CHALMERS

# Modelling of non-uniform washcoat in catalytic monolith reactors

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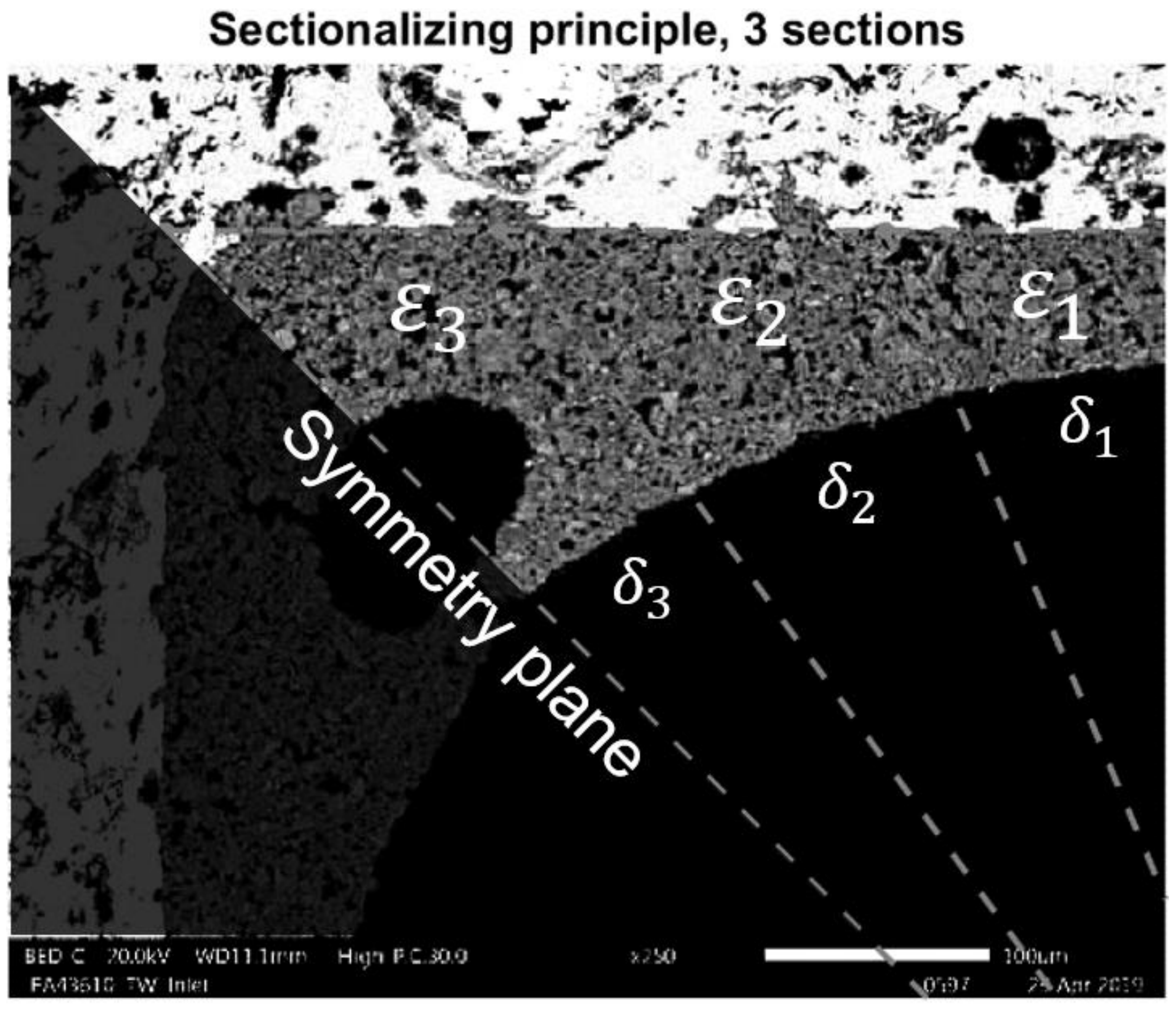
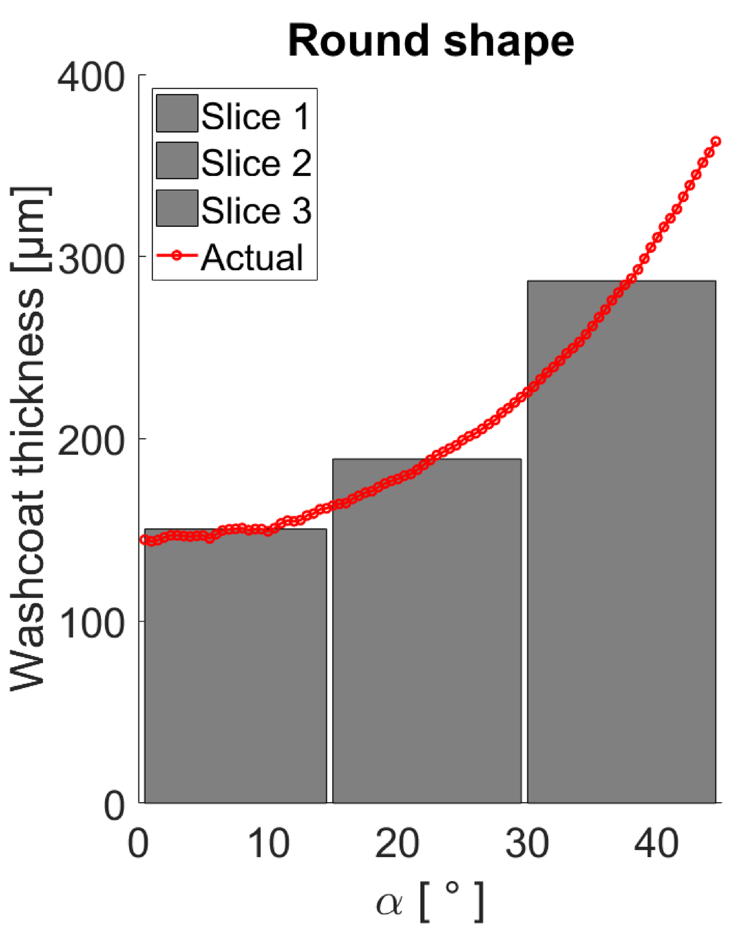
## WASHCOAT CHARACTERIZATION

