Erosion/deposition: WallDYN

Requirements for possible WallDYN-3D calculations for JET

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Summary of previous WallDYN calculations for JET-ILW

- In 2013-2015 2D WallDYN calculations were performed using DIVIMP for trace impurity transport [1]
  - Two **OSM based** plasma backgrounds generated by S. Lisgo
    - Ohmic L-mode plasma
    - H-mode plasma

- Based on this input and yield data from SDTrim.SP WallDYN calculates for each non recycling species (Be, W) as function time:
  - Total impurity source into the plasma due to sputtering & reflection: $\boldsymbol{\Gamma_{Be}^{Source}, \Gamma_{W}^{Source}}$
  - Total impurity influx onto the wall: $\boldsymbol{\Gamma_{Be}^{In}, \Gamma_{W}^{In}}$ due to plasma transport (re-distribution matrix approach)
  - Change of aral density $\boldsymbol{\delta_{ei}}$ $\boldsymbol{ei} \in \{\boldsymbol{Be, W}\}$ of impurities in the surface (material mixing, layer grown, surface erosion)

$$\frac{\partial \delta_{ei}}{\partial t} = \Gamma_{ei}^{In} - \Gamma_{ei}^{Refl} - \Gamma_{ei}^{Ero} - \Gamma_{ei}^{Bulk}$$

$\frac{\partial \delta_{ei}}{\partial t} < 0$ → Net. Erosion

$\frac{\partial \delta_{ei}}{\partial t} > 0$ → Net. Deposition (mixed layer growth)

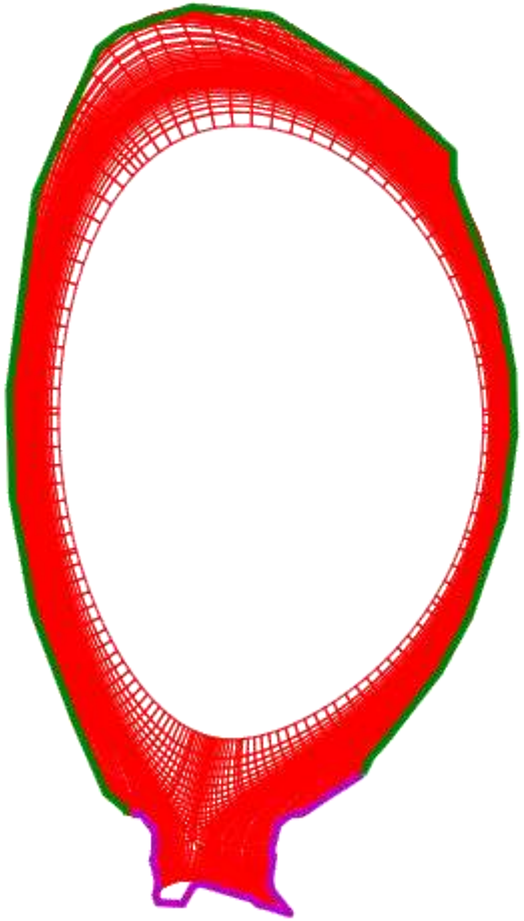
Self consistent evolution of impurity fluxes, surface composition and material balance

[1] K. Schmid et al Journal of Nuclear Materials 463 (2015) 66

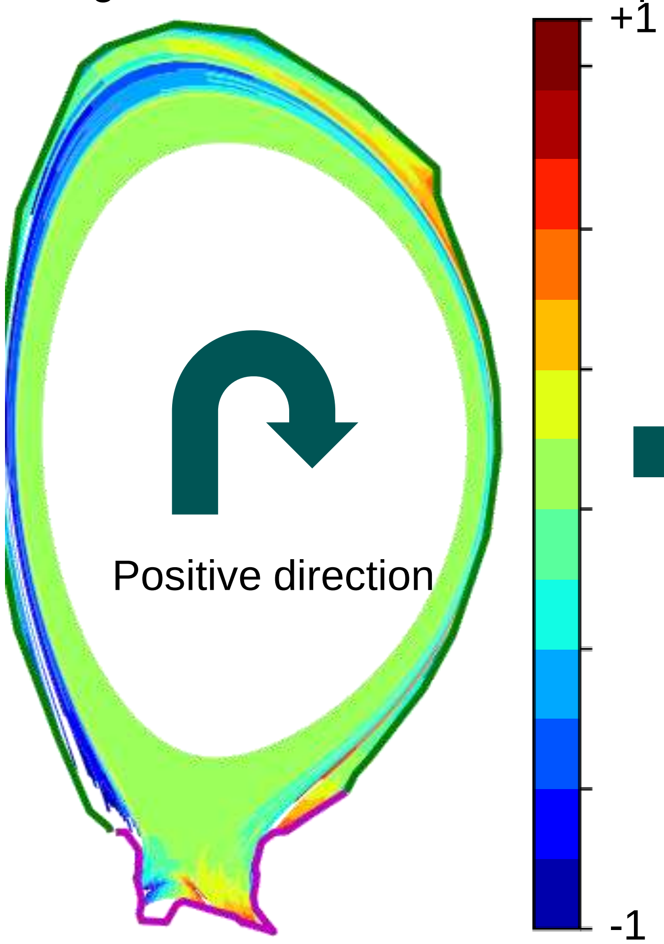
Summary of previous WallDYN calculations for JET-ILW

