UNIVERSITEIT GENT

FACULTY OF ENGINEERING AND ARCHITECTURE

Computational Fluid Dynamic design of steam cracking reactors: extrusion method for simulation of dynamic coke layer growth

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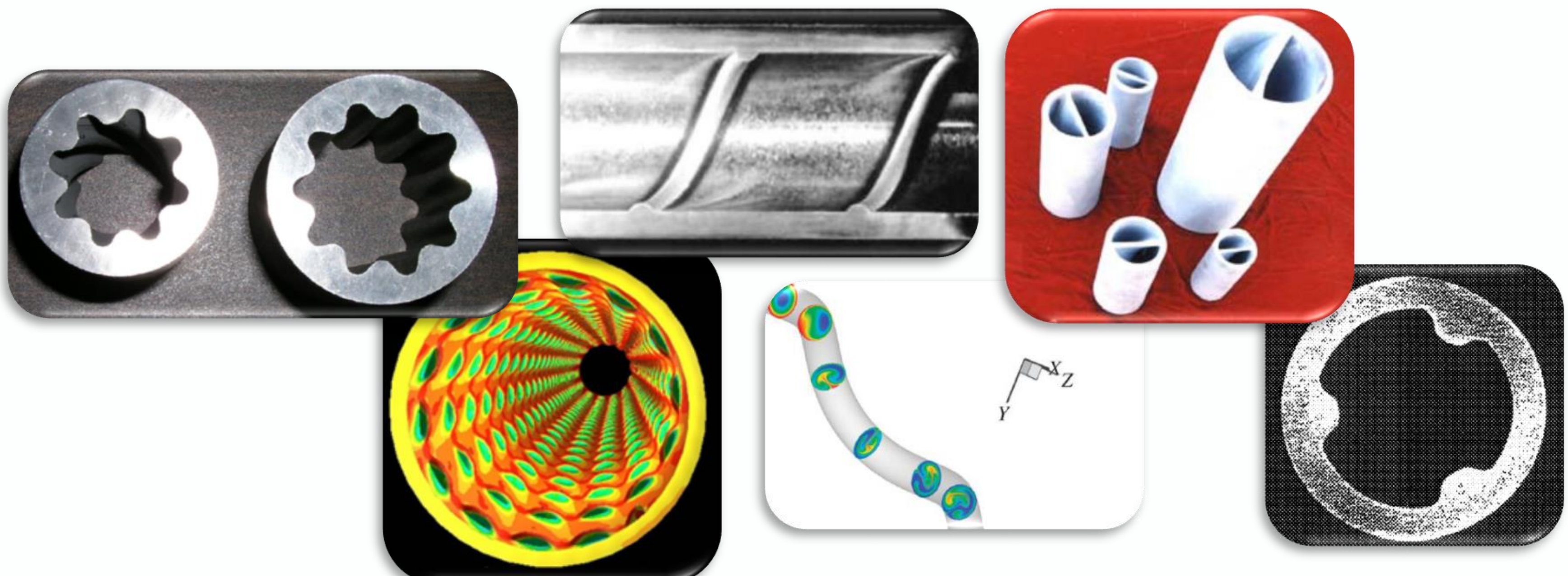
Coke reduction methods

- Feed additives
- Metal surface technologies
- 3D reactor technology

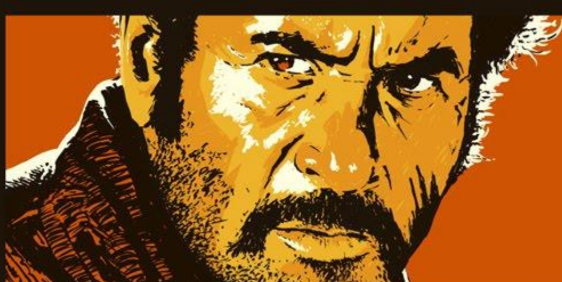


3D reactor technology | The Good, the Bad & the Ugly

Enhanced heat transfer & mixing → Less cokes?

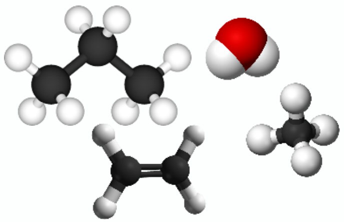
Increased pressure drop

Lower olefin selectivity?

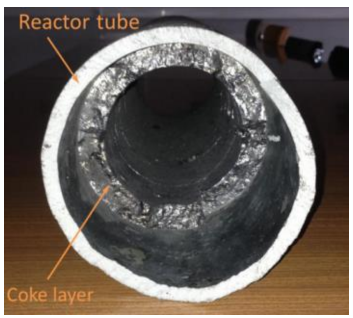


Long term performance and stability?

Where are we?

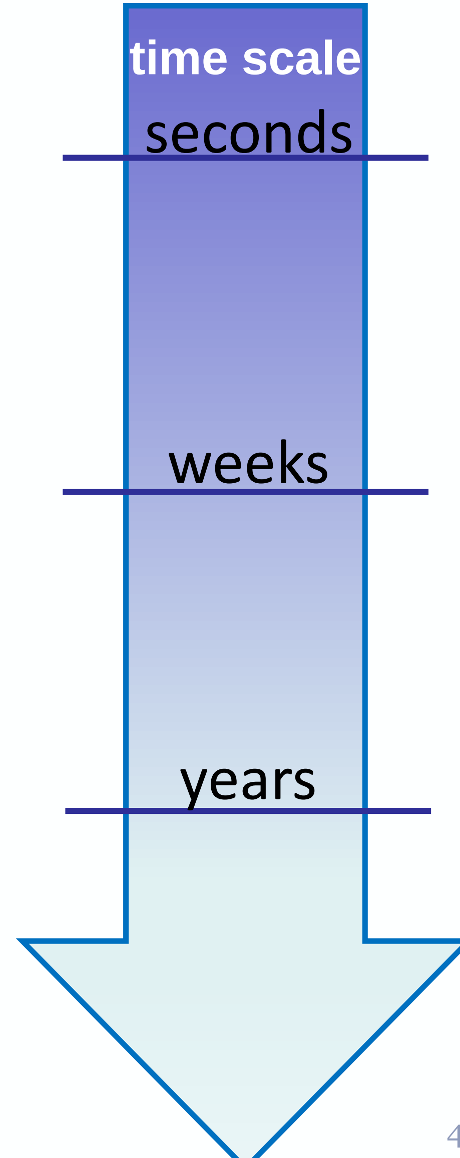


- Short term performance
  - Reactor residence time
  - Product yields, selectivities



- Intermediate term performance
  - Reactor run length
  - Coking rate, pressure drop, TMT

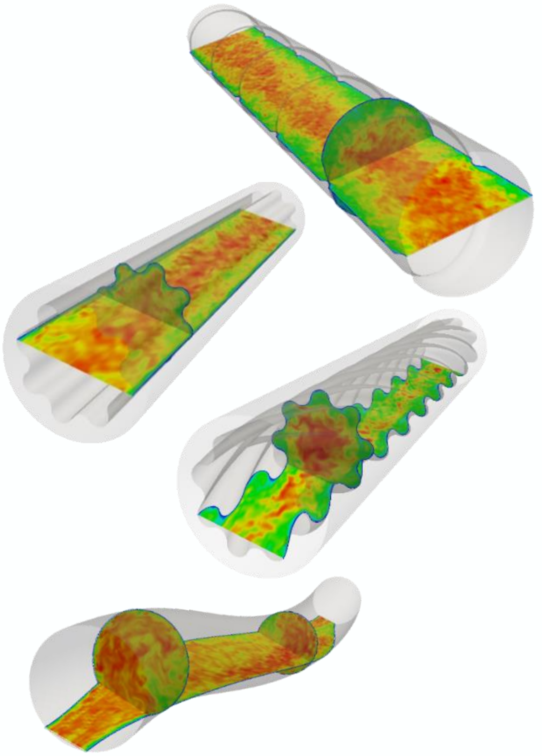
- Long term performance
  - Reactor stability & lifetime
  - Deterioration of reactor material