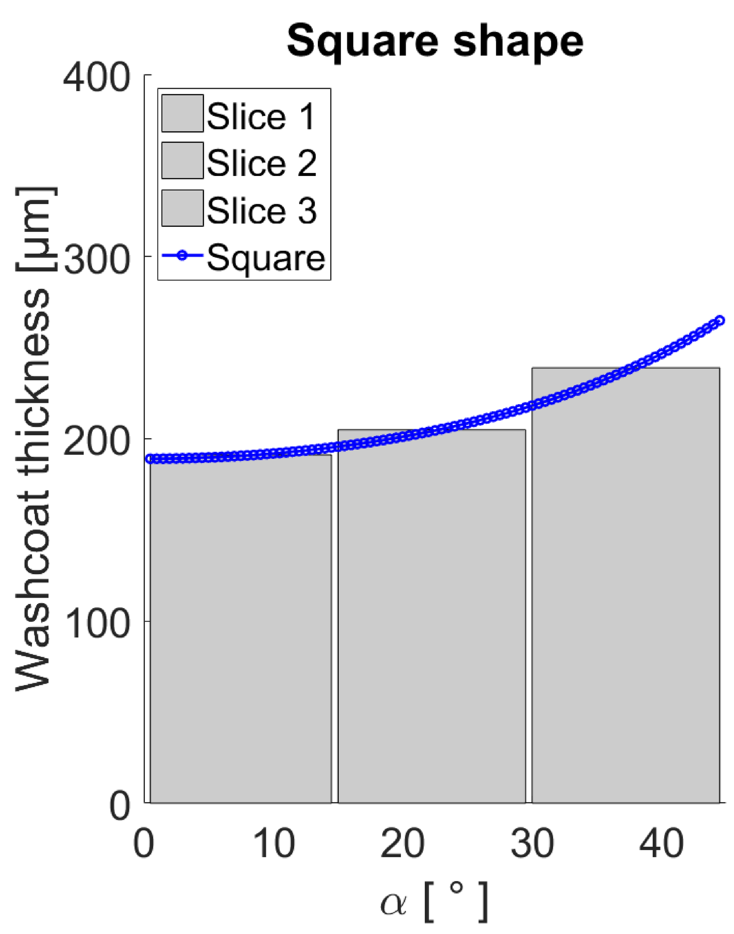
- Most 1+1d models assume uniform washcoat with global properties
- SEM (Scanning Electron Microscope) to approximate *global* and *local* porosity using *imageJ*
- IGA (Intelligent Gravimetric Analysis) to measure washcoat diffusivity [1]
- Input for parallel simulations to account for non-uniformity and tangential variations in properties

