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

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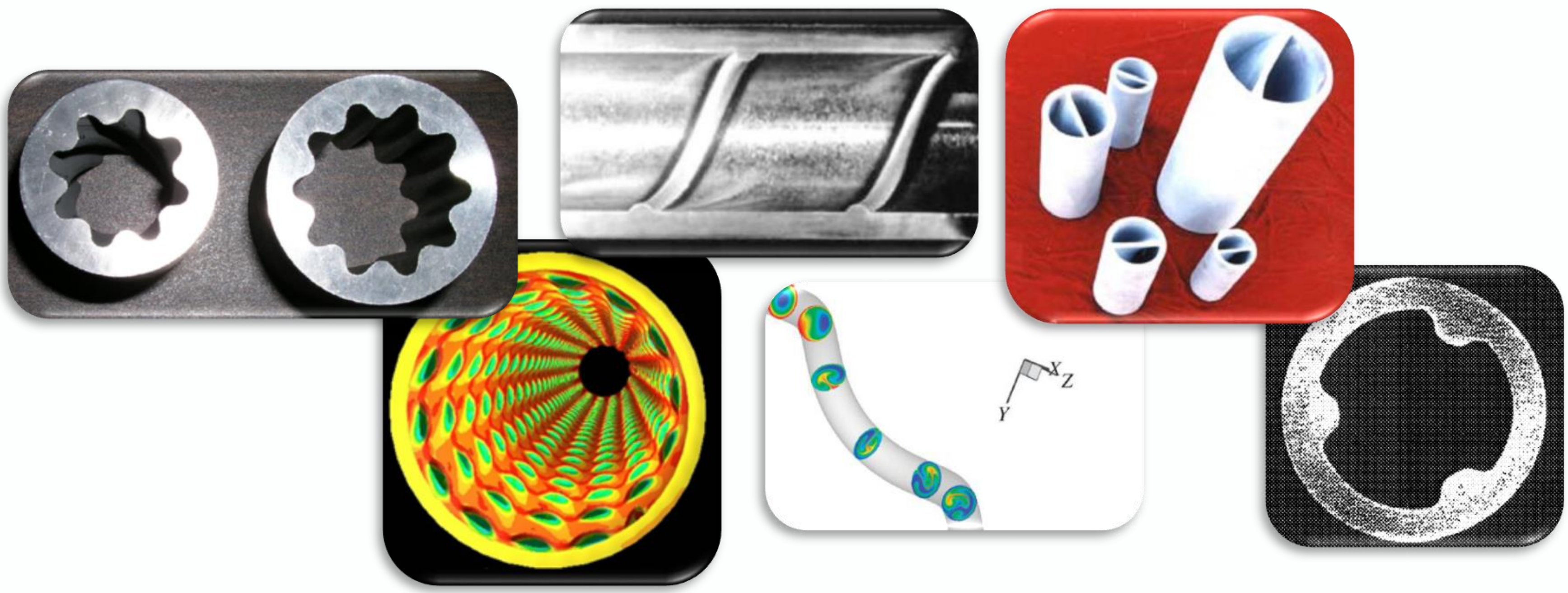
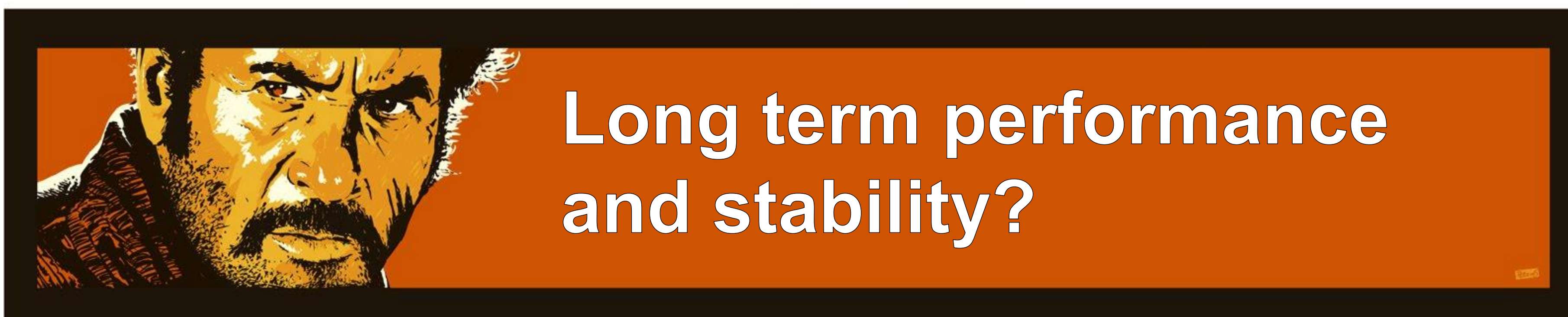
Coke reduction methods

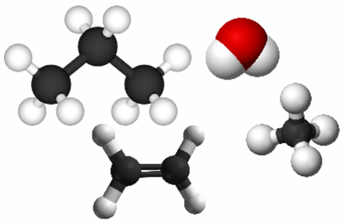
- Feed additives
- Metal surface technologies
- 3D reactor technologies



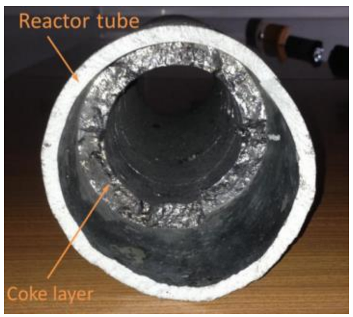
3D reactor technology | The Good, the Bad & the Ugly



Where are we?

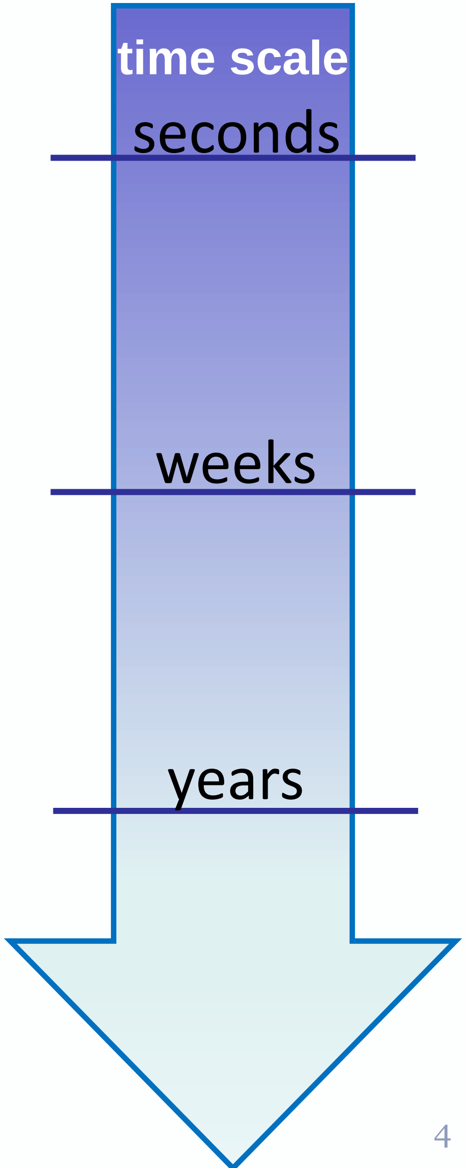


- Short term performance
  - Reactor residence time
  - Product yields, selectivities



