SDM-17

UNIVERSITEIT GENT

FACULTY OF ENGINEERING AND ARCHITECTURE

IMPROOF

LABORATORY FOR CHEMICAL TECHNOLOGY

IMPROOF: Integrated model guided process optimization of steam cracking furnaces

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1 GHENT UNIVERSITY 2 cnrs 3 DOW 4 CRESS 5 CERFACS CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE 6 POLITECNICO DI MILANO 7 JOHN ZINK HAMWORTHY COMBUSTION 8 S+C 9 ayming business performance consulting 10 AVGI 11 Emisshield 12 TechnipFMC

SDM-17, Bologna, Italy, 28/04/2017

ERIC

IMPROOF

Sep 2016 – Aug 2020

A H2020-SPIRE project

http://improof.cerfacs.fr

Project Coordinator: GHENT UNIVERSITY

- IND
- SME
- RTO
- UNI

Partners:

CRACKER: HEART OF A PETROCHEMICAL PLANT

Commercially important petrochemical process

The main source of ethylene, propylene and other valuable hydrocarbons (i.e. olefins and aromatics)

Steam cracker

Ethylene

Propylene

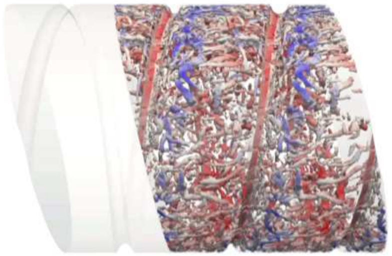
Butadiene

Benzene

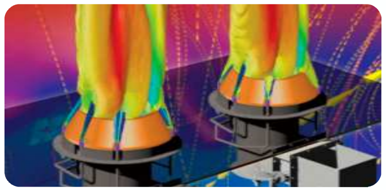
Polyolefin plants,…

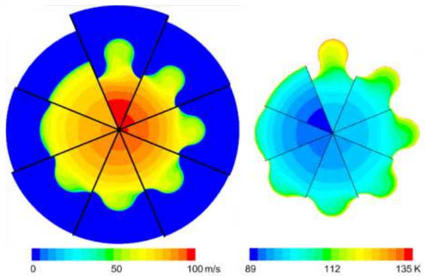
IMPROOF IS ALL ABOUT

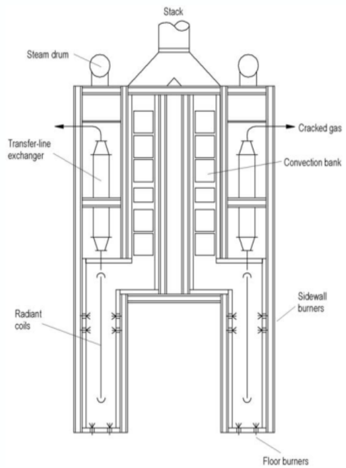
Renewable fuel characterization
- experimental activity
- kinetic mechanisms



Innovative Furnace System developments and integration
- oxy-fuel combustion
- coke formation
- emissivity coating
- 3D reactor testing





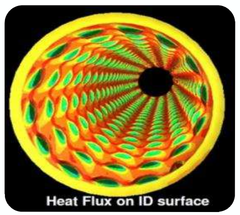


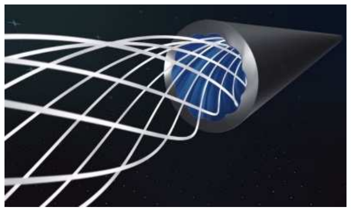
Upscaling and Demonstration

TRL6

TRL5

Advanced 3D modeling
- CFD RANS/LES
- Reactor optimization
- pilot plant simulation





- Energy efficiency
- Greenhouse gases
- NO_X
- SO_X

OUTLINE

- Introduction
- Concept and Objectives
- High Emissivity Coatings
- 3D Reactor Technology
- Conclusions

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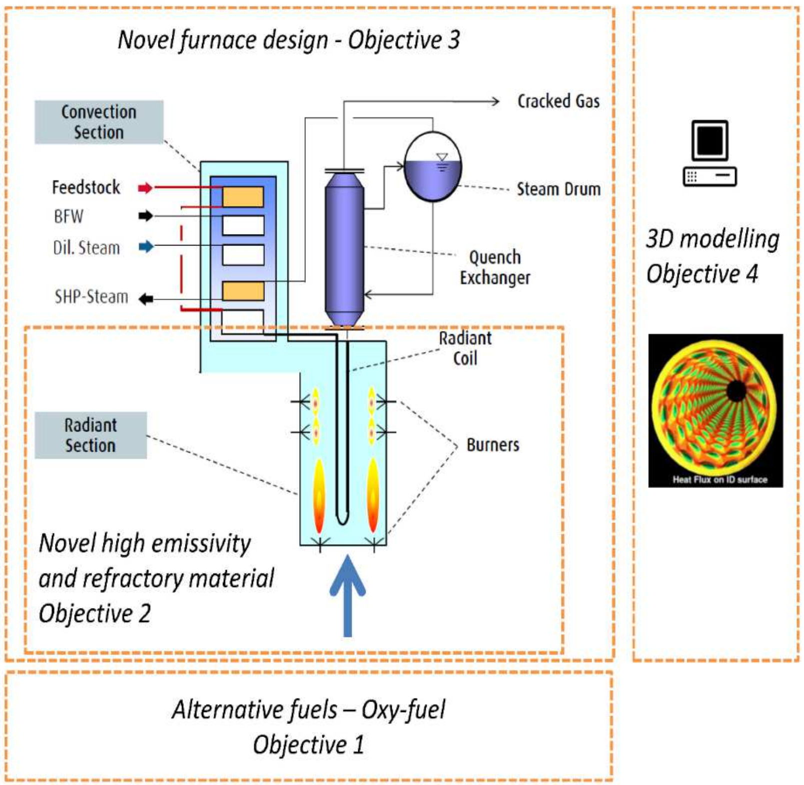
CONCEPT AND OBJECTIVES



1. Novel combustion technology using alternative fuels and oxy-fuel combustion
2. Demonstrate the individual impact of novel emissive, reactor and refractory materials and designs at pilot scale (TRL5)
3. Demonstrate the power of advanced process simulation (high performance computing and CFD) for furnace design and optimization
4. Demonstrate the technical economic and environmental sustainability of the IMPROOF furnace at TRL6
5. Coke formation reduction and real time optimization

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EMISSIVITY: RADIATIVE HEAT TRANSFER

Three fundamental mechanisms of heat transfer:

- Conduction
- Convection
- Radiation

$$E_{bb}(T) = \int_{\lambda=0}^{\lambda=\infty} L(\lambda, T)\mathrm{d}\lambda = \varepsilon(T)\sigma T^4$$

