Reactor design and optimization with OpenFOAM

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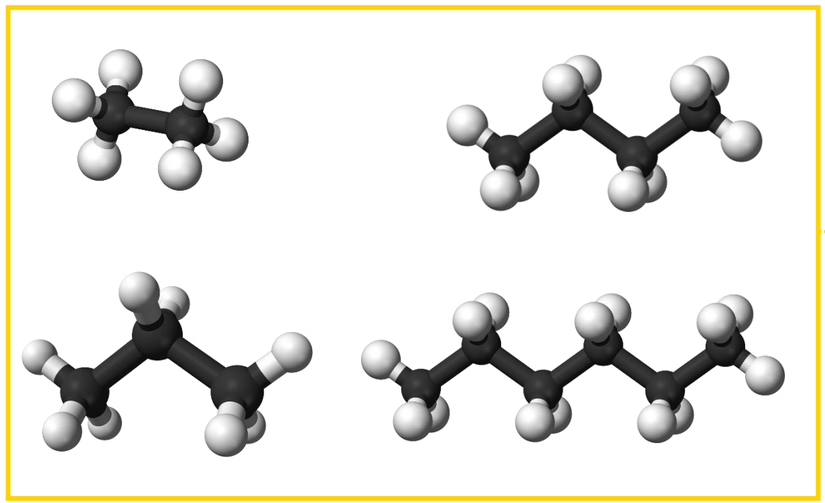
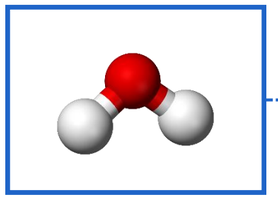
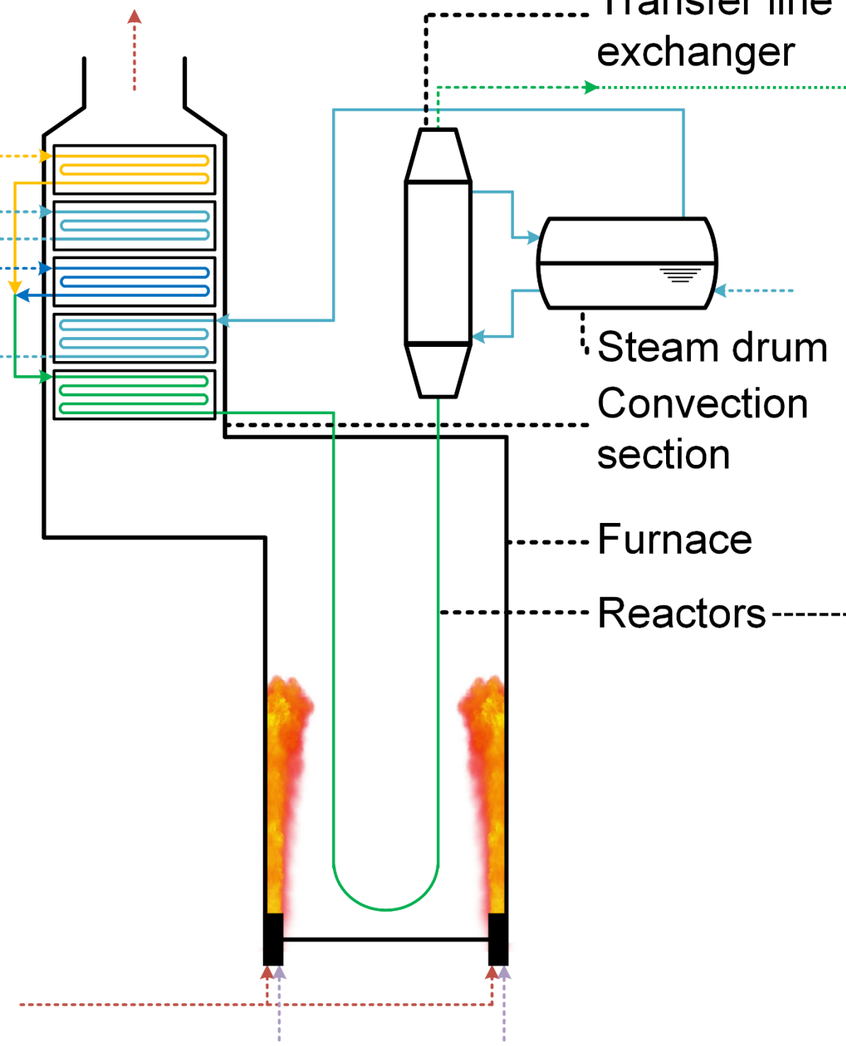
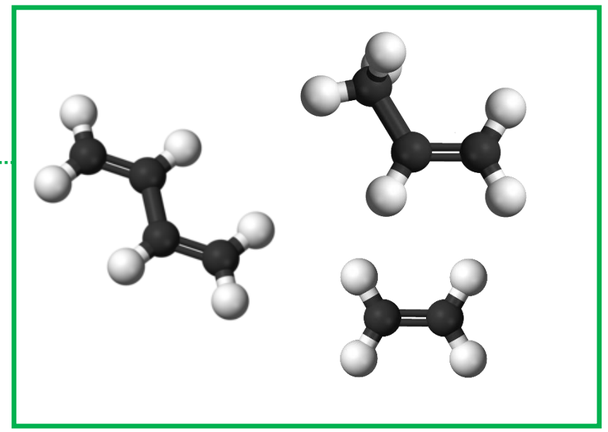
Steam cracking 101