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

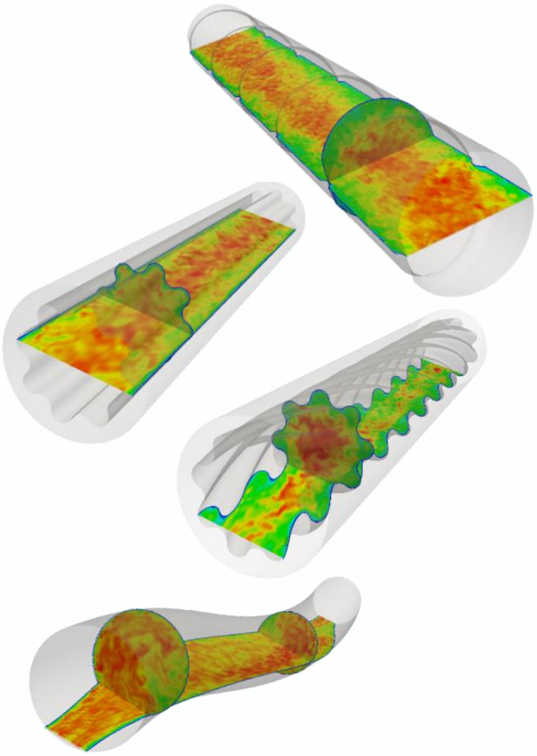
- Long term performance
  - Reactor stability & lifetime
  - Deterioration of reactor material



Short term reactor performance (1D vs. 3D)

- 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%	-34.0%	-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

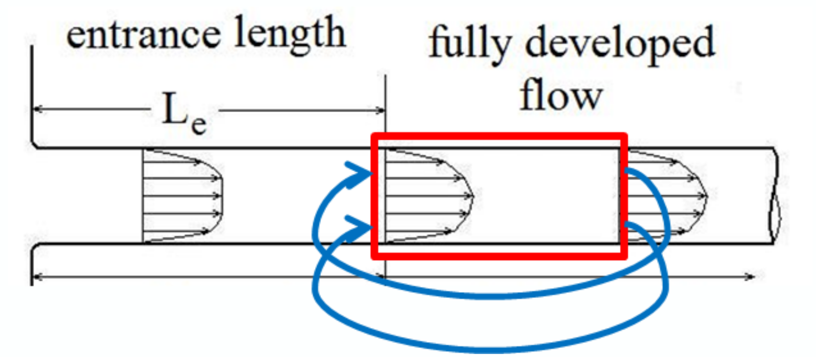
~ 1000 CPU hours

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

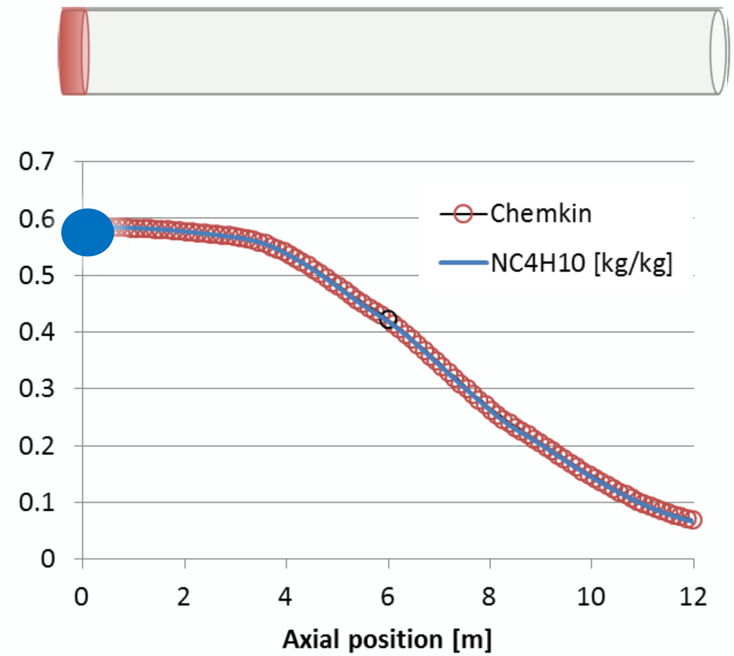
Periodic reactive simulations

- 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

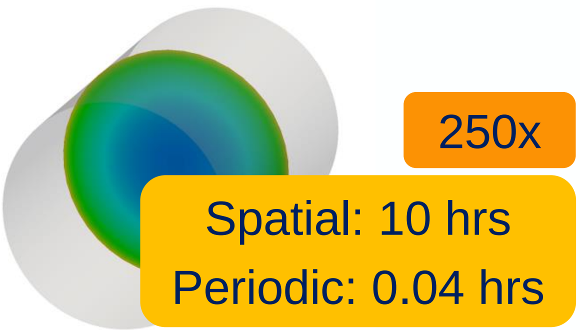
$$\Delta z = U_{bulk}\,\Delta t = \frac{\int_{\partial V} \rho u_z dA}{\int_{\partial V} \rho dA}\,\Delta t$$

Speedup factors of 200+



(Van Cauwenberge, 2015)

Periodic reactive | 3D Product yields

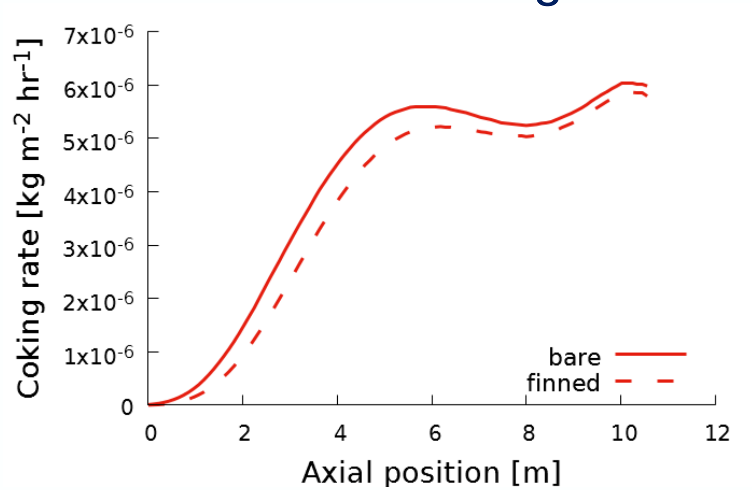


	Bare tube	Finned tube	Ribbed tube
COT [K]	1152.6	1151.6	1155.2
TMT [K]	1230.6	1222.7	1177.2
ΔP [Pa]	27682	29061	110001
Conversion	74.96%	74.99%	76.18%
CH4	13.96%	14.04%	14.54%
C2H2	1.64%	1.69%	1.55%
C2H4	27.60%	27.87%	27.74%
C2H6	1.23%	1.27%	1.32%
C3H6	22.91%	22.50%	23.52%
1,3-C4H6	2.91%	2.97%	2.88%