1D Reactor performance

- Does the **improved coking rate** outweigh the **loss of selectivity**?
- **In a 1D world…**

1D Simulation	Bare	Straight fins	Rifled	MERT	SFT
$\Delta P/\Delta P_{Bare}$	1.00	1.22	1.67	2.17	1.26
U/U_{Bare}	1.00	1.21	1.58	1.50	1.19
$T_{gas/cokes}$ [K]	1079.4	1066.4	1050.2	1054.5	1066.9
Rel. r_{coke}	-	**-4.8%**	**-34.9%**	**-43.1%**	**-24.1%**
Rel. yield C_2H_4	-	**-0.27%**	**-0.83%**	**-1.47%**	**-0.32%**
Rel. yield C_3H_6	-	+0.03%	+0.08%	+0.13%	+0.03%



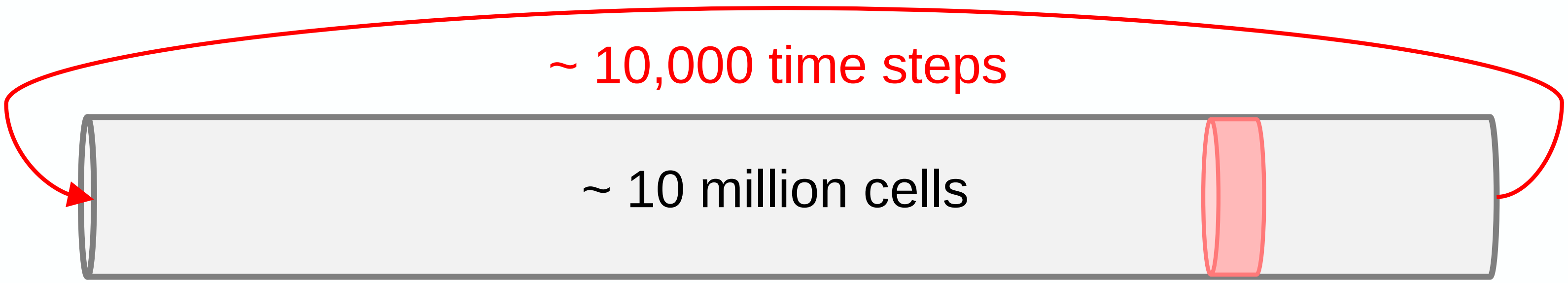
~ seconds

~ 1000 CPU hours

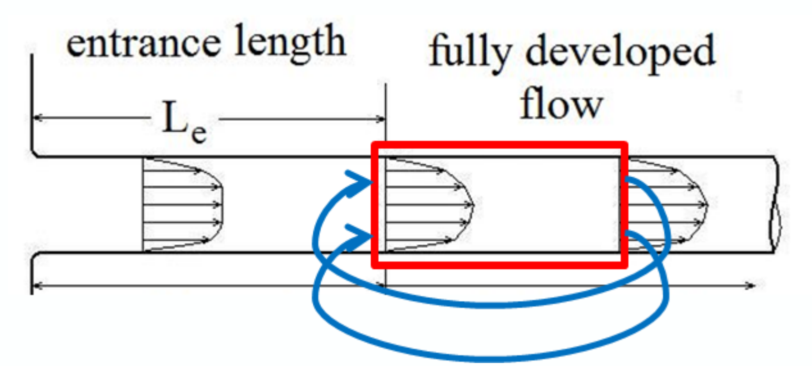
3D CFD simulations are **computationally very expensive**

Spatial vs. streamwise periodic

Full-scale reactor simulation



Trick: streamwise periodicity



⇨ Computational domain can be limited by using **streamwise periodic** boundary conditions

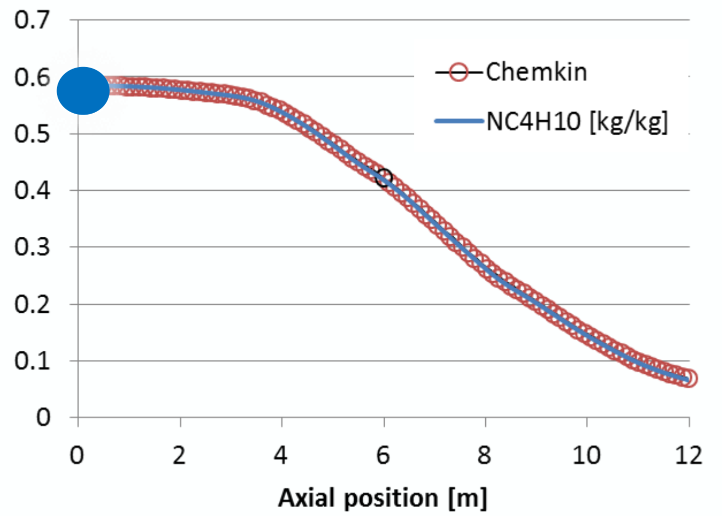
Periodic reactive simulations

- Assume **velocity fully-developed** over the short computational volume
- Use transient velocity field to evaluate **species and enthalpy radial mixing**
- Translate transient results back to the true steady-state by reconstructing the position from the bulk velocity:

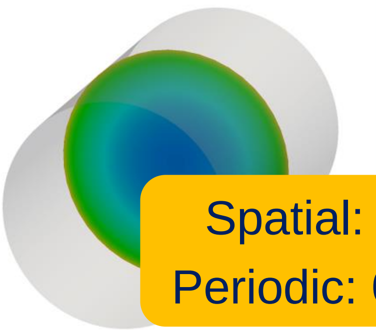
Transformation: Time → Position

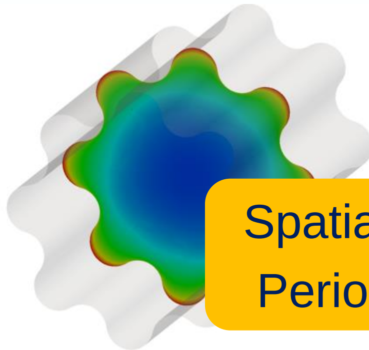
$$\Delta z = U_{bulk}\,\Delta t = \frac{\int_{\partial V} \rho u_z dA}{\int_{\partial V} \rho dA}\,\Delta t$$