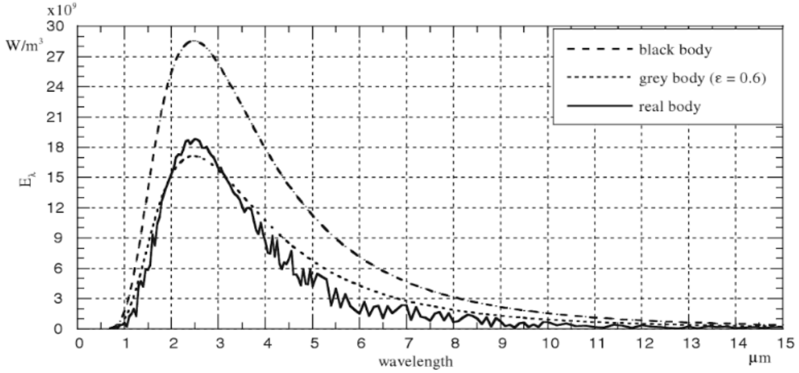
With σ the Stefan-Boltzmann constant
$\varepsilon(T)$ the total hemispherical emissivity

Over 90 % of the heat transfer from the steam cracking furnace to the reactor coils arises from radiation

Heynderickx, G.J. and M. Nozawa, *Banded gas and non-gray surface radiation models for high-emissivity coatings*. AIChE journal, 2005.

- In reality no object behaves as a perfect blackbody

The deviation of the spectral radiance from a perfect blackbody is given by the emissivity:



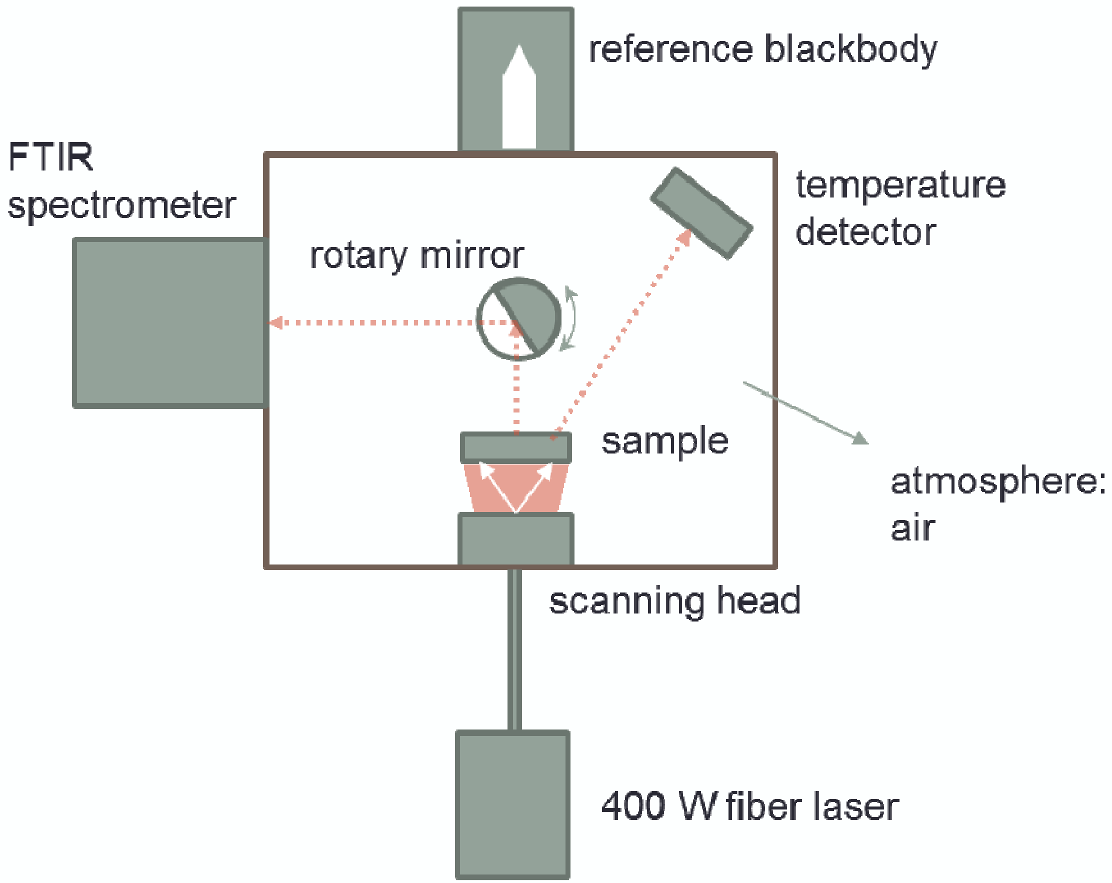
Annaratone, D. (2010). Engineering Heat Transfer, Springer Berlin Heidelberg.

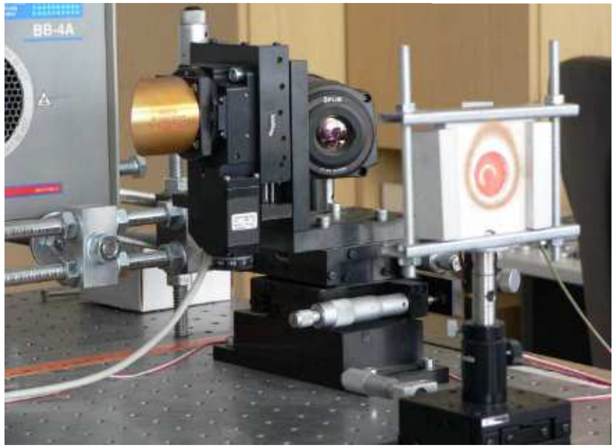
WHY EMISSIVITY COATINGS?

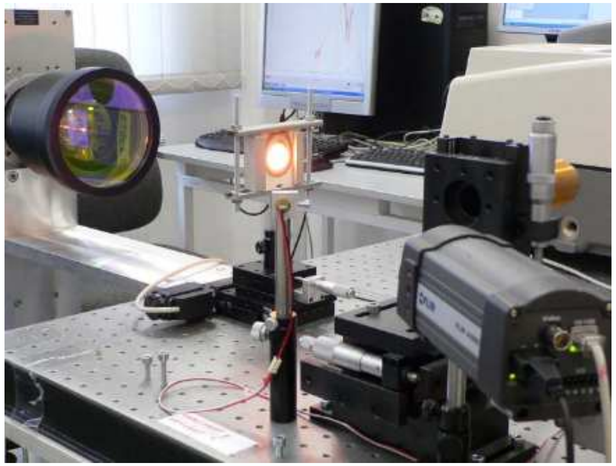
- To increase the thermal efficiency of a furnace, the use of **high-emissivity coatings** on reactor tubes and/or furnace walls has been suggested
- Applying a high-emissivity coating on a reactor tube decreases the amount of **reflected energy** and increases the amount of **absorbed** (and possibly re-radiated) **energy**
- Applying a high-emissivity coating on a **furnace wall** increases the amount of energy **absorbed** by the furnace wall which is transferred to **reactor tubes** through **re-radiation**
- An **increase** in the **thermal efficiency** of a furnace can be translated into an increase of throughput or a **decrease in fuel gas** input

Heynderickx, G.J. and M. Nozawa, *Banded gas and non-gray surface radiation models for high-emissivity coatings*. AIChE journal, 2005.