(Van Cauwenberge, 2015)

Coke formation | The Ugly

Start-of-run coking rate

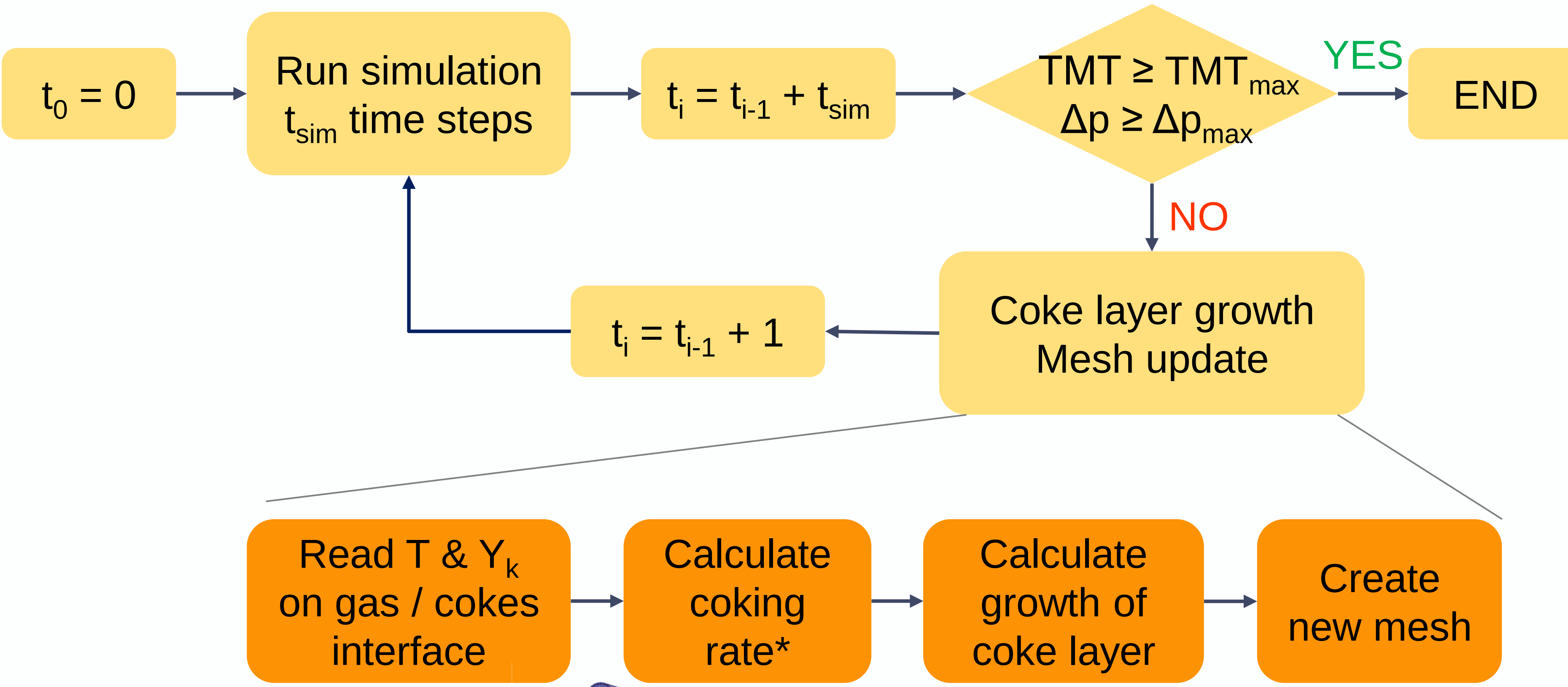


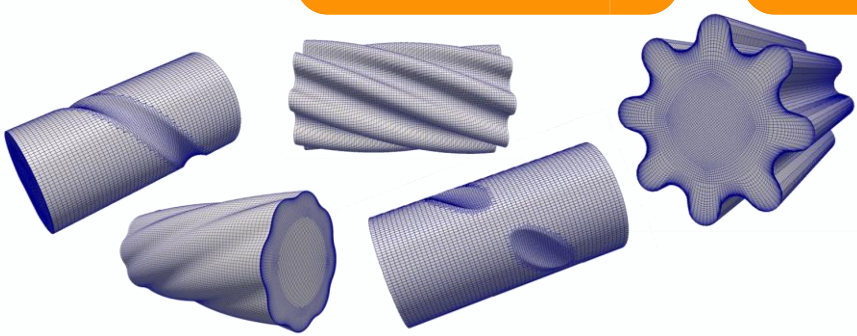
Evaluation of 3D reactor technologies requires tracking coke layer growth

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



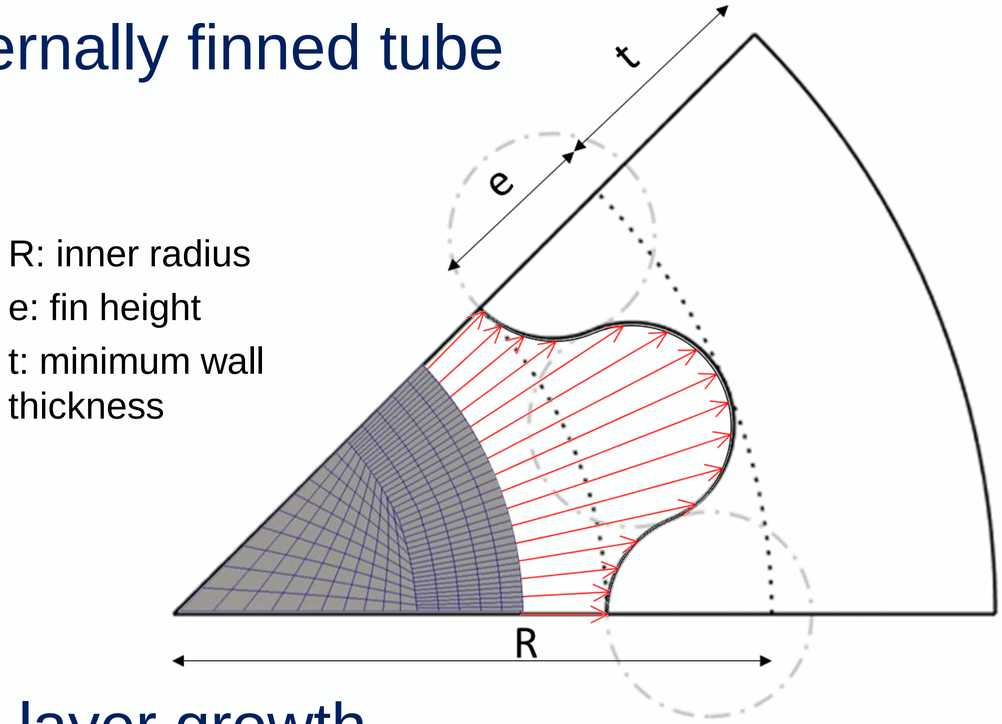


➔ New library of **extrusion models** in OpenFOAM, including a variety of 3D steam cracking reactor geometries