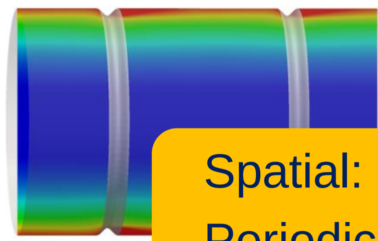
Speedup factors of 200+



Periodic reactive | 3D Product yields



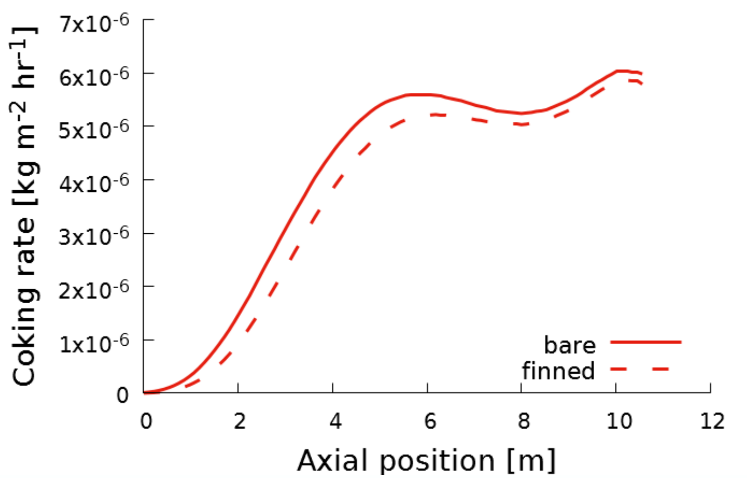




	Bare tube	Finned tube	Ribbed tube
COT [K]	1152.6	1151.6	1155.2
TMT [K]	1230.6	1222.7	1177.2
ΔP [Pa]	27682	29061	110001
Conversion	74.96%	74.99%	76.18%
CH4	13.96%	14.04%	14.54%
C2H2	1.64%	1.69%	1.55%
C2H4	27.60%	27.87%	27.74%
C2H6	1.23%	1.27%	1.32%
C3H6	22.91%	22.50%	23.52%
1,3-C4H6	2.91%	2.97%	2.88%

Coke formation | The Ugly

Start-of-run coking rate

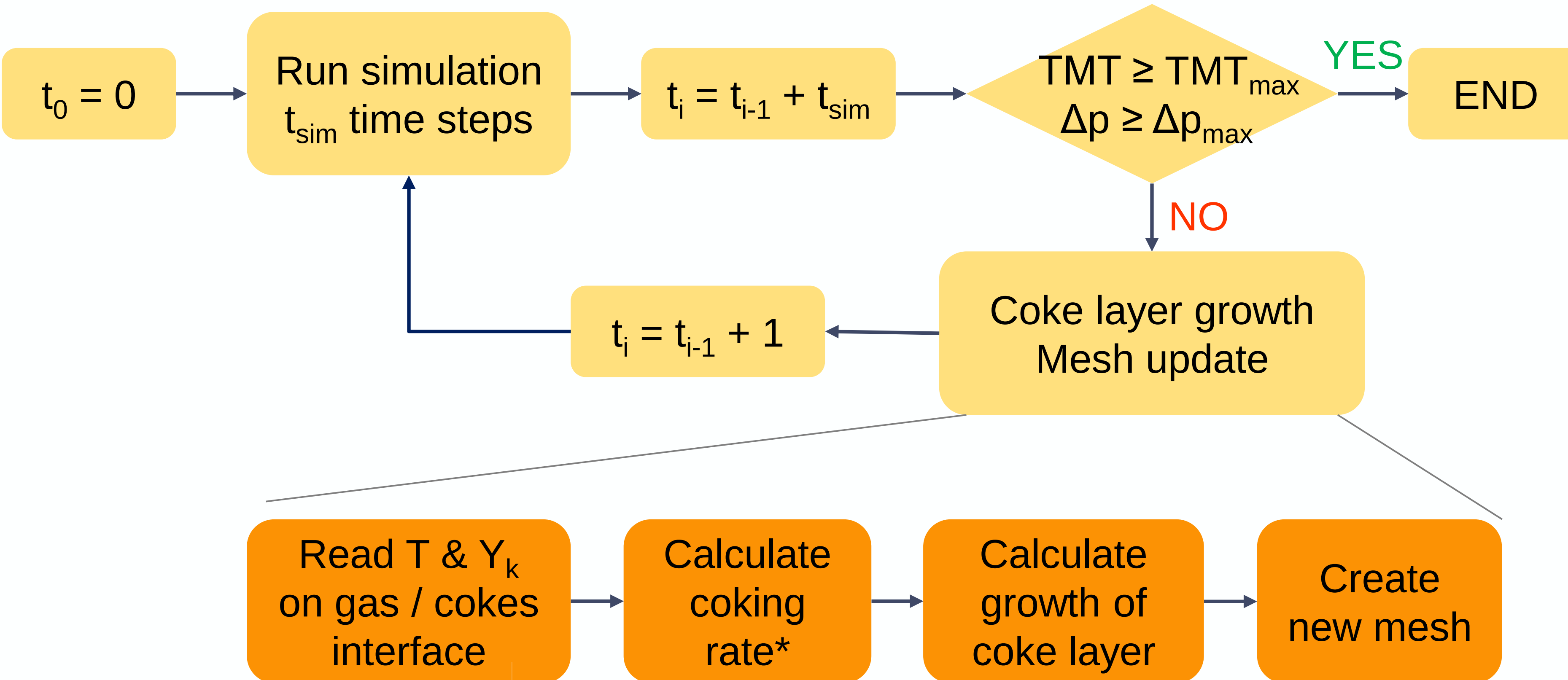


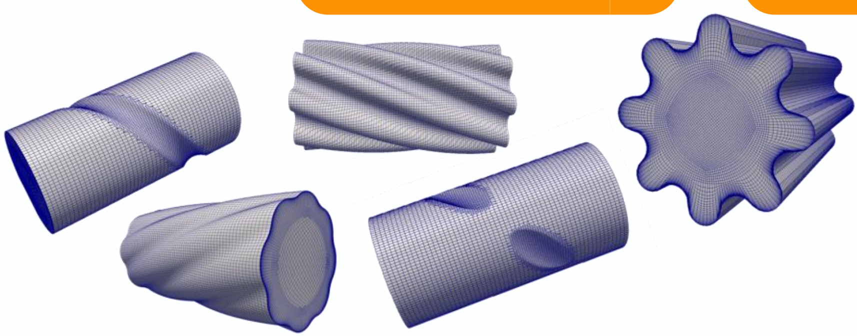
Evaluation of 3D reactor technologies requires tracking coke layer growth

NO streamwise periodicity
NO limitation of computational domain
NO fast periodic simulation approach

Tracking coke formation requires simulation of the entire geometry and is **computationally very expensive**