EMISSIVITY: EXPERIMENTAL SET-UP



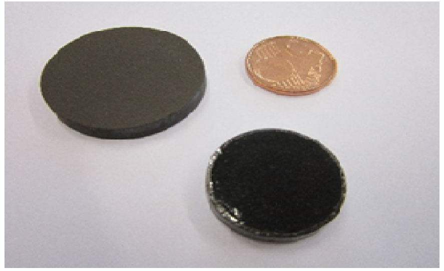




Honnerova et al., *New experimental device for high-temperature normal spectral emissivity measurements of coatings.*. Measurement Science and Technology, 2014.

EMISSIVITY: SAMPLES

Metal samples



(un)coated 304 stainless steel

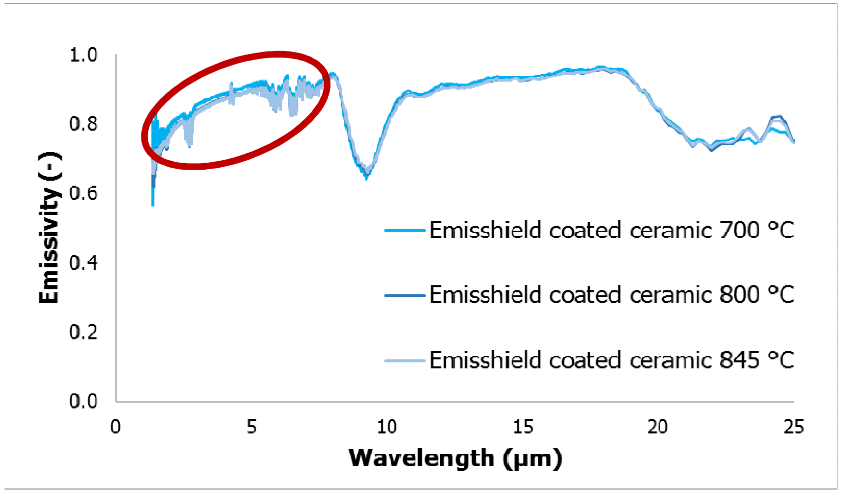
Ceramic samples

(un)coated Alamo®

- Two novel **high-emissivity** coatings by Emisshield designed for radiant **walls/floor** of furnace and process **coils/tubes**
- Reference 304 SS and Alamo® refractory bricks were measured

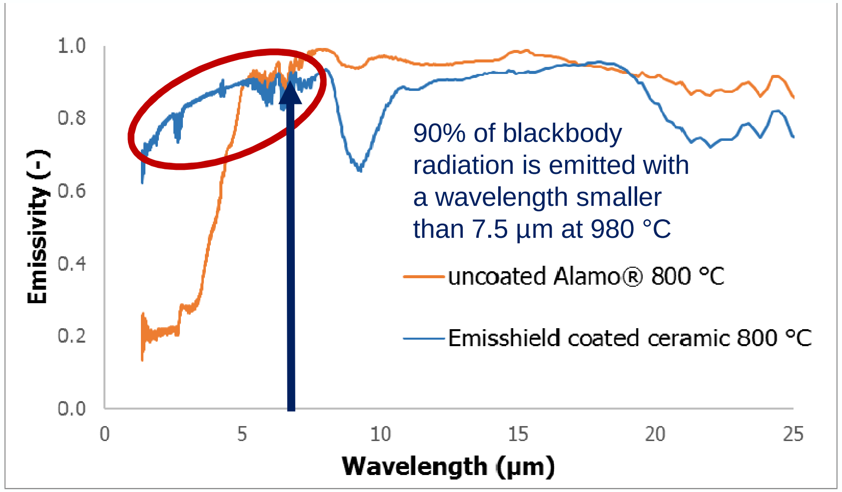
EMISSIVITY: CERAMIC SAMPLES

Emisshield Coated Alamo®



- Temperature independent in 700 – 850 °C
- Allows to measure at lower temperatures

Coated vs. Uncoated Alamo®

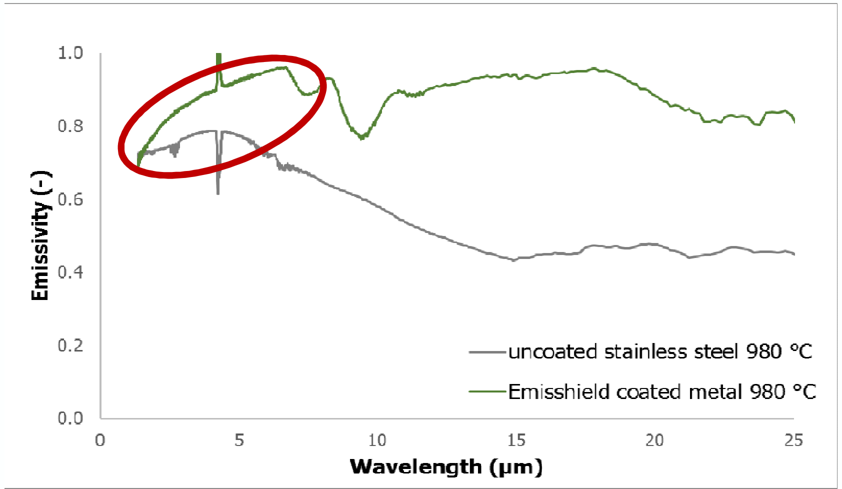


- Big difference in the sub 5 µm region
- Coating the **refractory wall** can significantly **improve** the thermal efficiency of a furnace

- Decrease of spectral emissivity is observed for wavelengths shorter than 5 µm.
- Method needs further **improvement** to evaluate this.