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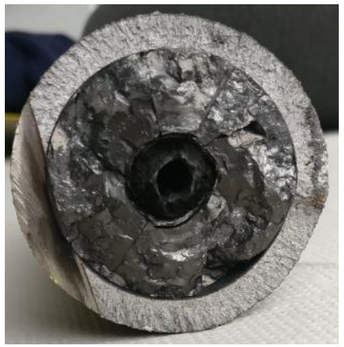
Process Intensification in steam cracking

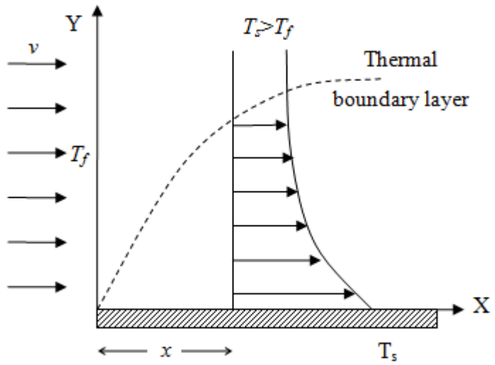
Improve reactor design by accelerating heat input

$$\dot{Q} = h\ A\ (T_{inner\ reactor\ wall} - T_{fluid})$$



- Thermal efficiency
- Product selectivity
- Decoking procedures

- More reactor material needed
- More friction with wall ~ Δp



- Disrupt the boundary layer

Fig.4.3: Thermal boundary layer flow past a flat surface

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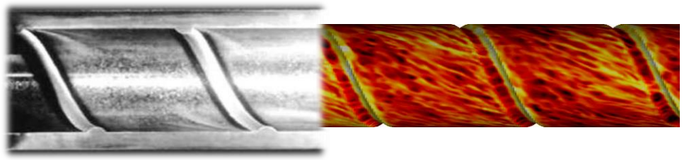
3D reactor technologies for flow modulation