- ❖ In 2013-2015 2D WallDYN calculations were performed using DIVIMP for trace impurity transport [1]

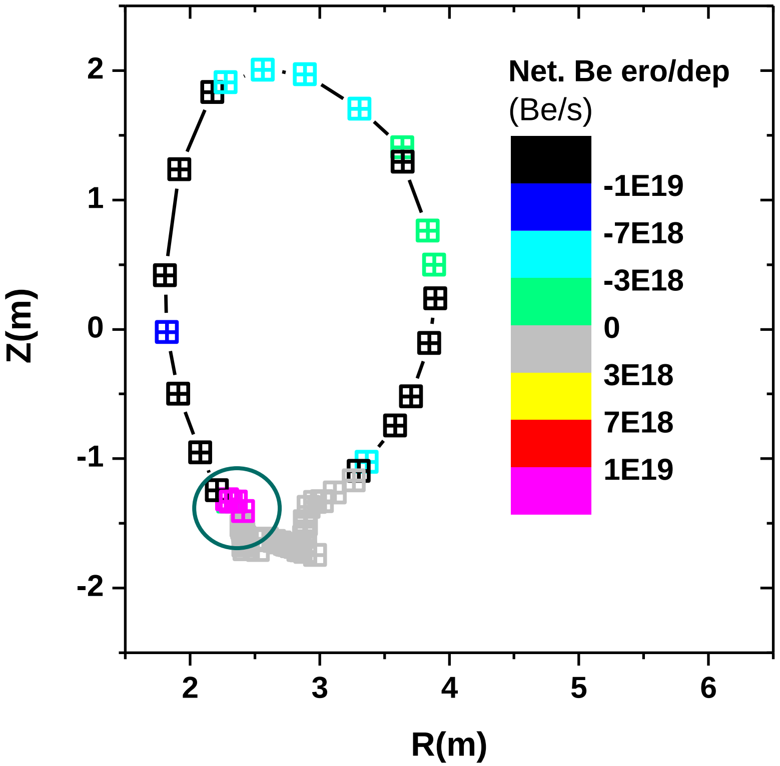
- ❖ Extended grid up to wall



- ❖ Strong flow towards inner baffle „apron“



- ❖ Strong deposition on apron



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Improvements of the WallDYN surface models

- The WallDYN surface model tries to match the output of a dynamic SDTrim.SP calculation

- Erosion and reflection fluxes $\boldsymbol{\Gamma_{ei}^{Refl}}$, $\boldsymbol{\Gamma_{ei}^{Ero}}$ are determined based on pre-calculated (by SDTrim.SP) yield tables

$$\Gamma_{ei}^{Ero} = \Gamma_{Proj}^{In} \times Y_{Partial}\left(E_{Proj}, \alpha_{Proj}, C\right)$$

- Partial sputter yield and reflection yield depends on surface composition C, impact energy E & angle α