Dynamic modeling of coke formation



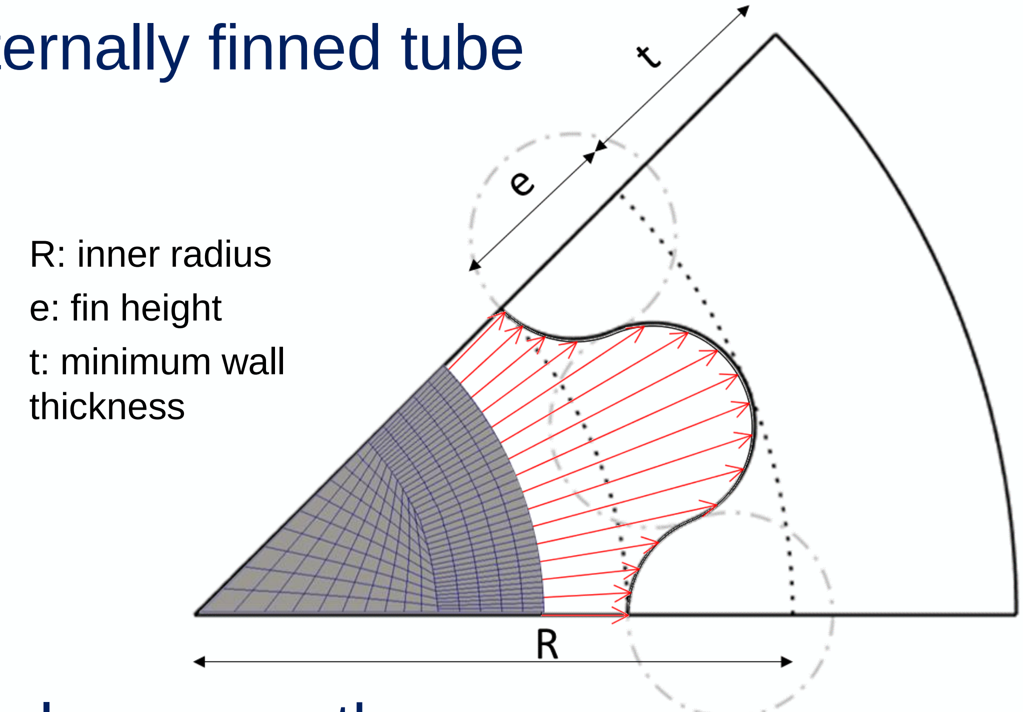


➔ New library of extrusion models in OpenFOAM, including a variety of 3D steam cracking reactor geometries

*P.M. Plehiers, Laboratorium voor Petrochemische Techniek, Rijksuniversiteit Gent, 1989

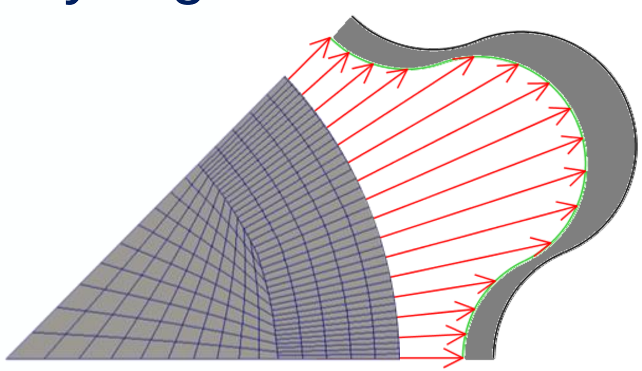
Extrusion of 3D reactor geometries

Internally finned tube



1. Start from core cylindrical geometry
2. Extrusion to 3D surface

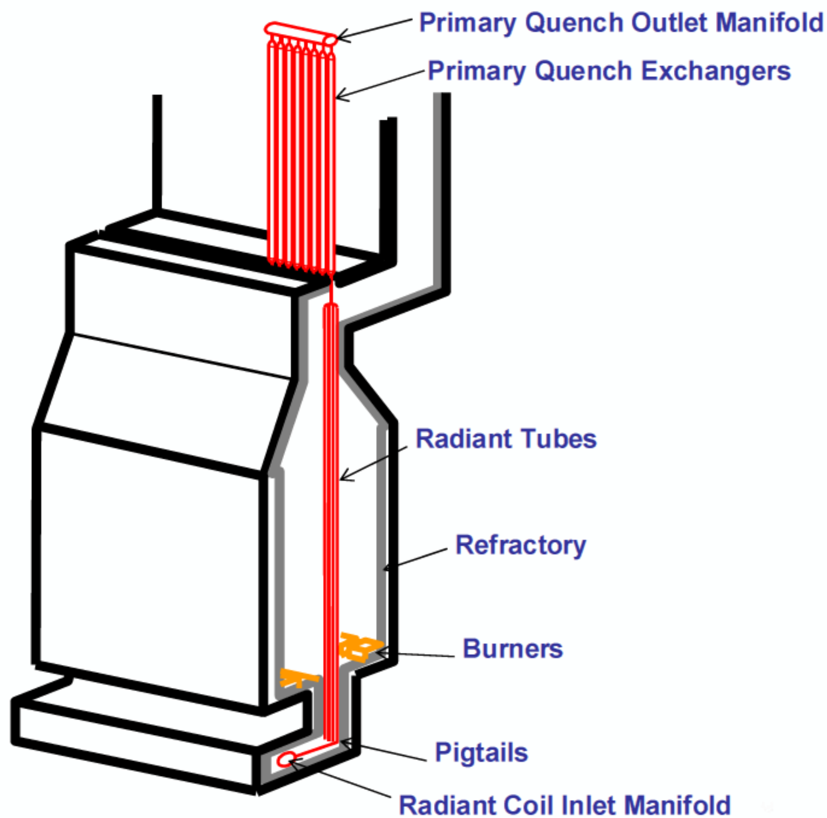
Coke layer growth



Extrusion of gas and cokes region from core cylinder wall to specified surface geometry, while taking into account calculated coke layer thickness

Test case | Millisecond propane cracker

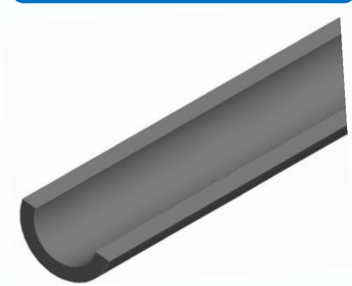
- Feedstock 118.5 kg/h propane
- Propane conversion 80% (± 0.05%)
- Steam dilution 0.326 kg/kg
- CIT 903.7 °C
- COP 170 kPa