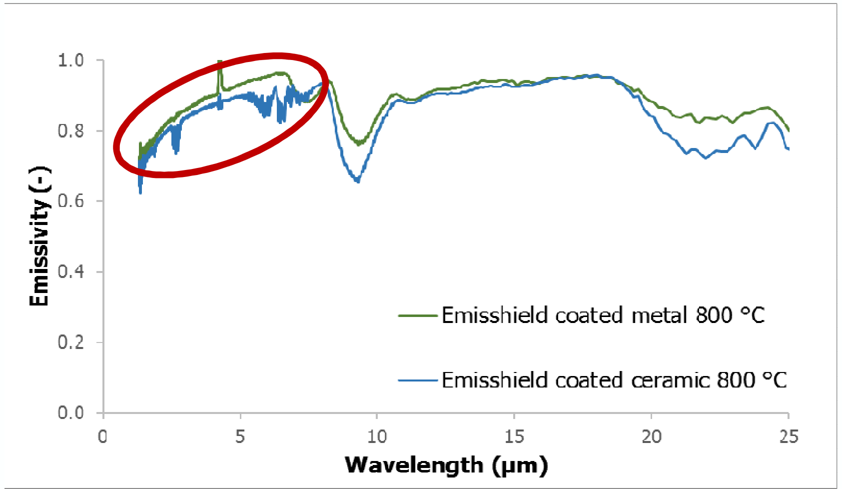
EMISSIVITY: METAL SAMPLES

Coated vs. Uncoated 304 SS



- **<u>Clear difference</u>** exists between the samples throughout the entire range of wavelengths
- Once the 304 SS material is **oxidized**, spectral emissivity will **increase** and close the gap
- Emissivity of 304 SS is slightly **higher** than in literature – due to **<u>roughness</u>**

Metal Coating vs. Ceramic Coating



- Two coatings designed for **metal** and **ceramics**
- Although **different** in composition they have **<u>very similar</u>** emissivity

- <u>Decrease</u> of spectral emissivity is observed for wavelengths shorter than 5 µm.

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COKE FORMATION

Deposition of a carbon layer on the reactor surface

- Thermal efficiency
- Product selectivity
- Decoking procedures

[Muñoz, 2013]

Estimated annual cost to industry: $ 2 billion

Optimization by
- Feed additives
- Metallurgy & surface technology
- 3D reactor technology

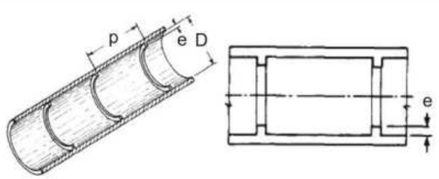
L. Benum, "Achieving Longer Furnace Runs at NOVA Chemicals," in AIChE Spring National Meeting, 14th Annual Ethylene Producers’ Conference, New Orleans, Louisiana, 2002.

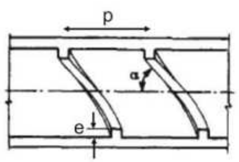
3D REACTOR TECHNOLOGY

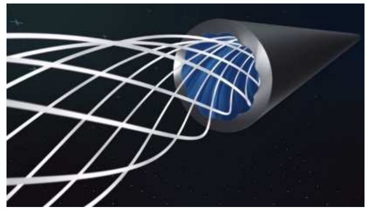
Improve the reactor by decreasing $T_{gas/coke}$

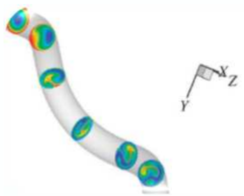
$$Q = U \cdot A \cdot \left(T_{gas/coke} - T_{bulk}\right)$$

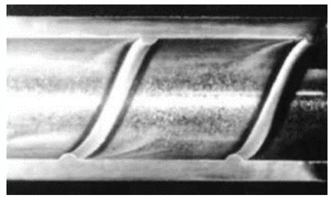
- ➢ Increase tube area (A) — finned tubes
- ➢ Increase heat transfer coefficient (U) — ribbed tubes