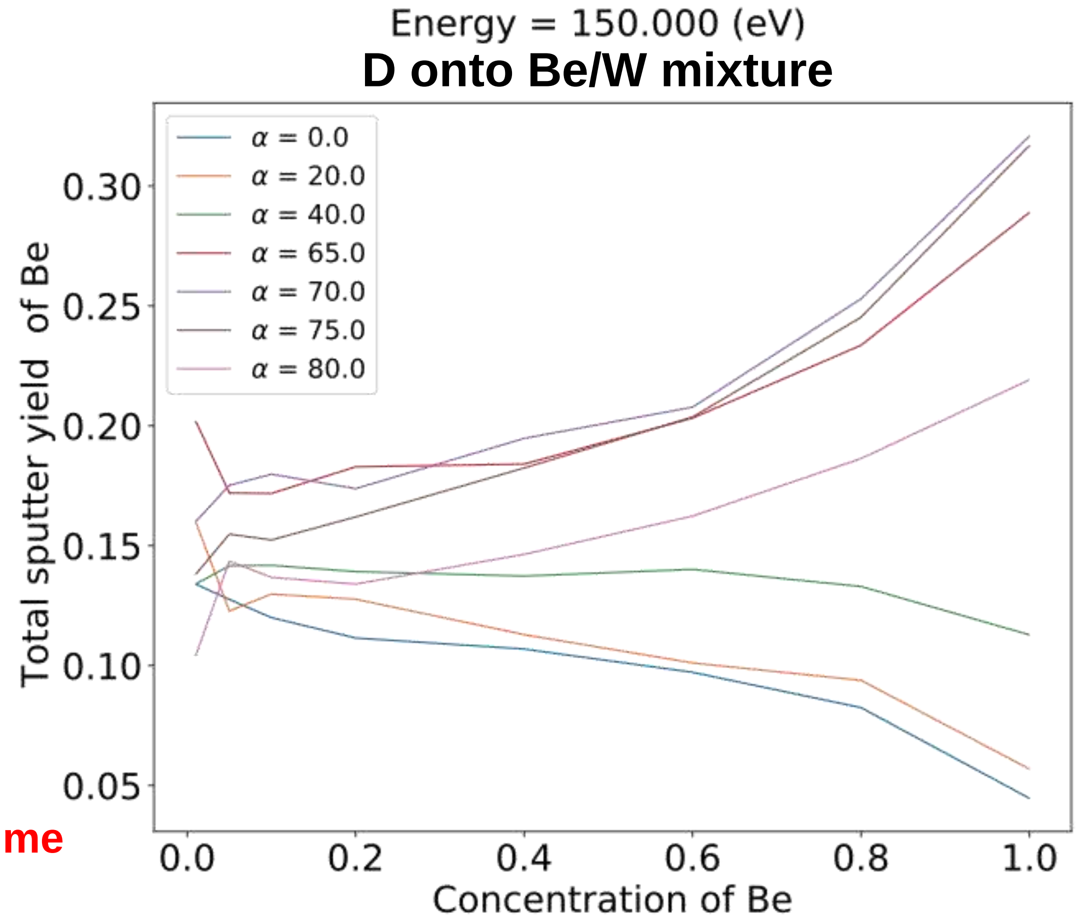
- The partial sputter yield is thereby **often approximated** by a **linear** dependence on composition

$$Y_{Partial}\left(E_{Proj}, \alpha_{Proj}, C\right) \approx C \times Y_{Total}\left(E_{Proj}, \alpha_{Proj}\right)$$

- However for light elements in a heavy matrix (e.g. Be in W) **this is not true**

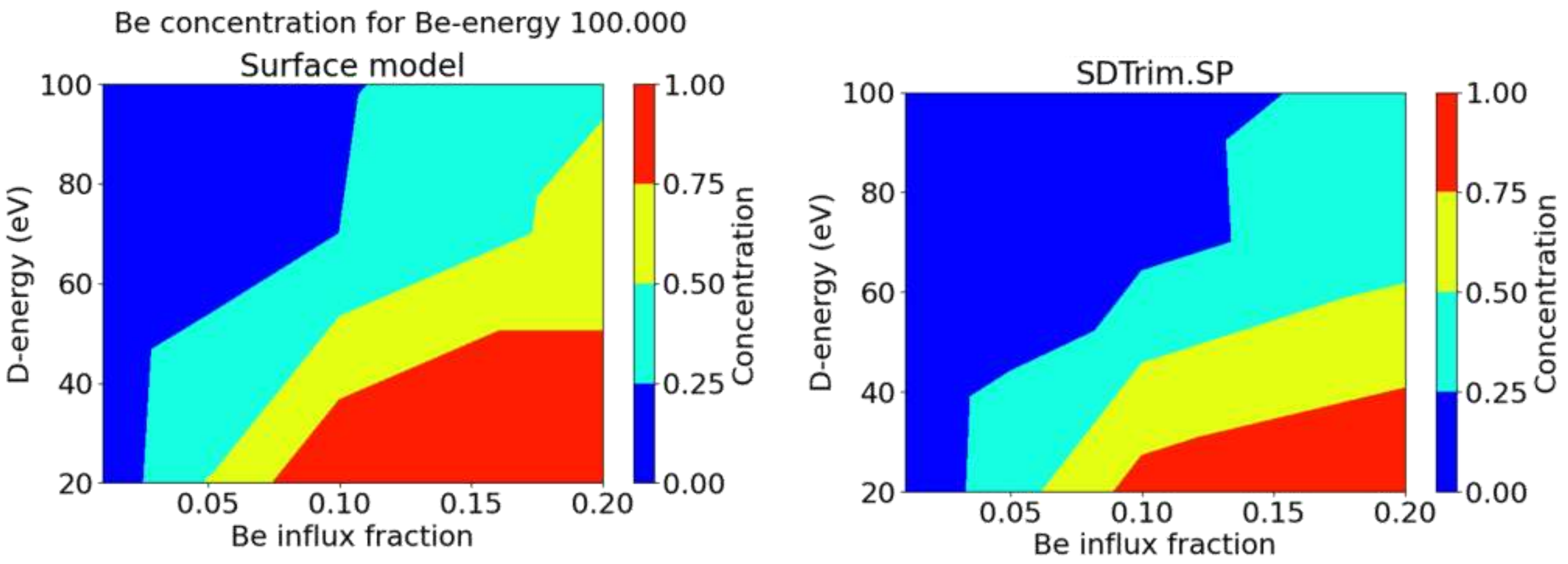
WallDYN has allways included non linear dependence of sputter yield on composition