Two geometries were simulated

- Same reactor volume
- Same axial length
- Same minimal wall thickness

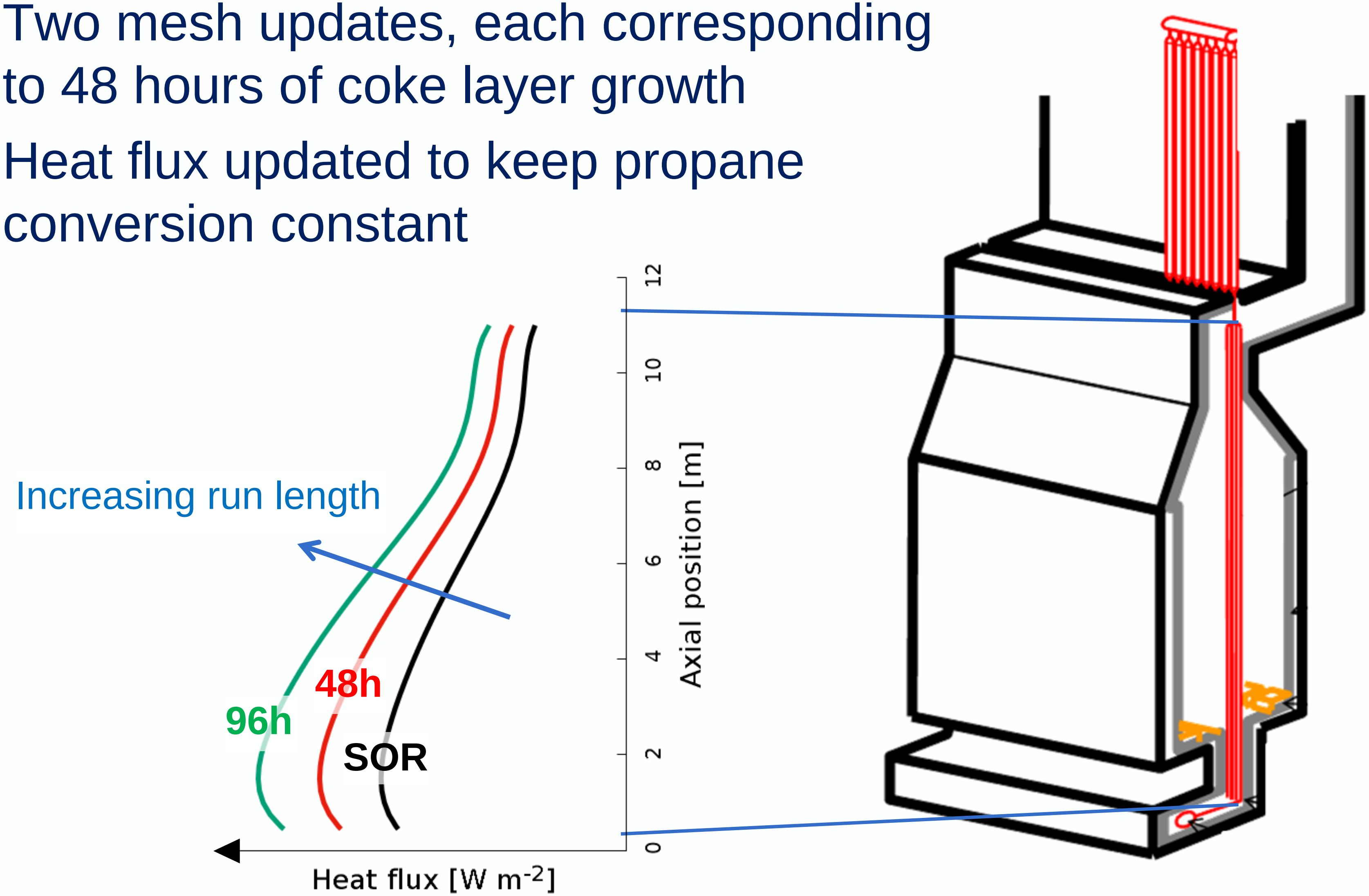
Bare



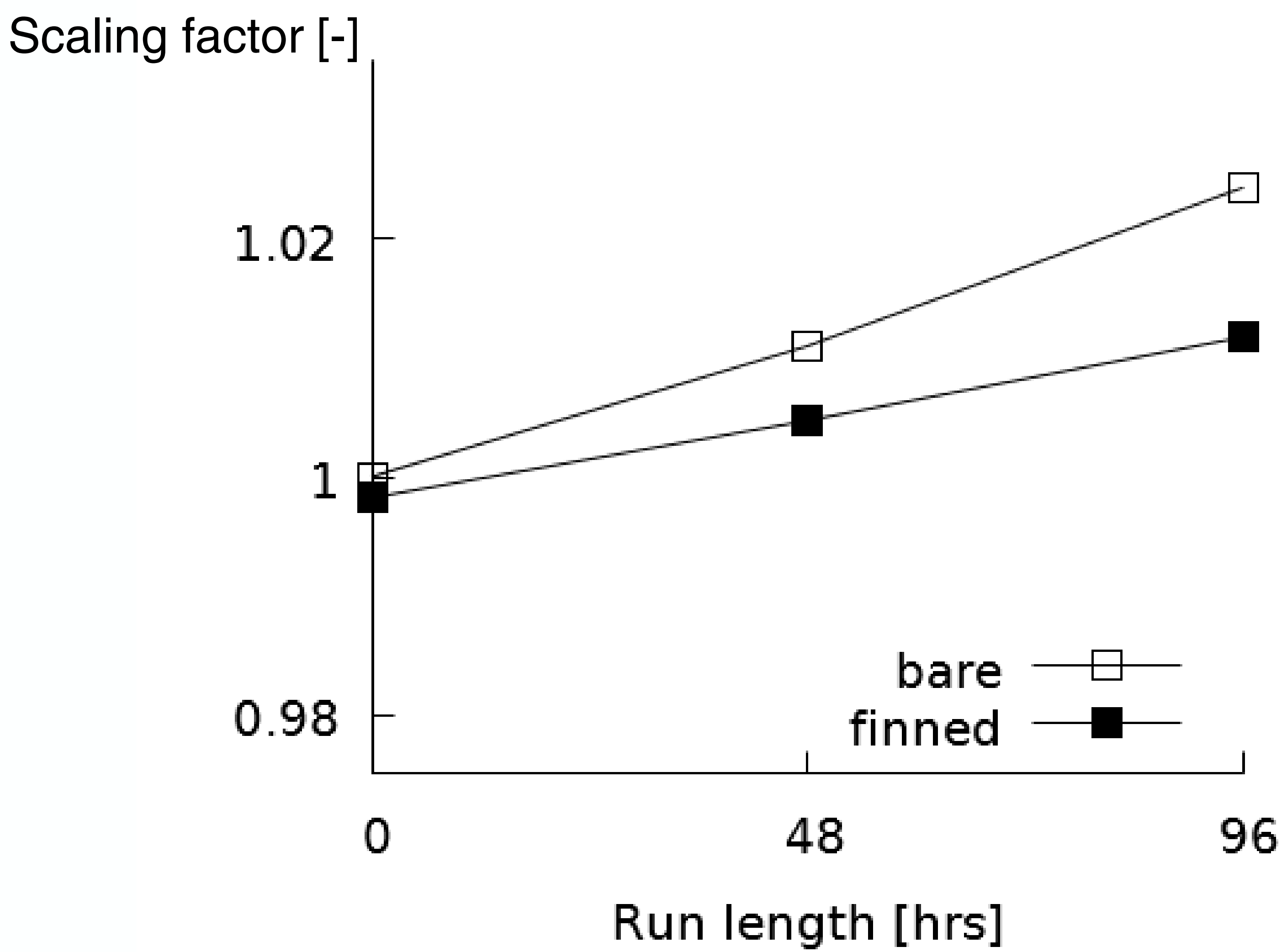
Straight fin

Run length simulation

- Two mesh updates, each corresponding to 48 hours of coke layer growth
- Heat flux updated to keep propane conversion constant



Heat flux correction



CFD model | Setup

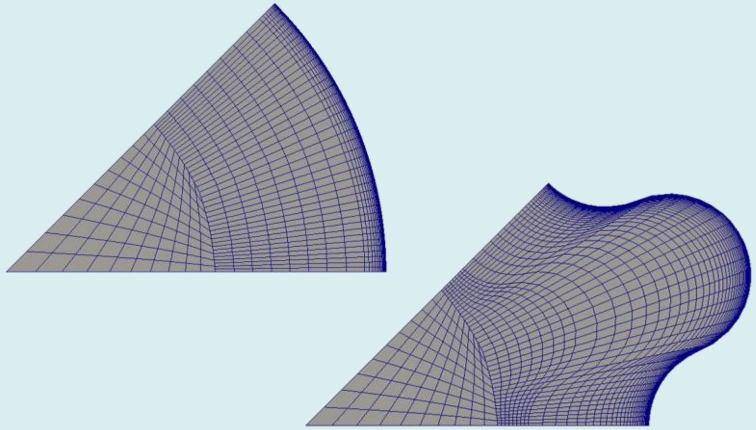
OpenFOAM

Turbulence modeling
- RANS: k–ω SST model (Menter, 2001)