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

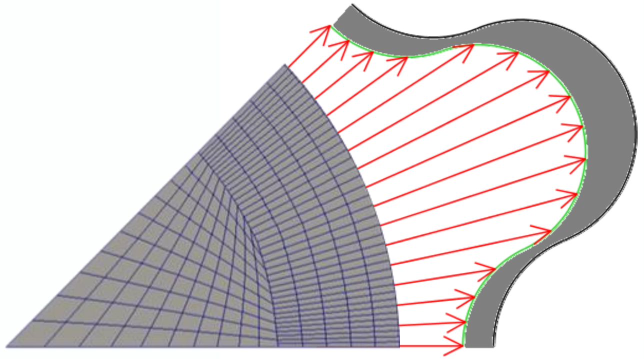
Extrusion of 3D reactor geometries

Internally finned tube



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

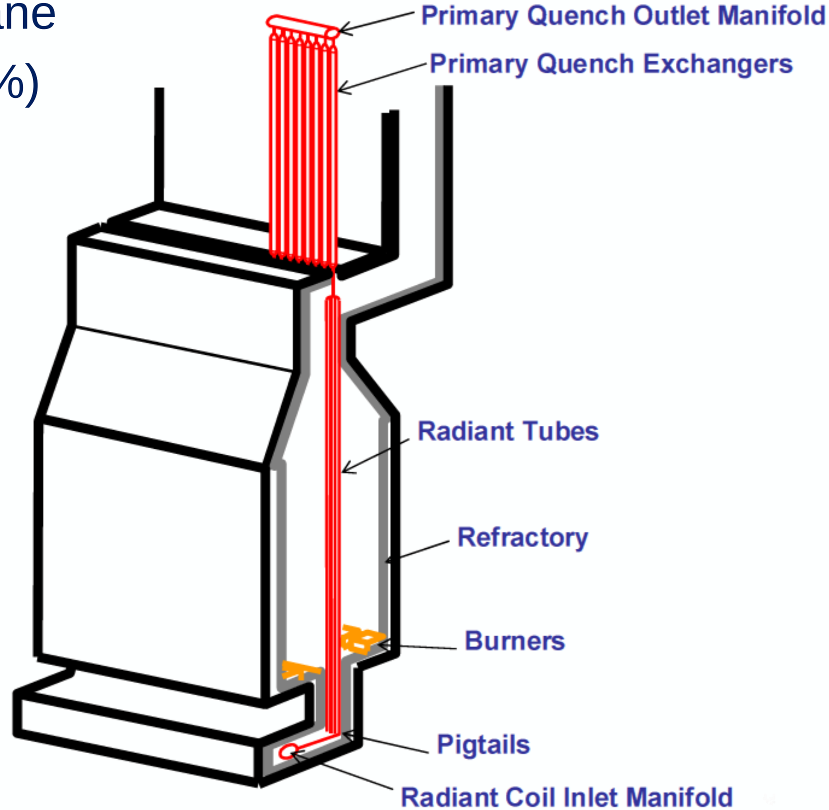
Coke layer growth



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

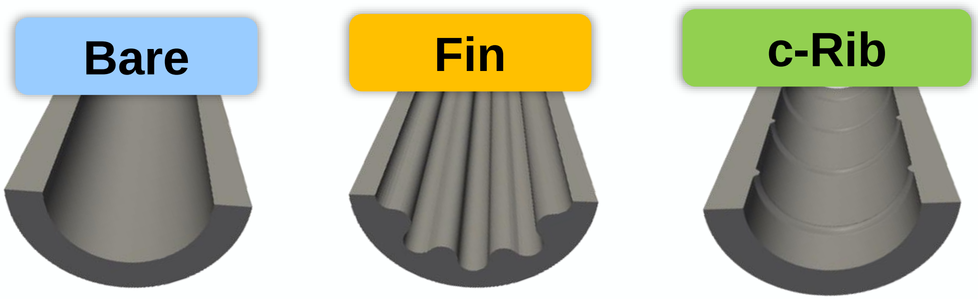
Test case | Millisecond propane cracker

- Feedstock 118.5 kg/h propane
- Propane conversion 80.15 % (± 0.05%)
- Steam dilution 0.326 kg/kg
- CIT 903.7 °C
- COP 170 kPa