**Sectionalizing principle, 3 sections**




- Tortuosity, $\tau \approx 4$
- Porosity, $\varepsilon \approx [0.81 \quad 0.83 \quad 0.86]$
- Unused washcoat showed up to 6.2 % higher local porosity in corners




- Washcoat thickness, $d_{wsc}$ 92 % higher in corners
- N = 3 slices gives good tradeoff

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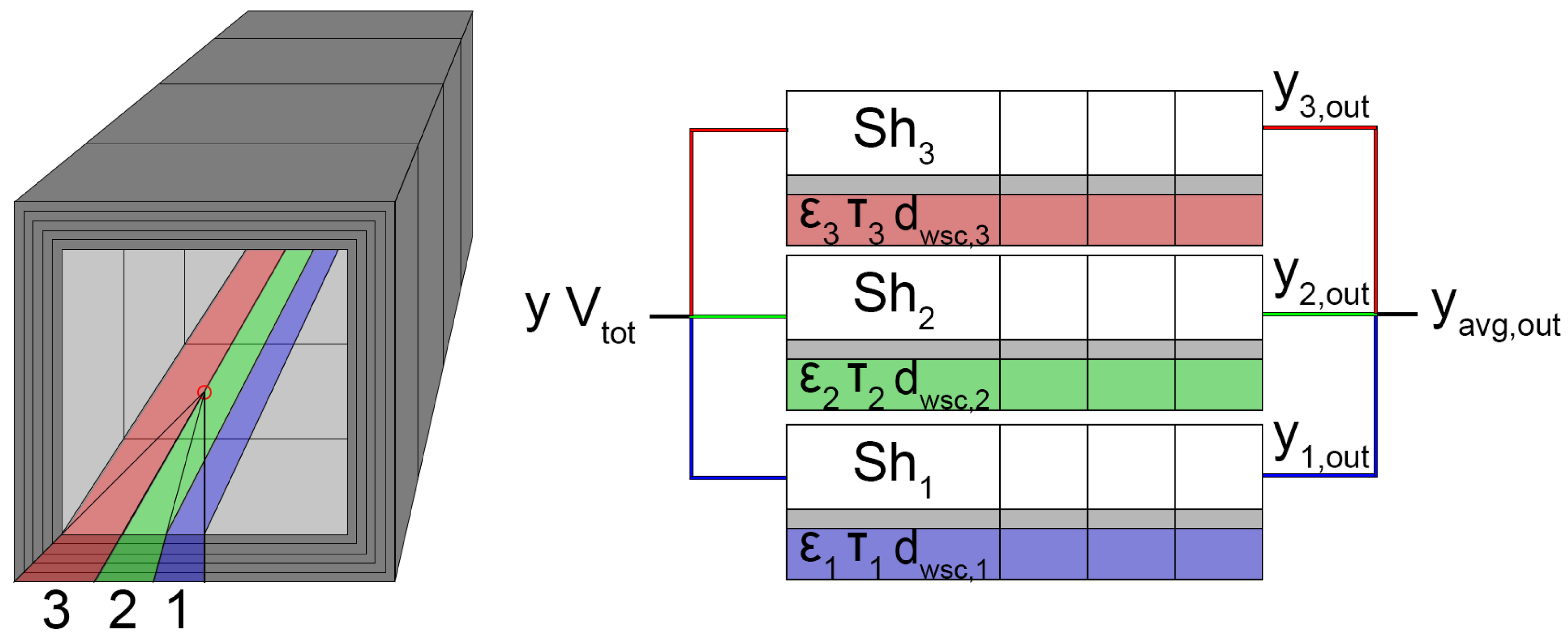