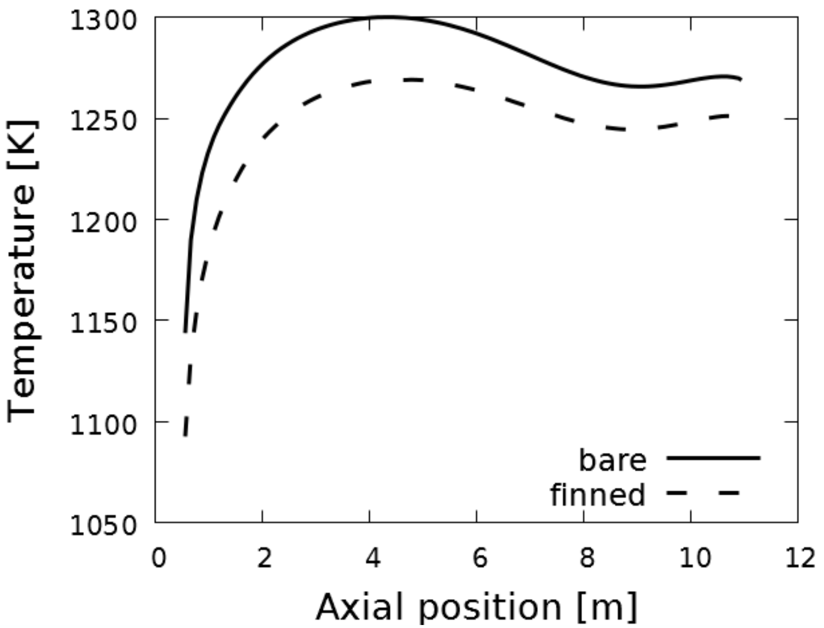
Numerical setup
- Steady-state
- SIMPLE algorithm
- 2nd order central differencing spatial discretization scheme

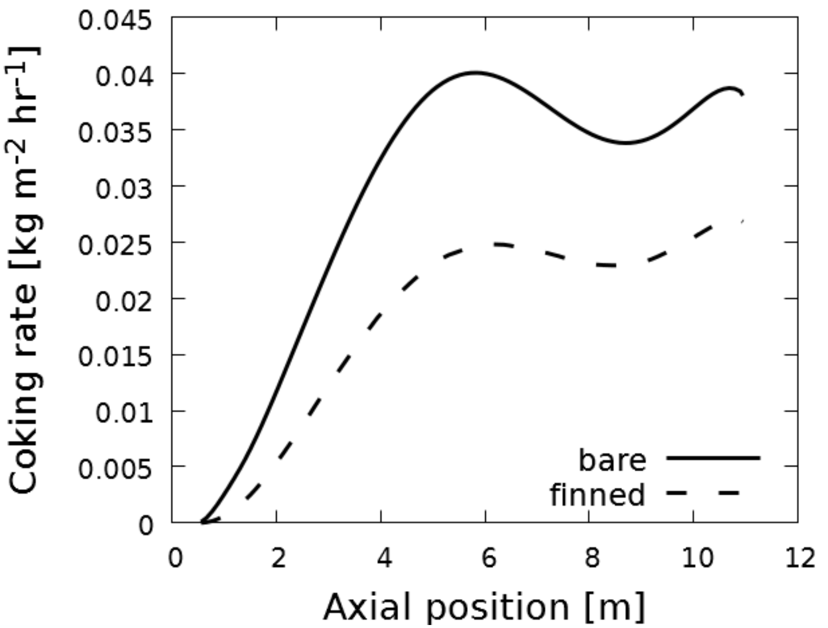
Chemistry model
- Full single-event microkinetic CRACKSIM model reduced to core for propane cracking:
  - 151 reactions
  - 29 species (13 radicals)

Meshing
- Structured grids for improved grid spacing control and cell orthogonality
- 1/8th of the tube's cross section
- Near wall grid resolution satisfying $y^+ < 1$



SOR Performance



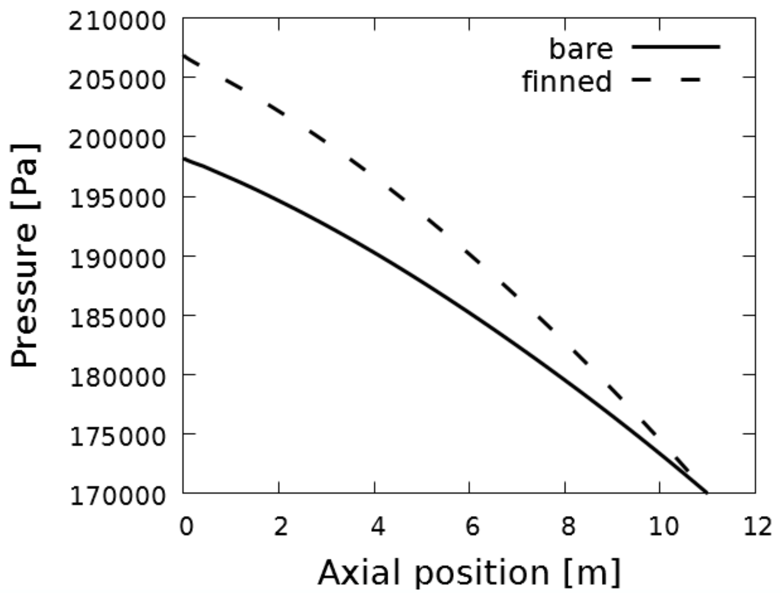


Max. TMT finned: 30 K lower

Max. coking rate: 32.5% lower

Increased run length?

Product selectivities

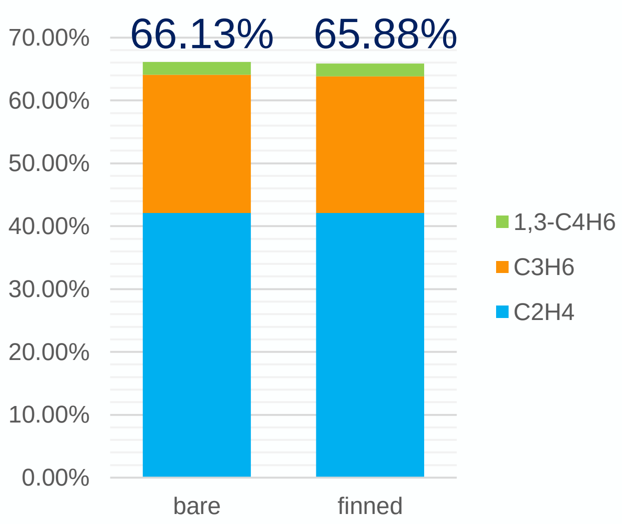


Reactor pressure drop 30% higher

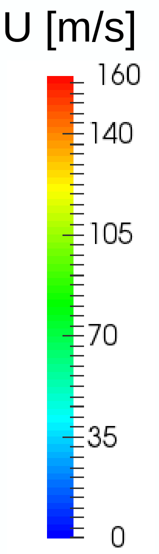
Lower olefin selectivity?