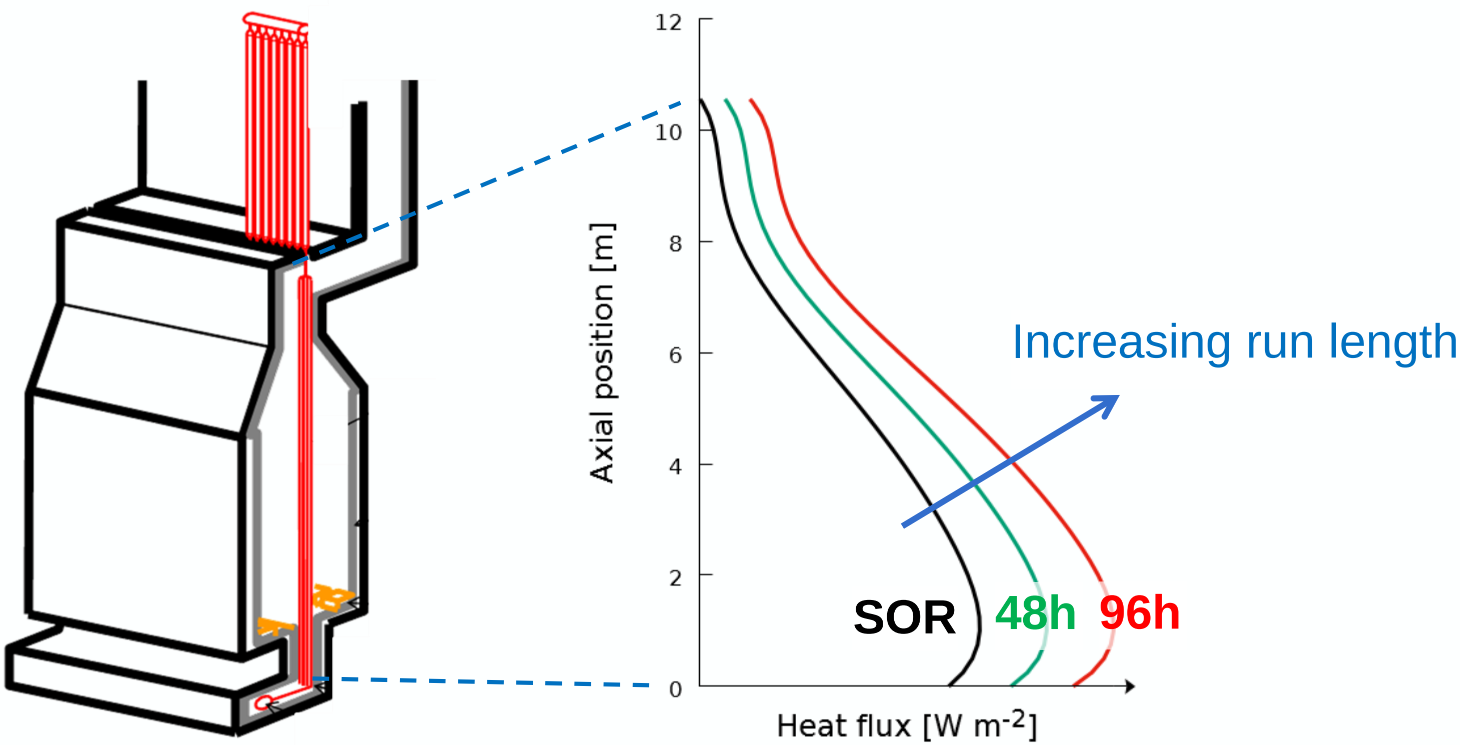
Different geometries simulated

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



Run length simulation

- Several mesh updates, each corresponding to 24 hours (c-rib, bare) or 48 hours (fin) of coke layer growth
- Heat flux updated to keep propane conversion constant



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)

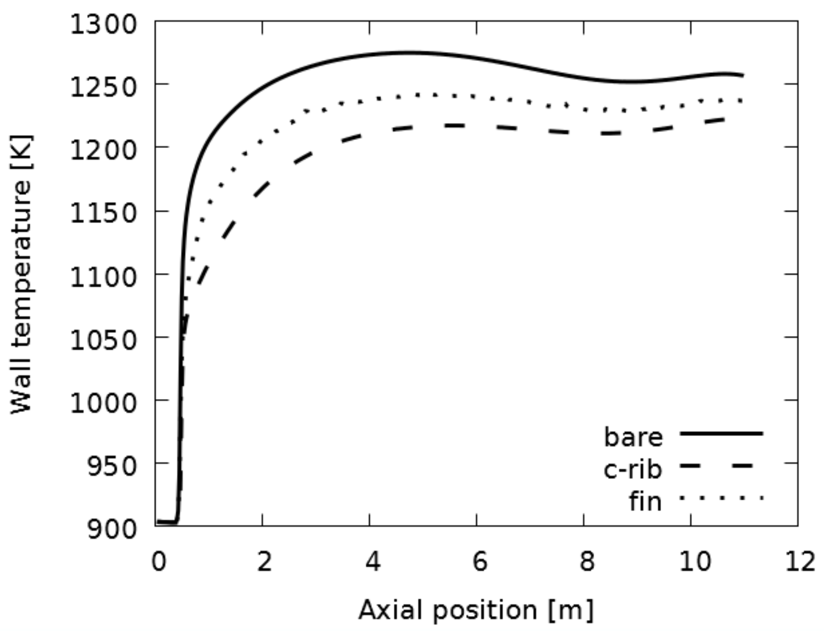
Meshing

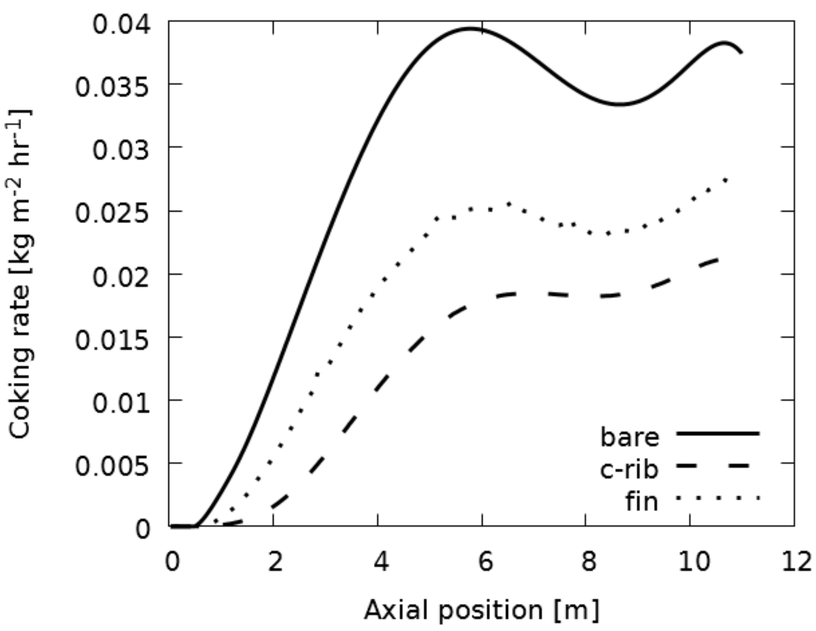
- Structured grids for improved grid spacing control and cell orthogonality

- Symmetry:
  - Wedge for bare, c-Rib
  - 1/8th for finned geometry

- Near wall grid resolution satisfying $y^+ < 1$

SOR Performance



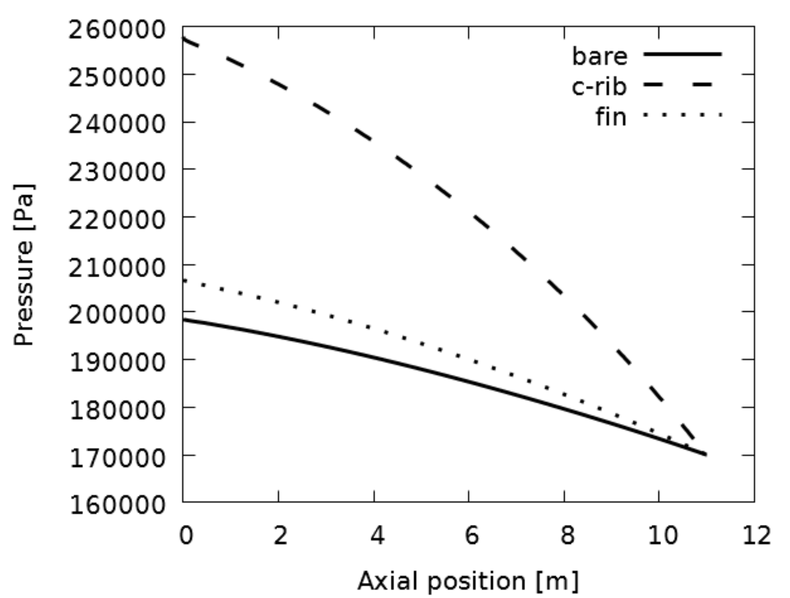


Max. TMT 3D geometries: >30 K lower

Max. coking rate: >32.5% lower

→ Increased run length?

