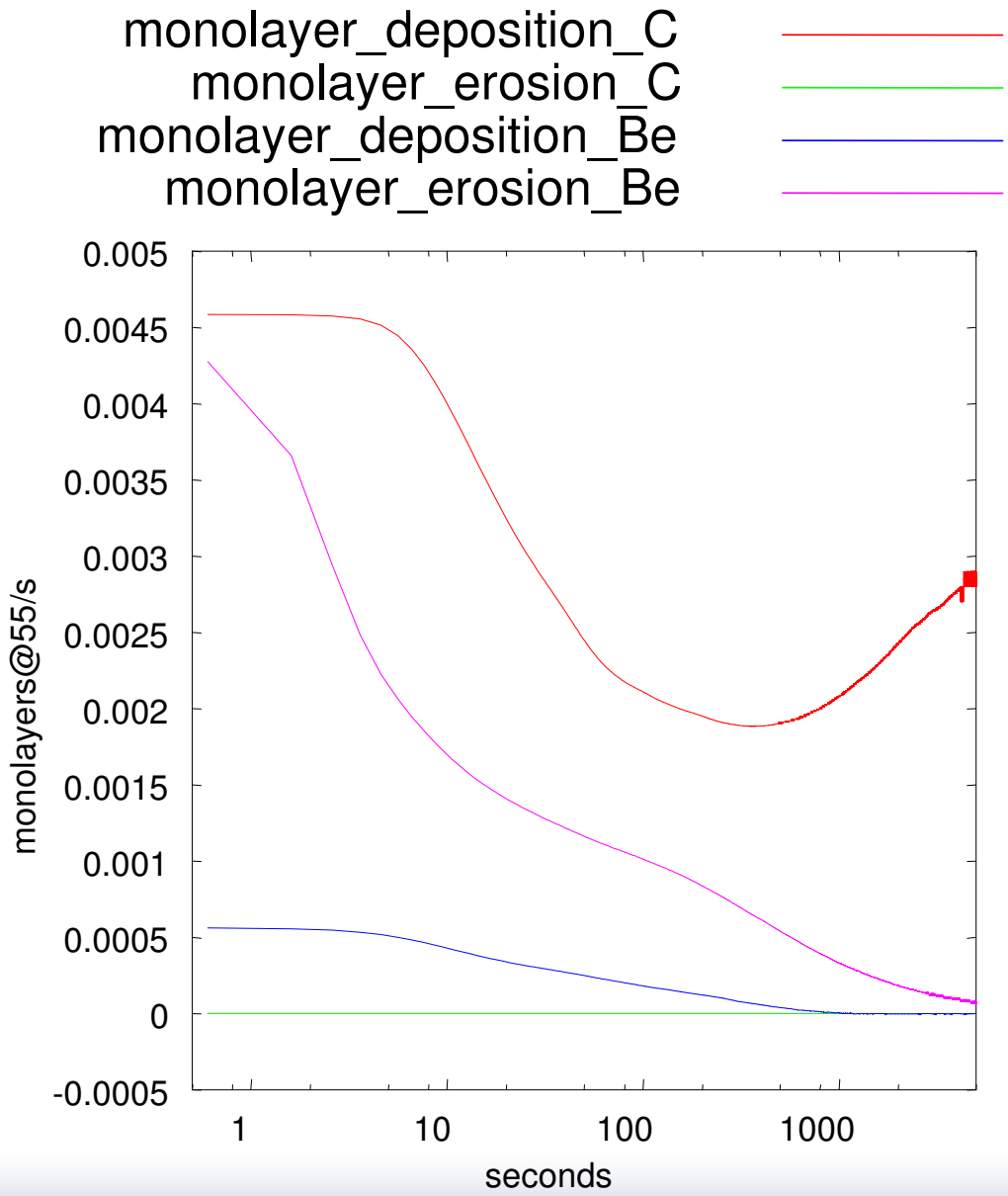
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