Minor effect on ***total*** olefin selectivity

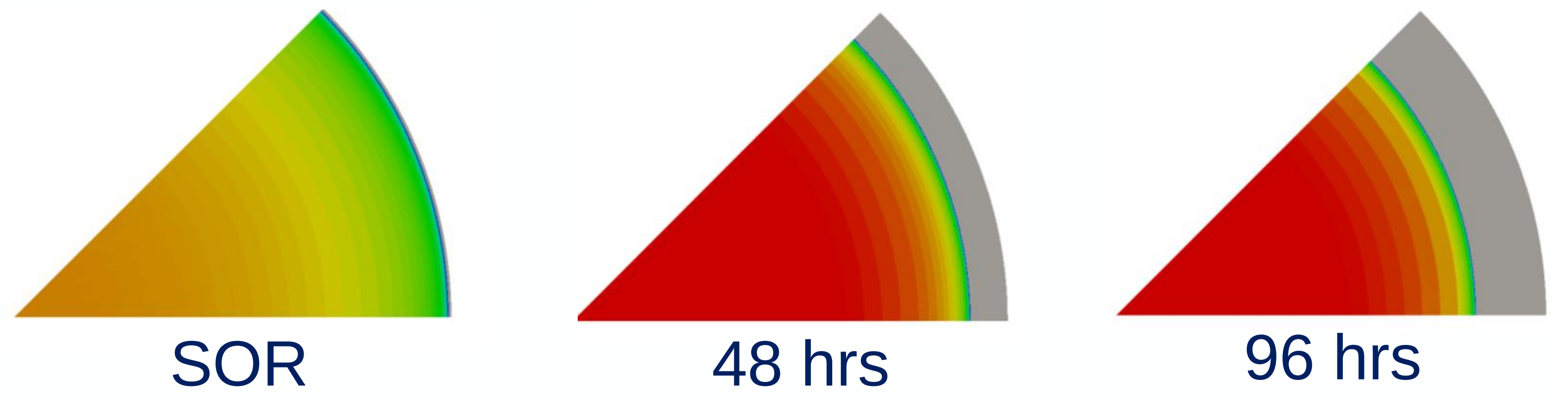
Radial mixing effects cannot be predicted based on 1D simulations only

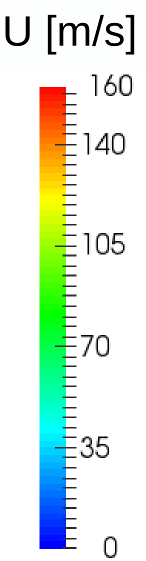


Coke layer growth

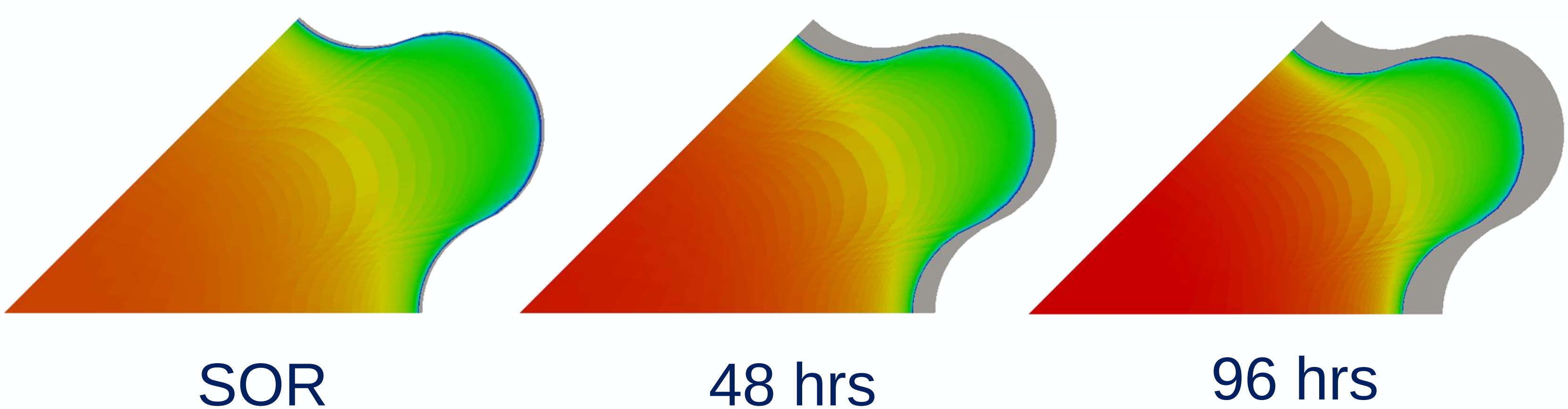


Bare tube: velocity magnitude contours @ z= 6 m



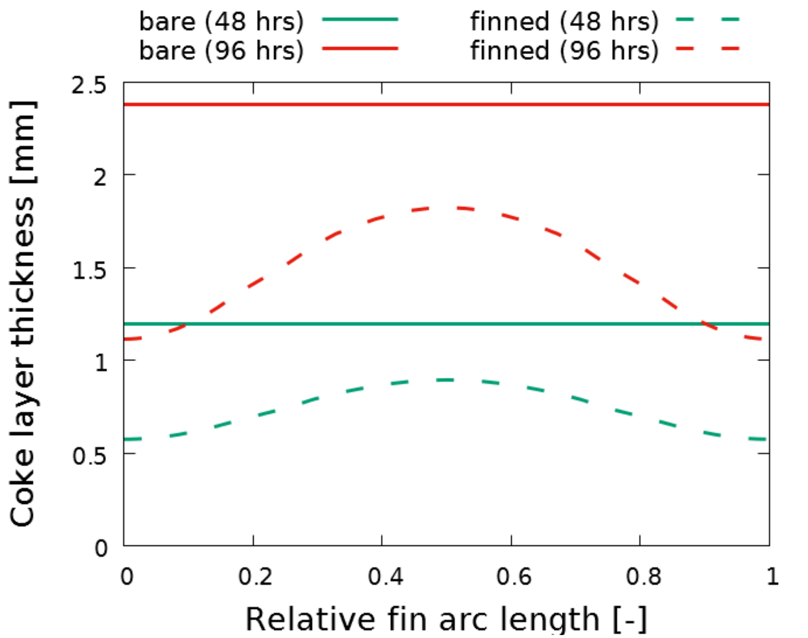


Finned tube: velocity magnitude contours @ z= 6 m



Coke layer growth

z = 6 m



Large difference in coke layer thickness BUT greater internal surface area

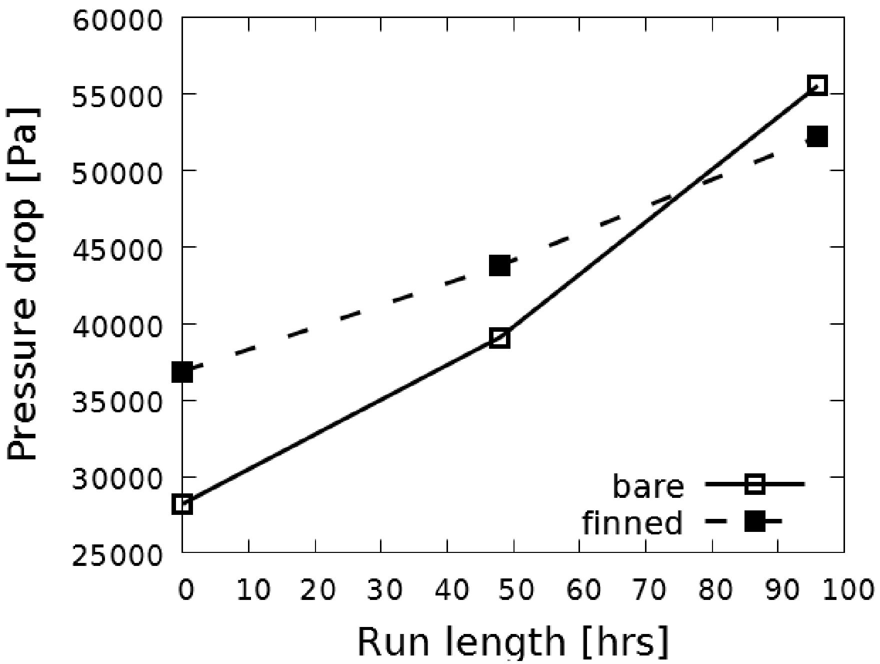
Small difference in effective coke volume