Product selectivities

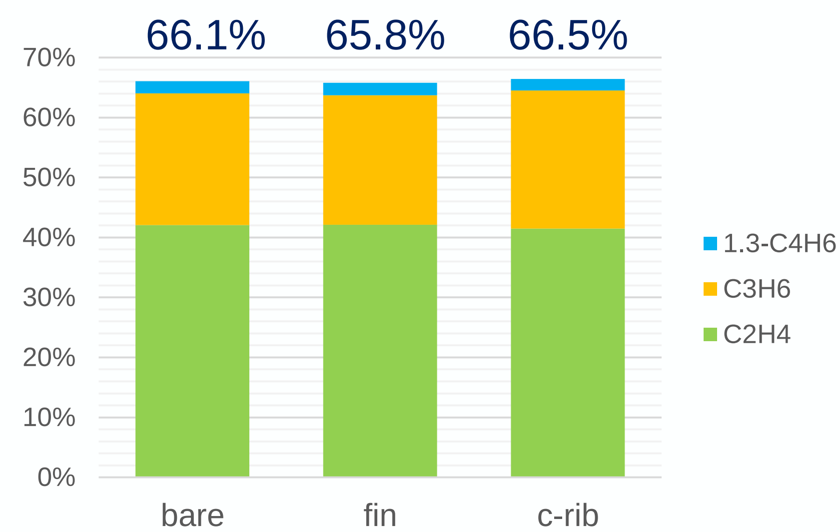


Reactor pressure drop

30% higher (fin)

300% higher (c-Rib)

~~1D: “Lower olefin selectivity”~~

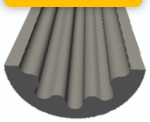


Minor effect on ***total*** olefin selectivity

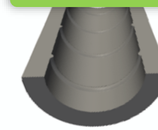
Radial mixing effects cannot be predicted based on 1D simulations only

Non-uniform coke layer growth

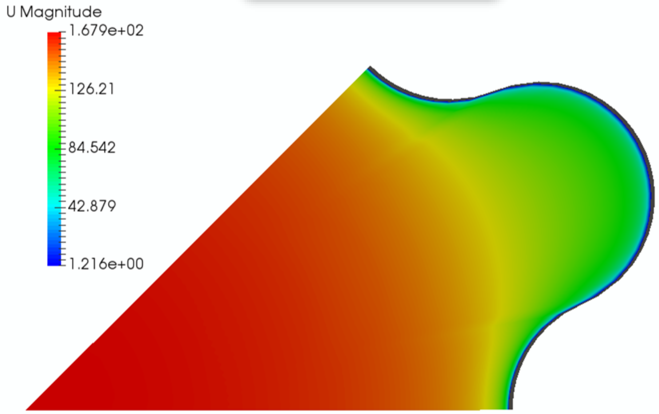
Fin



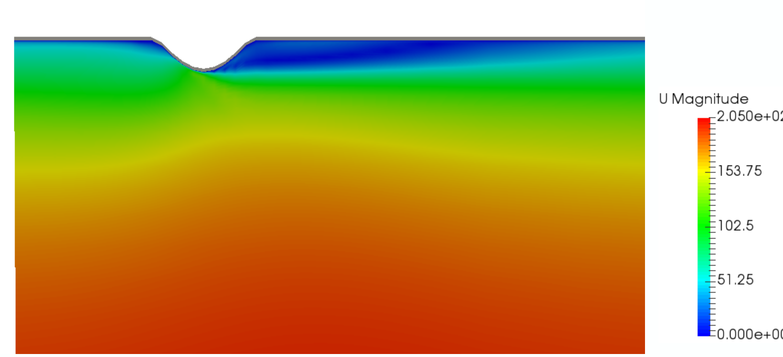
c-Rib



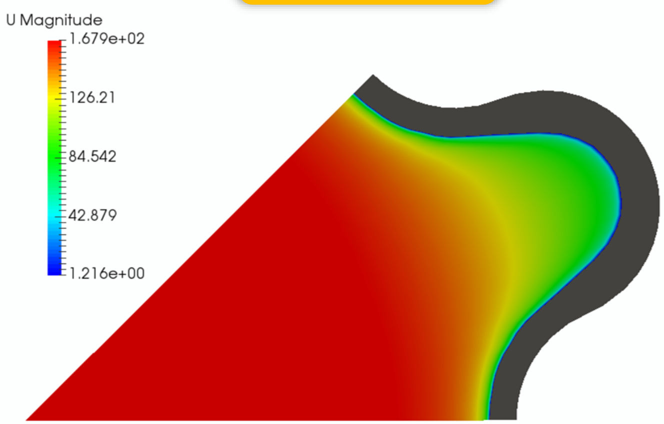
SOR (0 hrs)