→ Yields need to be interpolated from pre-calculated tables at runtime



Improvements of the WallDYN surface models

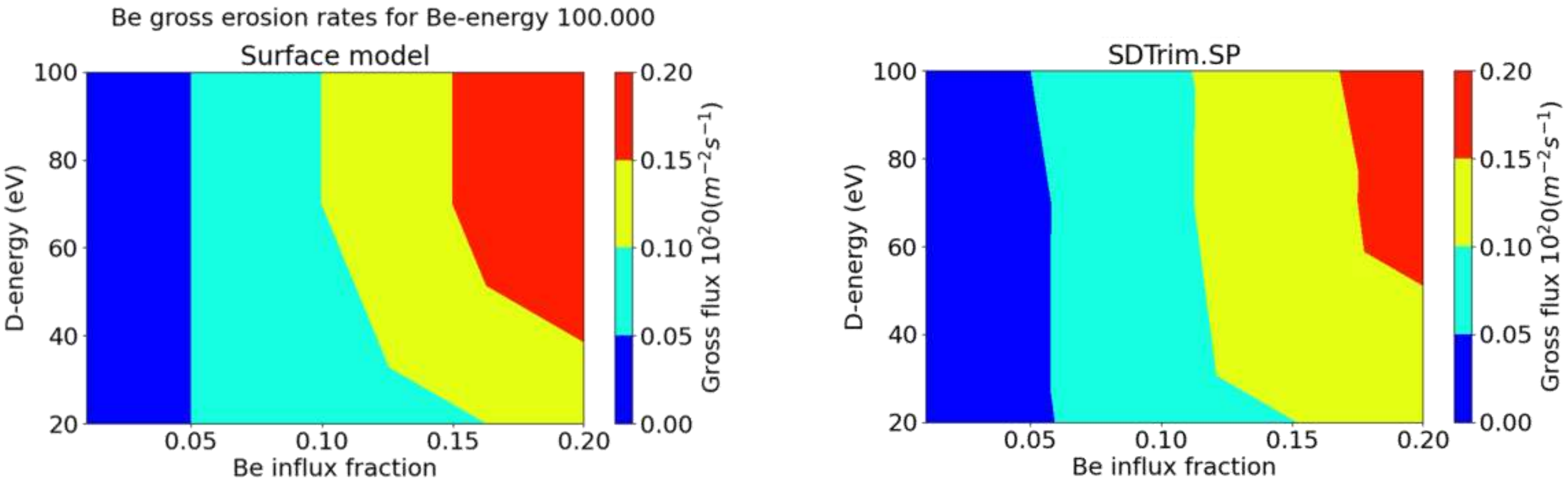
- ❖ For large 3D geometries (2000 vs 50 first wall elements) Mathematica version of WallDYN is insufficient
    - ➢ An MPI/OpenMP parallel C++ version of WallDYN was developed
        - ➢ **Features a new sputter and reflection yield interpolation model**
- ❖ Benchmark WallDYN surface model against SDTrim.SP
    - ➢ Bombard pure W surface with Be/D mixed plasma
    - ➢ Compare final Be surface **concentration** & gross flux into plasma