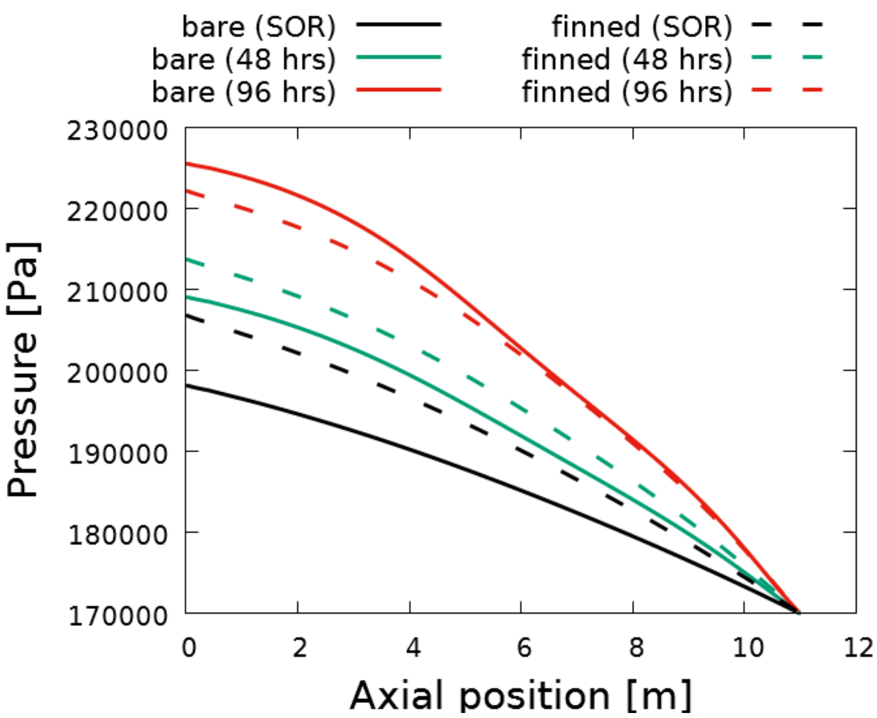
Coke volume at z = 6 m [$cm^3\ m^{-1}$]

	Bare	Finned
48 hrs	12.98	11.84
96 hrs	23.59	23.24

Total coke volume for finned tube still smaller than for bare tube

Pressure drop

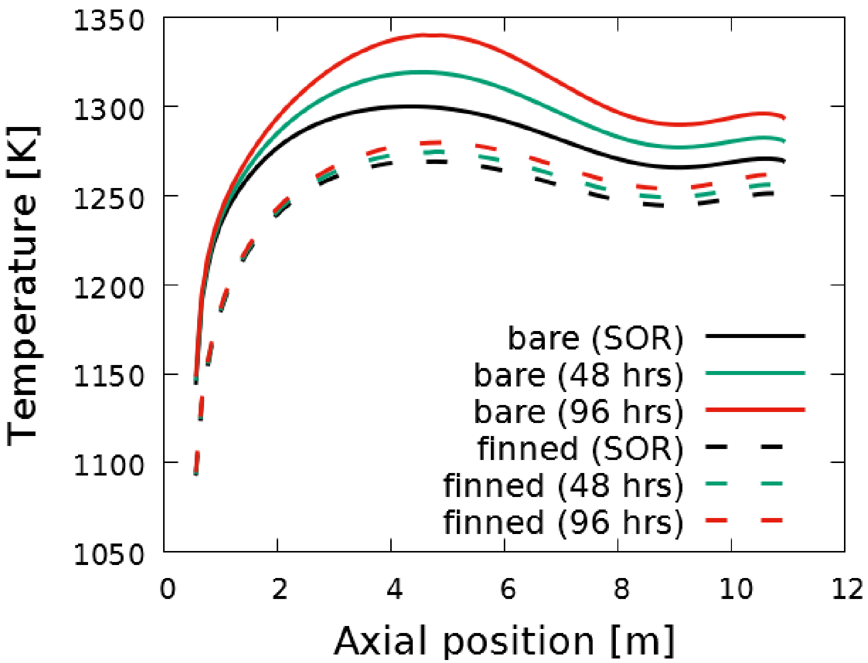


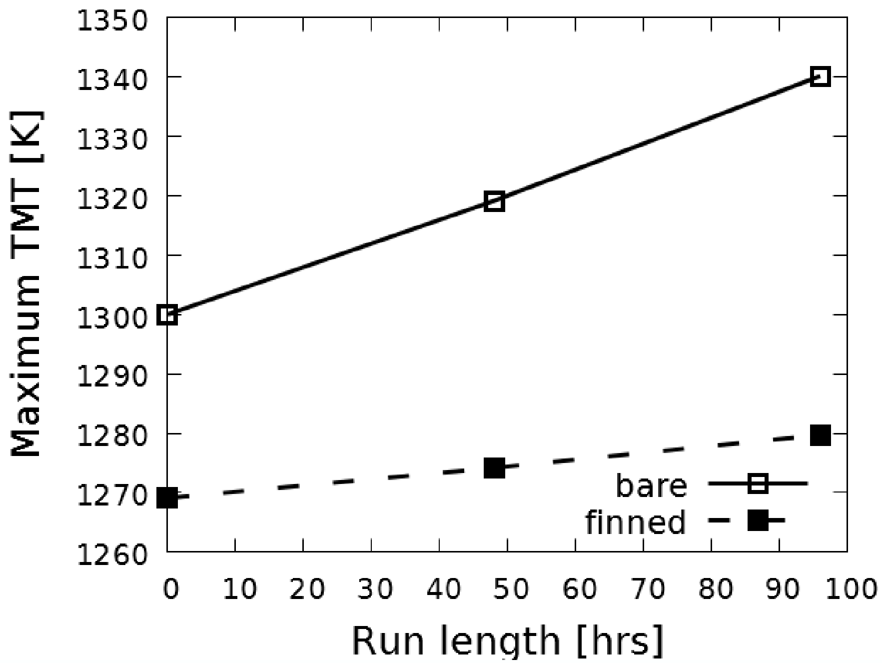


Cross-sectional flow area decreases → Pressure drop increases

Pressure drop increase for bare tube almost 2x faster than for finned tube

Tube metal temperature





Thermal resistance coke layer → Max. TMT increases

TMT increase for bare tube 4x faster than for finned tube

Conclusions & future work

- 3D computational fluid dynamic simulations allow optimization of industrial steam cracking reactors
- New method to perform yield & run length simulations of industrial steam crackers was developed
  - Combination with streamwise periodic simulations not possible
- Proof-of-concept reactive simulation of industrial propane cracker: bare vs. finned tubes
  - Strongly non-uniform formation of cokes in fins
  - Pressure drop increases faster in bare tube
  - TMT increases faster in bare tube
- Advantages of other 3D geometries (e.g. MERT) over finned tubes to be evaluated

Acknowledgements

- FWO Flanders, PI-FLOW Project
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Thank you for your attention!

Questions ?