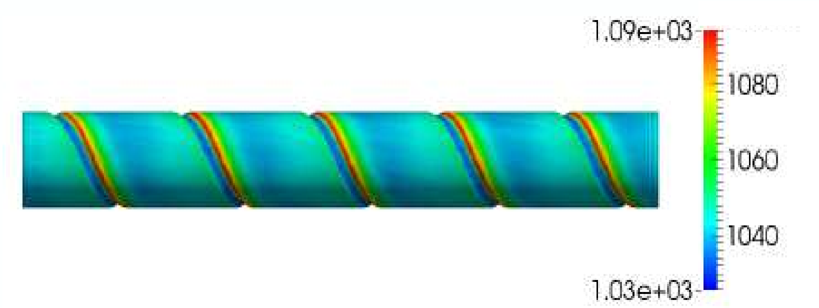



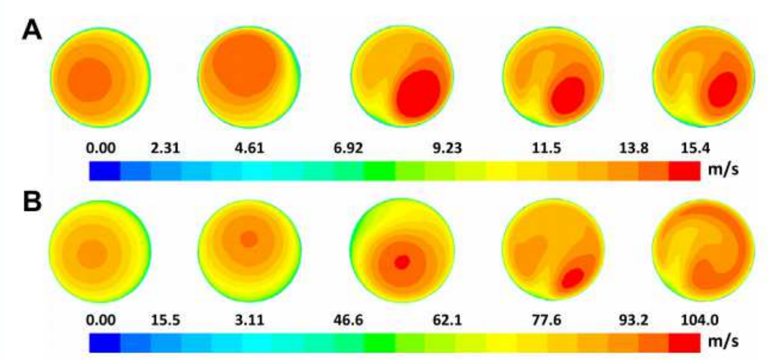


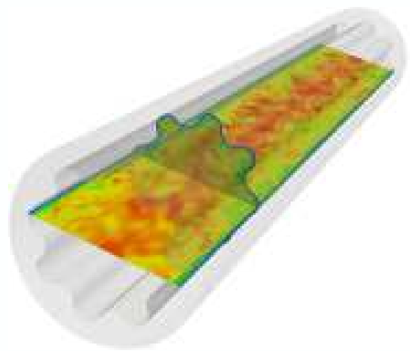



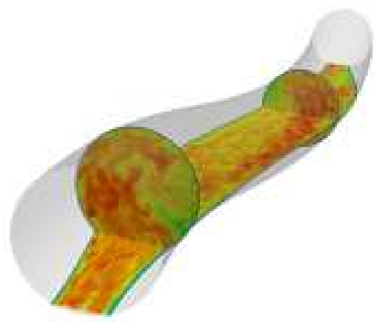

M. Zhu, "Large eddy simulation of thermal cracking in petroleum industry," 2015.

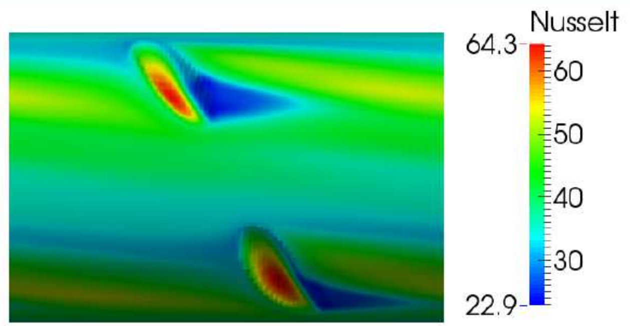
(3D) SIMULATION ARE NEEDED







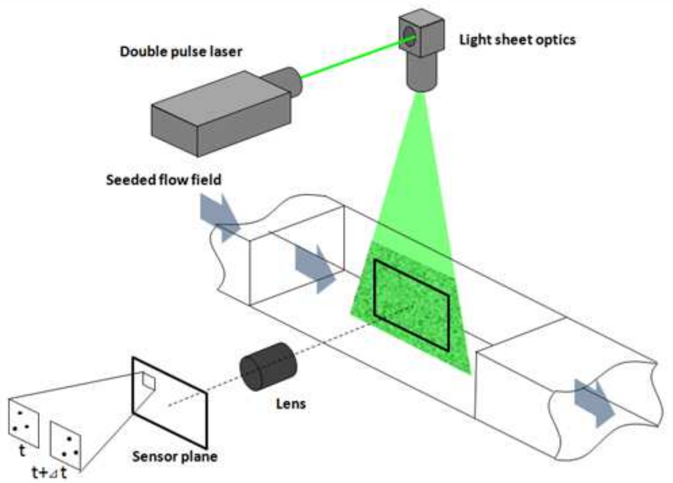




NEED VALIDATION!!!

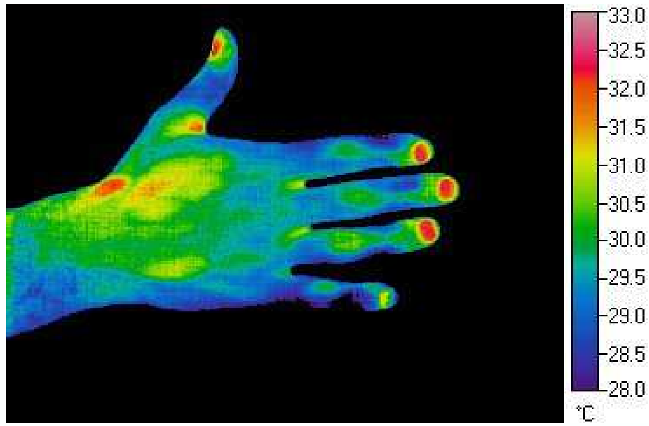
EXPERIMENTS

PIV



Measuring velocity
and 3D flow profile

Liquid Crystal Thermography



Measuring tube wall temperature
and heat transfer

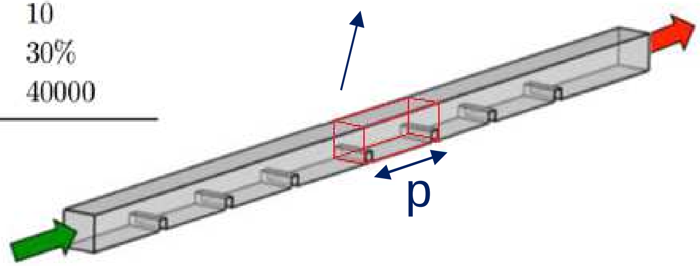
The von Karman Institute
for Fluid Dynamics

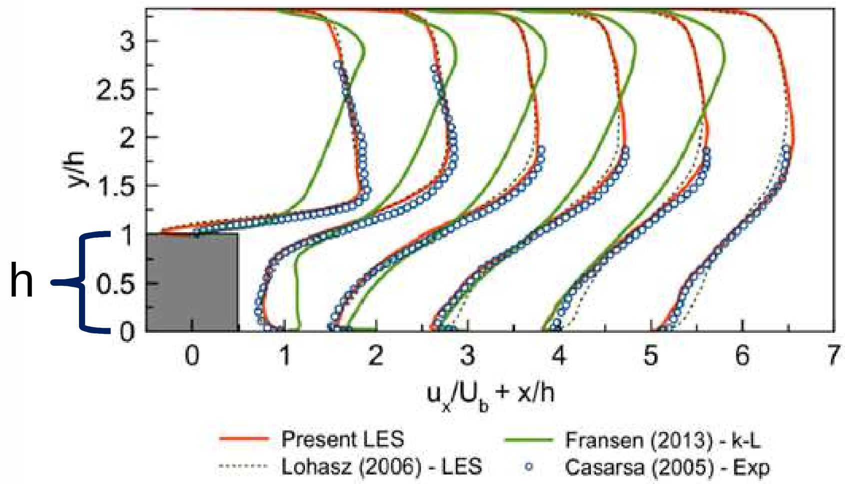
Both experiments were performed at the
von Karman Institute for Fluid Dynamics

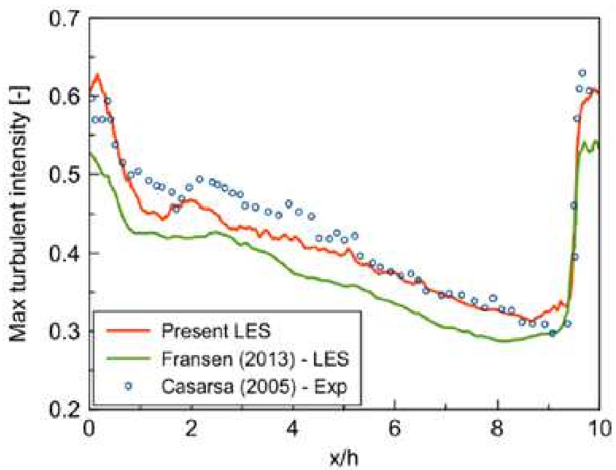
LES vs RANS – RIBBED DUCT (Re=40 000)

Channel section	square	Fluid	*Air*
Hydraulic diameter D_h	0.1 m	Inlet bulk velocity U_b	$8.8\ \mathrm{m \cdot s^{-1}}$
Number of ribbed wall	1	Inlet bulk temperature	293 K
Ribs angle	90°	p/h	10
Ribs height h	0.03 m	h/D_h	30%
Ribs pitch p	0.3 m	Re	40000