Improvements of the WallDYN surface models

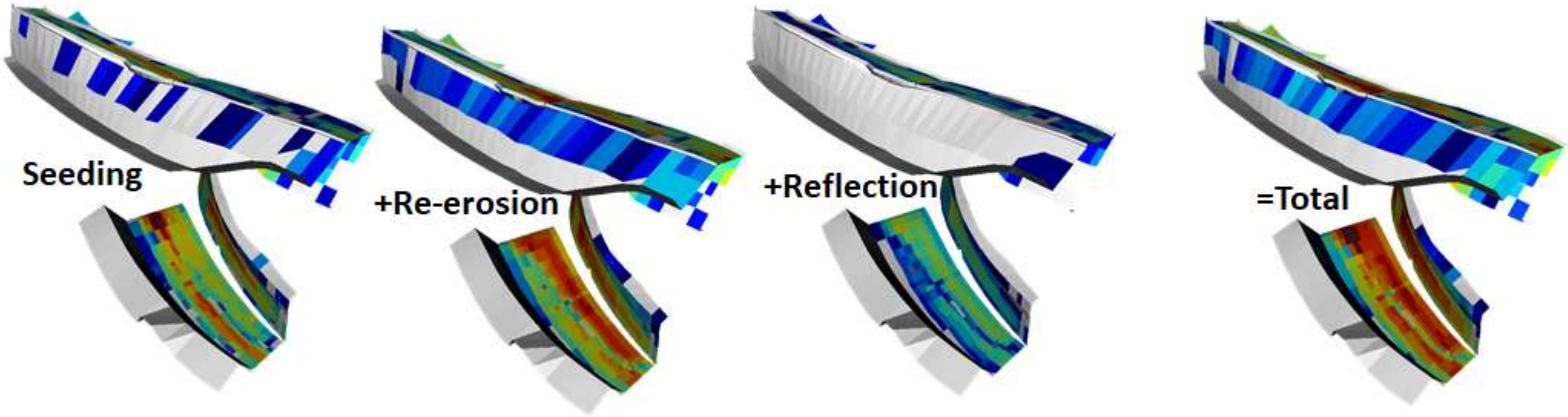
- For large 3D geometries (2000 vs 50 first wall elements) Mathematica version of WallDYN is insufficient
  - An MPI/OpenMP parallel C++ version of WallDYN was developed
    - **Features a new sputter and reflection yield interpolation model**
- Benchmark WallDYN surface model against SDTrim.SP
  - Bombard pure W surface with Be/D mixed plasma
  - Compare final Be surface concentration & **gross flux into plasma**

WallDYN well reproduces SDTrim.SP result



Required input for 3D calculations

- WallDYN is now 3D and uses a customized EMC3-Eirene version for impurity transport [1,3]
  - Example: **^{13}C influx in W-7X due to different sources**



→ Re-erosion dominates over seeding
→ Need a dynamic wall model
→ Also important for JET-ILW:
re-erosion of Be from W divertor tiles

[1] K. Schmid et al. Nucl. Mat. and Energy Vol 17 (2018) p. 200
[2] K. Schmid et al Phys. Scr. T171 (2020) p. 014006

Required input for 3D calculations

- WallDYN is now 3D and uses a customized EMC3-Eirene version for impurity transport [1,2]
  - Needs a 3D plasma background **all the way to the first wall**
  - Otherwise main chamber erosion cannot be properly modeled

  → Currently this means an EMC3-Eirene based plasma solution

- Internally WallDYN can also map arbitrary plasma solutions onto EMC3 3D grids
  - Derives wall plasma fluxes from local n_e, cs(T_e, T_i) and M (Hutchinson Model)
  - Computes wetted patterns on 3D wall elements based on connection length cut-off
  - Derives CX fluxes from a single EIRENE run („neutral iteration“) from within EMC3

  → This still needs a 3D EMC3 grid/equilibrium and wall definition!

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Required input for 3D calculations

- WallDYN is now 3D and uses a customized EMC3-Eirene version for impurity transport [1,2]

  → Ideally a full EMC3-Eirene based plasma solution

  → At least 3D EMC3 grid/equilibrium and wall definition!

- Possible simulation output:

  - Be layer deposition and resulting co-deposition (using different version of D/Be scaling laws)
  - Be plasma concentration due to calculated impurity influxes into the plasma (virtual spectroscopy available)
  - Comparison of Be deposition with 3D-poloidal rib-limiters vs. perfectly toroidally symmetric quasi 2D JET-ILW

    → Are 3D simulations nescessary for JET-ILW?

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[2] K. Schmid et al Phys. Scr. T171 (2020) p. 014006

Summary & Outlook

- **WallDYN now has a very fast C++ based implementation that can handle thousands of coupled wall elements**

- **The yield interpolation for the surface model was improved and benchmarked against SDTrim.SP**

- **The combination of a low-Z first wall with a high-Z divertor requires a dynamic surface model to handle low-Z recycling in the divertor**

- **To model JET-ILW with WallDYN3D an EMC3-Eirene based plasma solution is needed**