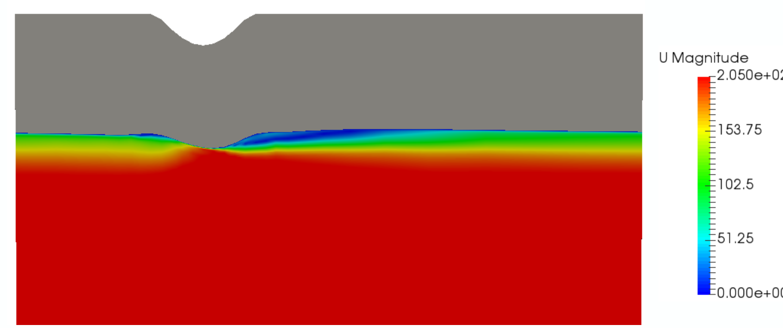
SOR



48 hrs

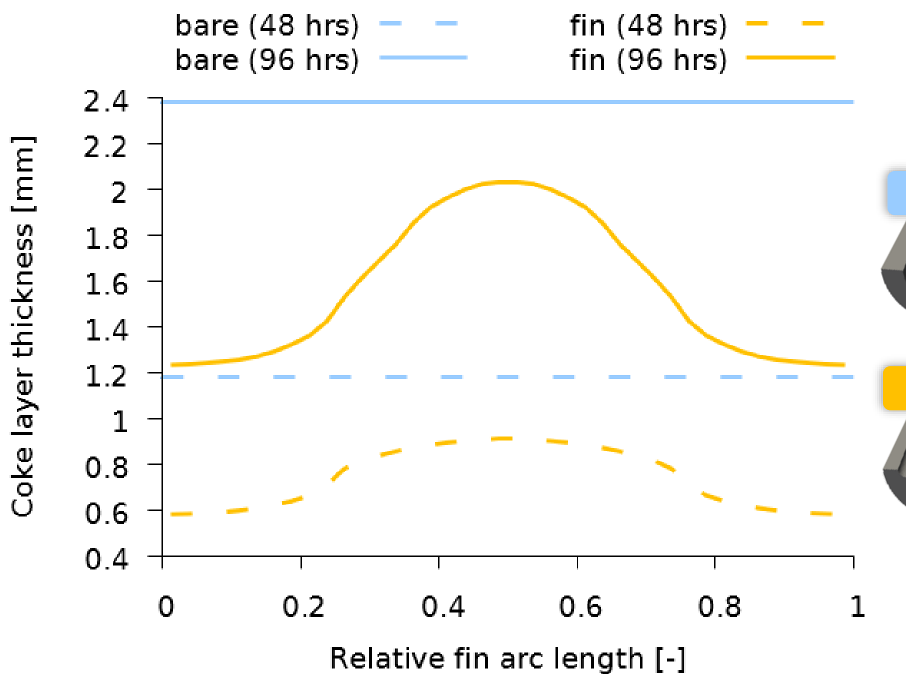


10 days



Coke layer growth

z = 6 m



Thinner coke layer for finned tube compared to bare tube

BUT:
larger internal surface area

Total coke volume in reactor [dm³]

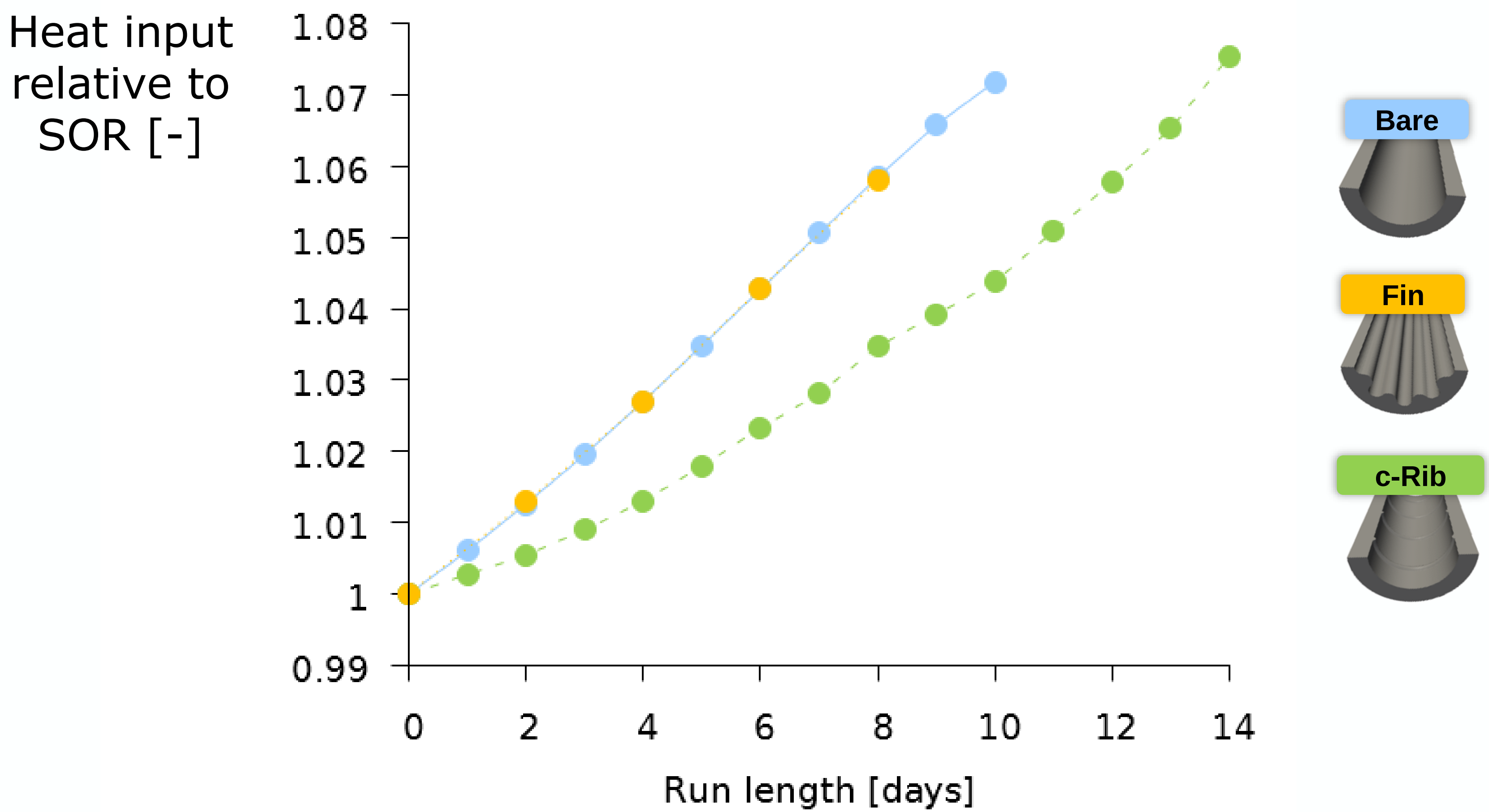
	Bare	Finned
48 hrs	0.844	0.887
96 hrs	1.652	1.739