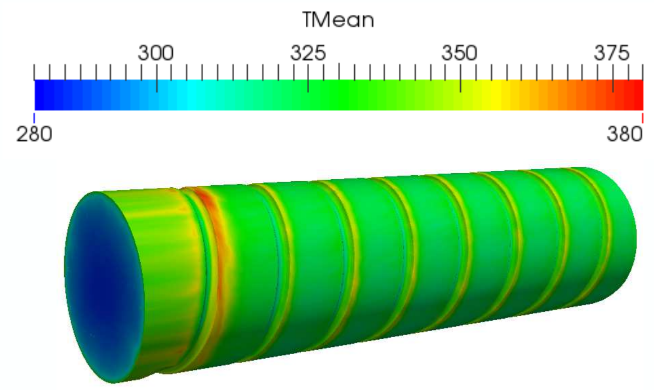
Computational domain
5 000 000 cells

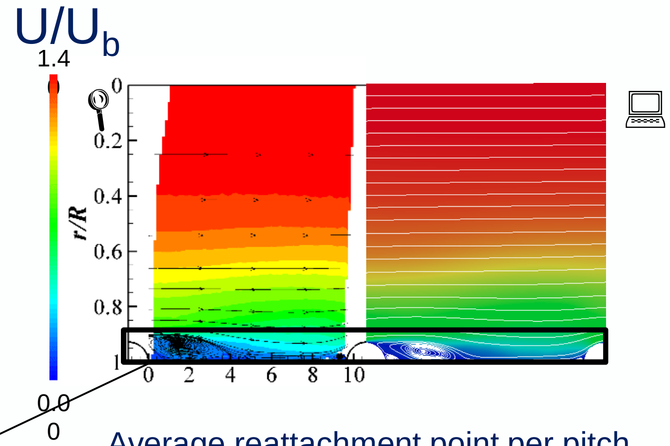


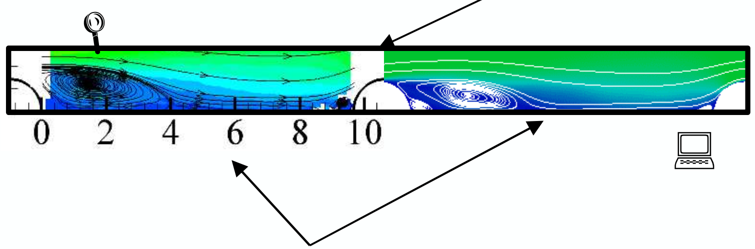




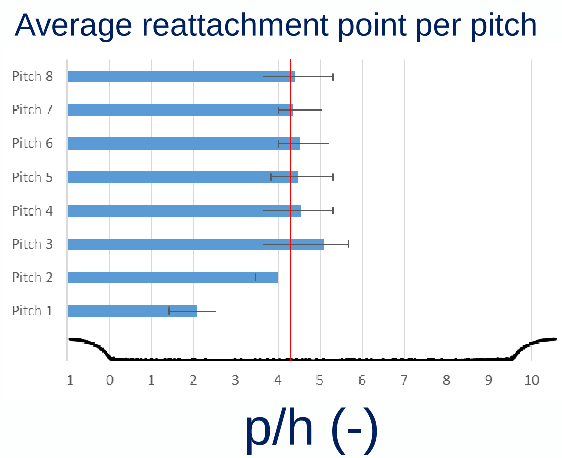
LES SIMULATIONS





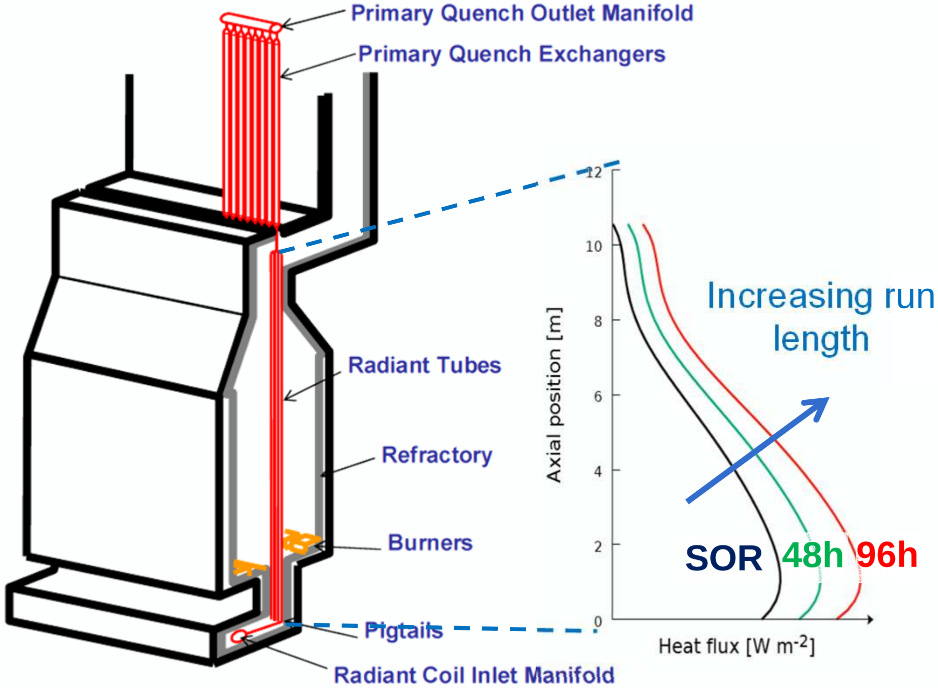


Reattachment behavior differs along the rib



MILISECOND PROPANE CRACKER SIMULATION

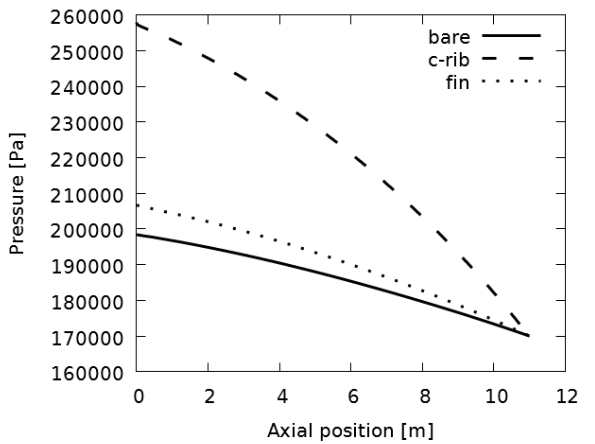
• Feedstock	33 g/s propane
• Propane conversion	80.15 % (± 0.05%)
• Steam dilution	0.326 kg/kg
• CIT	903.7 K
• COP	170 kPa



Different geometries simulated

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

PRODUCT SELECTIVITIES



Reactor pressure drop

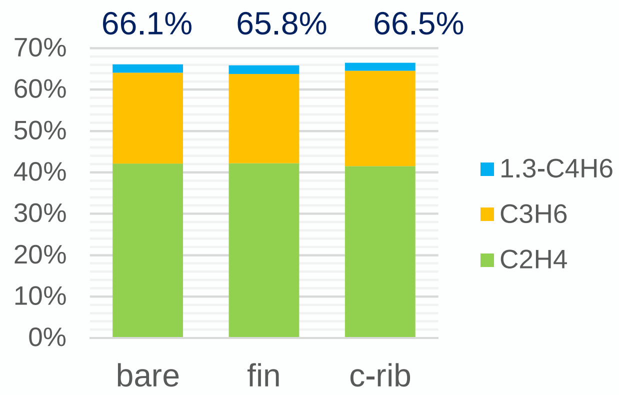
30% higher (fin)