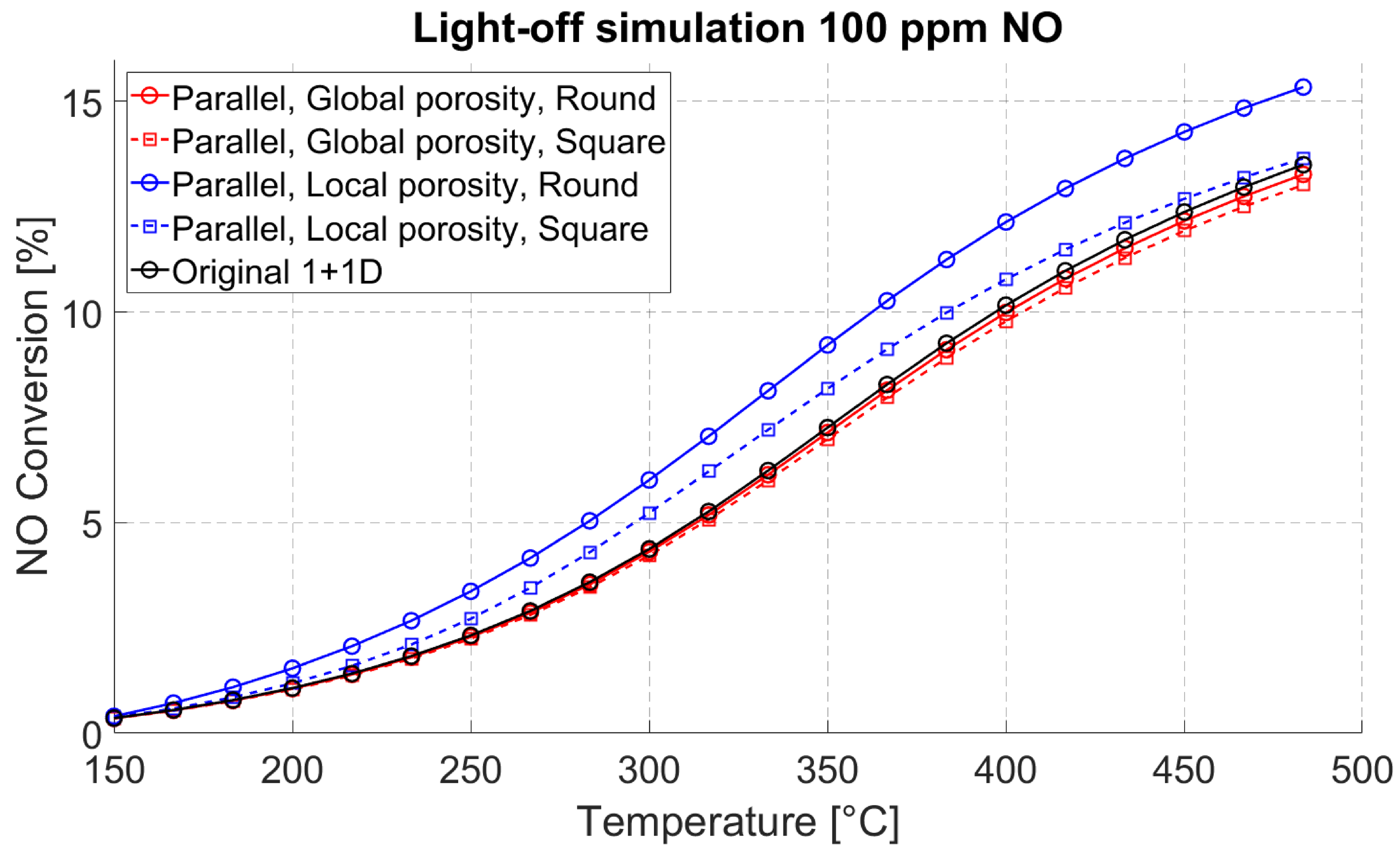
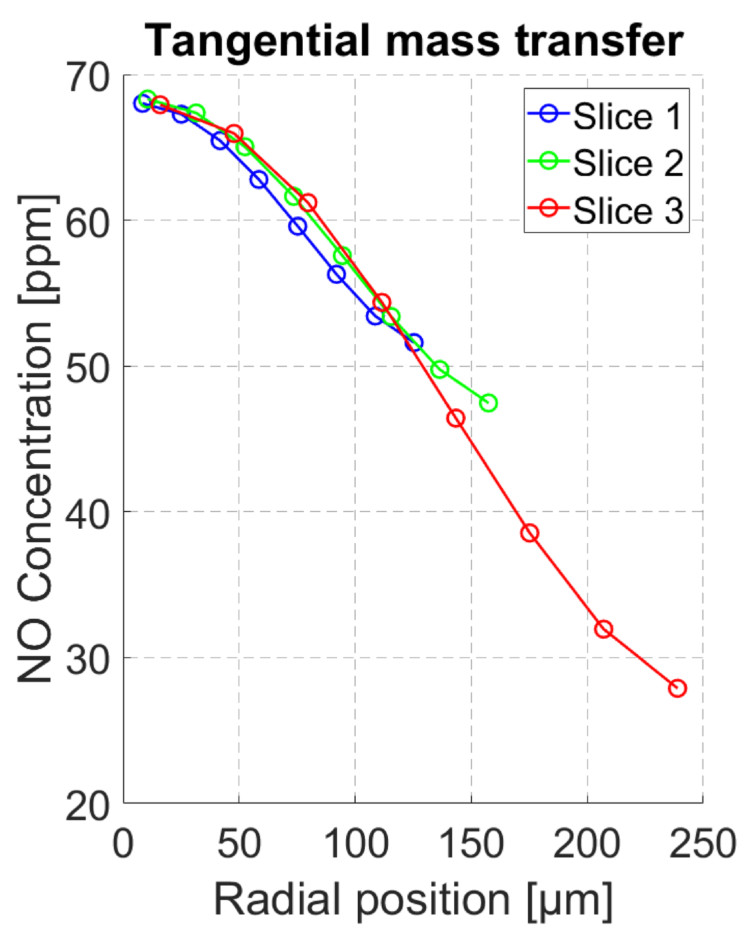
## PARALLEL 1+1D MODEL

- Sectioning principle based on equal angle
- Assumes no tangential mass transfer (between slices)




- Tangential concentration profiles are similar
- Ratio Radial : Tangential = 83
- Ratio Radial : Axial = 14 000

## CONCLUSIONS

- IGA and SEM enabled tangentially resolved washcoat diffusivities – important for highly predictive reactor models.
- With global porosity, conversion decreases due to slightly thicker washcoat.
- With local porosity, conversion increases due to higher diffusivity in corners.

**References:**
[1] – Ruthven DM. Diffusion in type A zeolites: New insights from old data. Microporous and Mesoporous Materials. 2012;162:69-79.