Total volume of cokes more or less the same

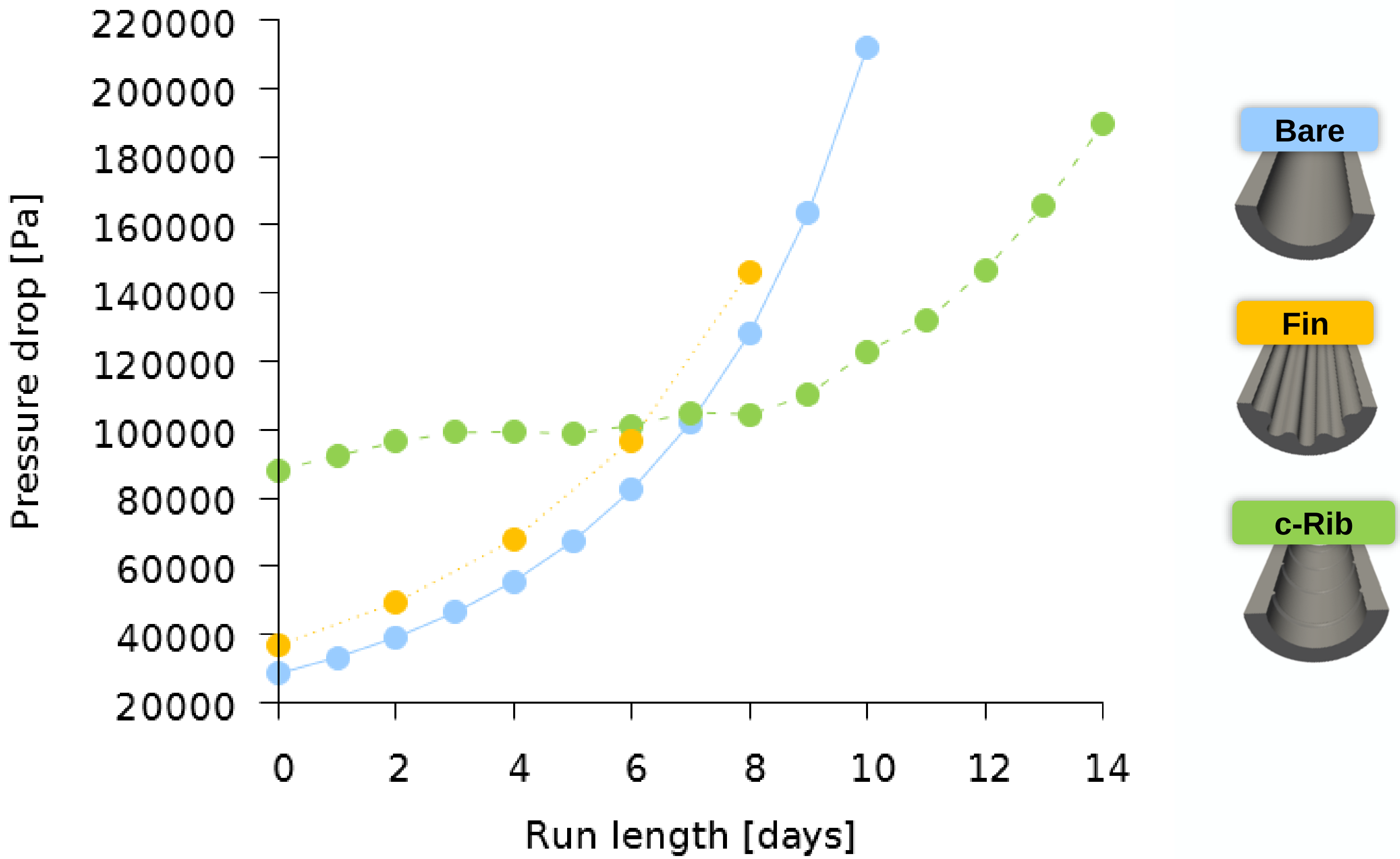
Or, even more cokes for finned tube

Increased heat input

Heat input to the reactor is updated after each mesh update, to keep the propane conversion constant: **more cokes = more heating.**



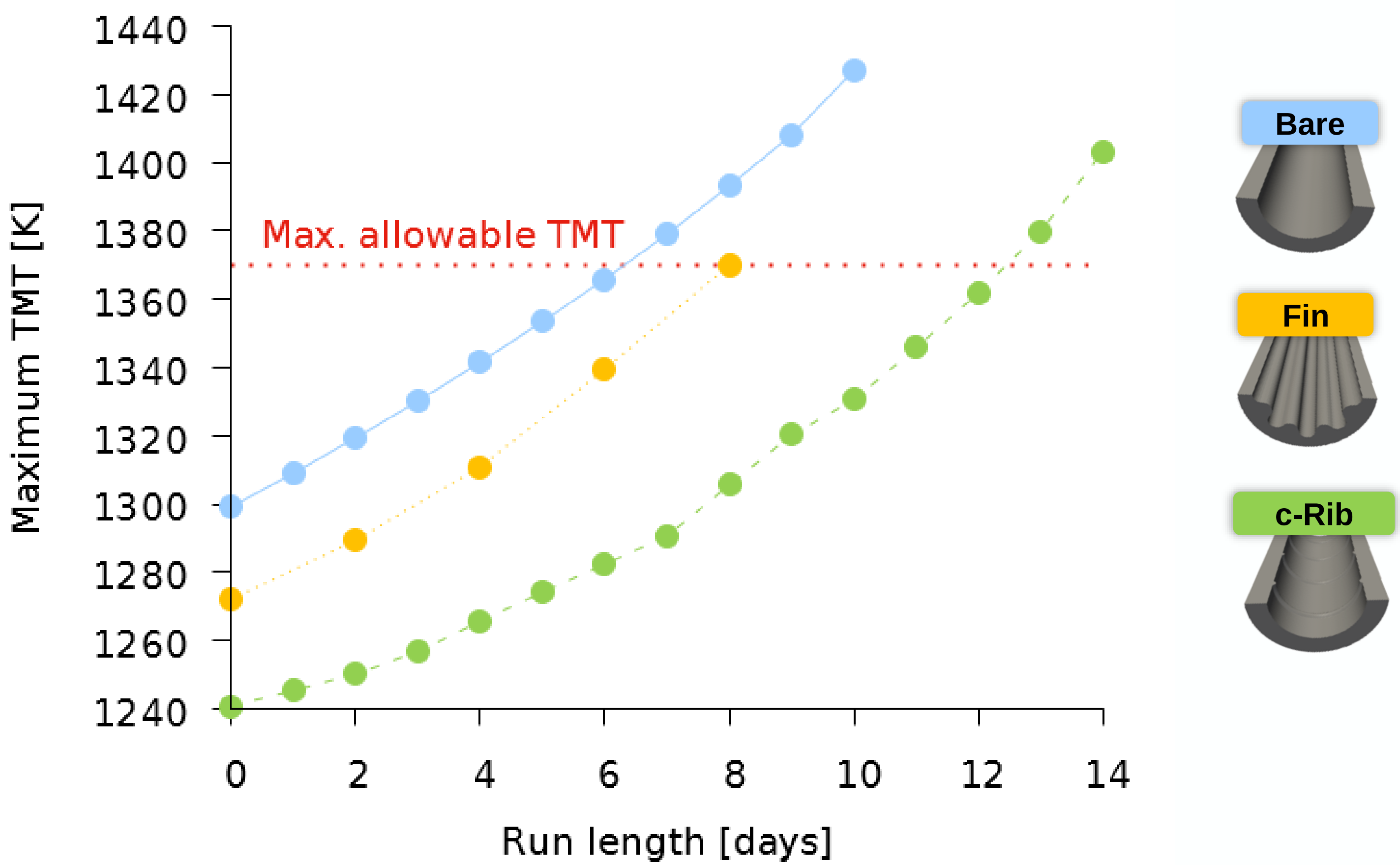
Pressure drop



Cross-sectional flow area decreases due to coke → Pressure drop increases

Less fast increase for **c-rib** compared to bare and finned geometry

Tube metal temperature



Thermal resistance coke layer → Max. TMT increases

TMT increases at the **same rate** for all geometries, but **absolute max. TMT lower** for 3D geometries

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 vs. ribbed tubes
  - Strongly non-uniform formation of cokes in fins and on ribs
  - Pressure drop increases faster in bare and finned tube compared to ribbed tube
  - Max. allowable TMT is reached earlier for bare tube
- Advantages of other 3D geometries (e.g. intermittently ribbed tube) over finned tubes to be evaluated

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Opening new horizons

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HPC UGENT

Vlaams Supercomputer Centrum

- IMPROOF: Integrated Model guided PROcess Optimization of steam cracking Furnaces. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 723706

Acknowledgements | IMPROOF

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