300% higher (c-Rib)

~~1D: “Lower olefin selectivity”~~

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

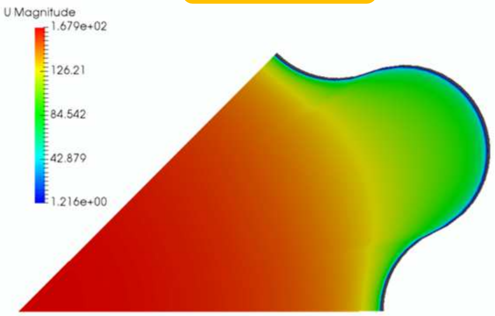
Radial mixing effects cannot be predicted based on 1D simulations only



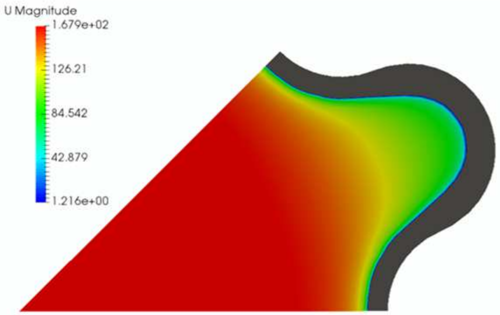
NON-UNIFORM COKE LAYER GROWTH

Fin

SOR (0 hrs)

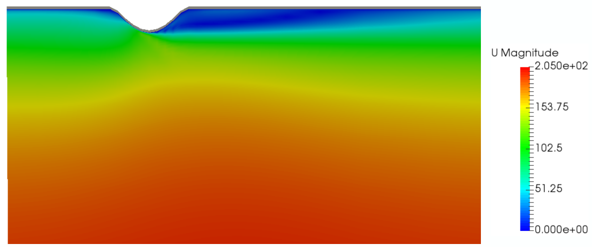


48 hrs

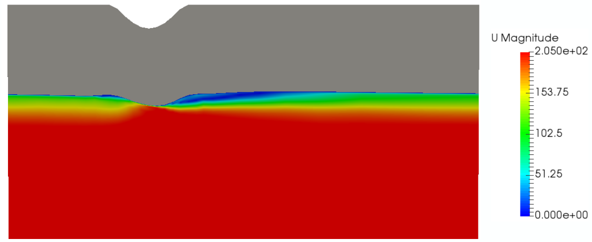


c-Rib

SOR

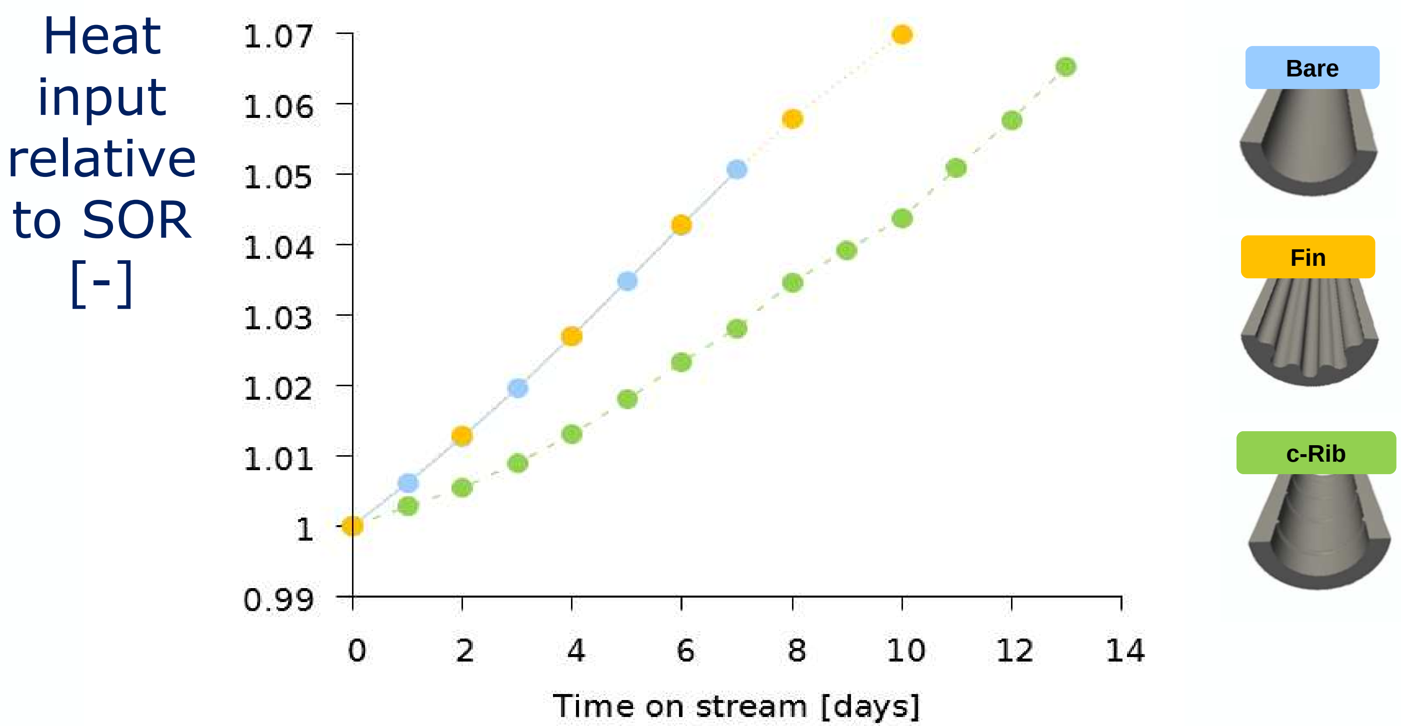


10 days

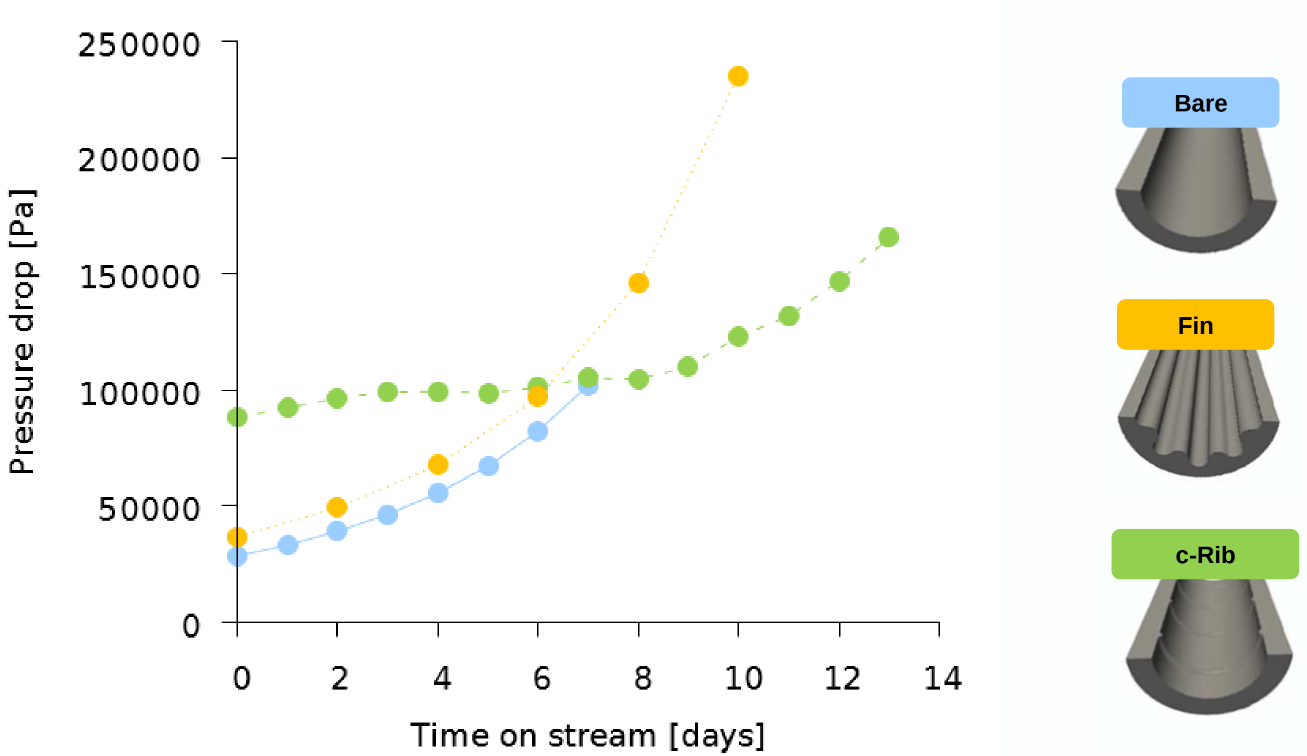


INCREASED HEAT INPUT

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



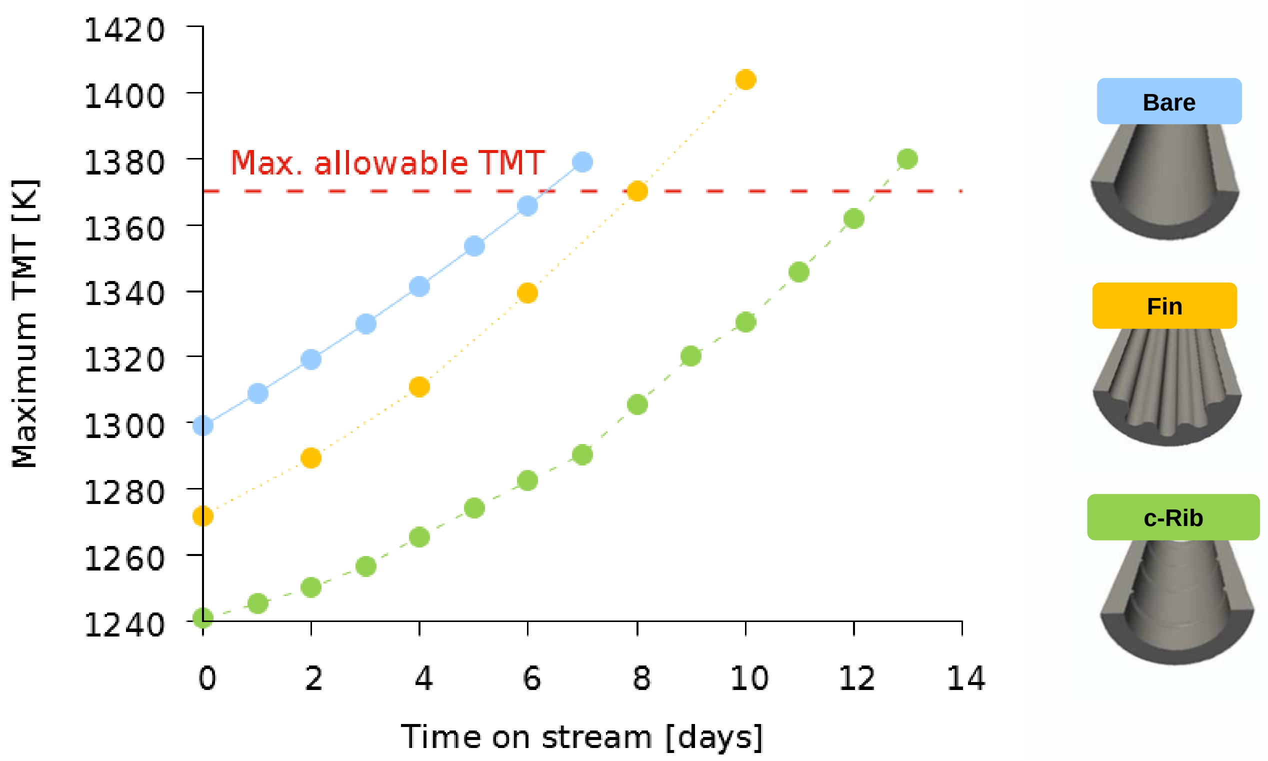
PRESSURE DROP



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

Slower 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 is lower** for 3D geometries

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CONCLUSIONS

- IMPROOF aims at <u>improving</u> the **energy efficiency**, at the same time <u>reducing</u> the **greenhouse** and **air-pollution** emissions

- The **high-emissivity** coatings significantly **<u>increase</u>** the spectral normal emissivity
  - Most of the **profit** will come from coating the **<u>refractory wall</u>**
  - Further investigation of the **<u>sub 5 µm</u>** region and study on the **<u>effective directional emissivity</u>**
  - Selection of the **<u>best</u>** out of 5 different coating for **<u>wall</u>** and **<u>reactor</u>** and benchmarking their performance in the pilot plant cracker at UGent

- Application of novel **3D reactor designs** can lead to:
  - ✓ more uniform heat transfer
  - ✓ increased run lengths
  - ✓ longer lifetime of the furnace

Acknowledgment

- The work leading to this invention has received funding from the European Union Horizon H2020 Programme (H2020-SPIRE-04-2016) under grant agreement n°723706.

- My colleagues Jens Dedeyne, Stijn Vangaever, Laurien Vandewalle and David Van Cauwenberge

Thank you for your attention!