Bumps or dents throughout the reactor wall

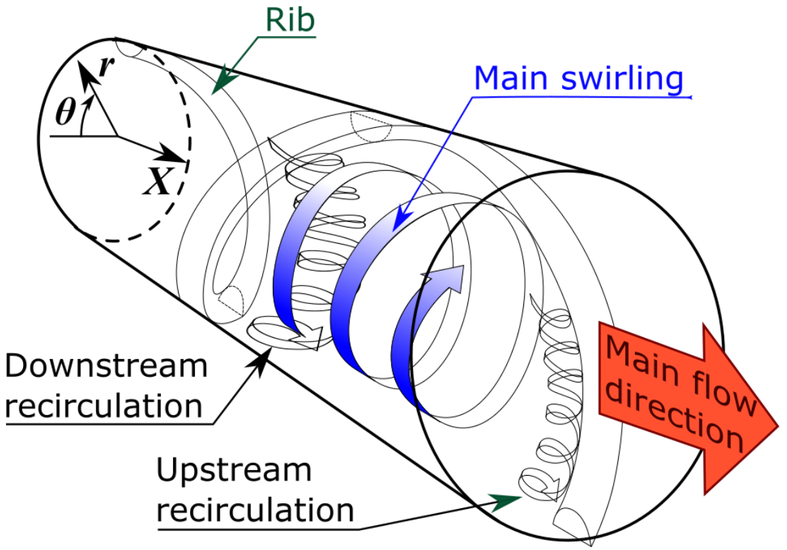


MERT

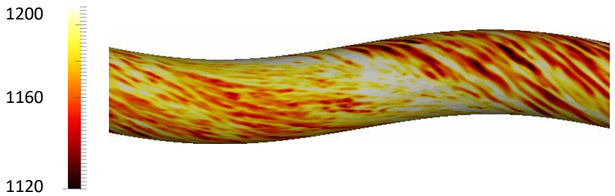
Finned tube

X-MERT

SCOPE



Contort the entire reactor wall



SFT

Static mixers to create decaying swirl

IHT

HCD

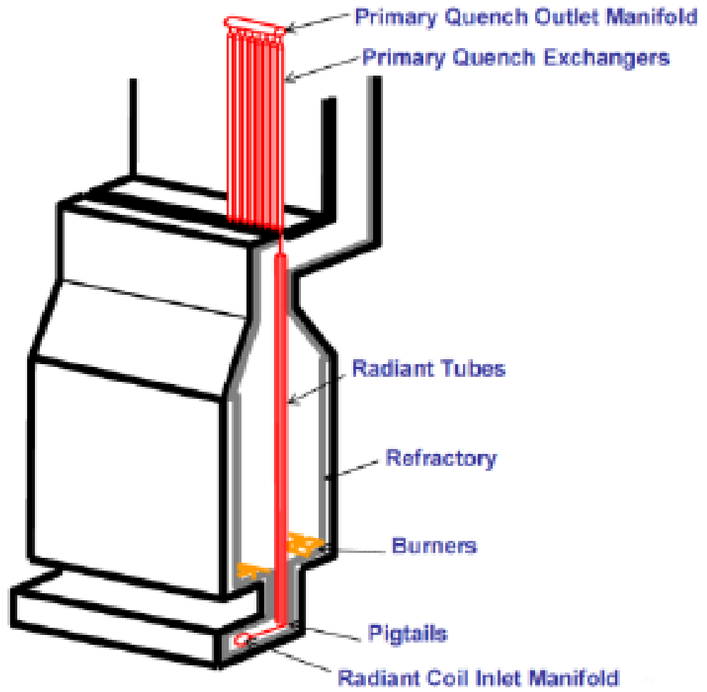
I. Mayo, B. C. Cernat, M. Virgilio, A. Pappa, T. Arts, and Asme, "Aerothermal Investigation of the Flow and Heat Transfer in a Helically Corrugated Cooling Channel," (in English), *Proceedings of the Asme Turbo Expo: Turbine Technical Conference and Exposition, 2016, Vol 5b,* Proceedings Paper p. 11, 2016.

D. Bai, Y. Zong, M. Zhou, L. Zhao, “Novel cracking coil design based on positive constructing of synergetic flowing field,” submitted to International Journal of Heat and Mass Transfer.

Methodology

Process conditions

Reactor length	11 m
Feedstock	118.5 kg/h propane
Steam dilution	0.326 kg/kg
Coil Inlet Temperature	903 K
Coil Outlet Pressure	170 kPa
Conversion	80.6 %

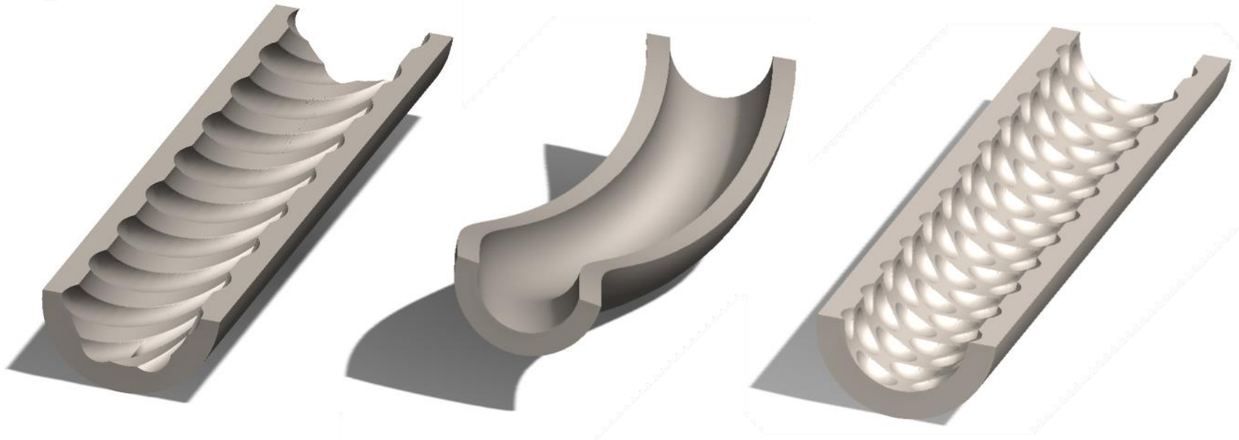


Chemistry

Reaction network reduced for propane cracking

151 reactions (16 molecules + 13 radicals)

QSSA applied for radicals



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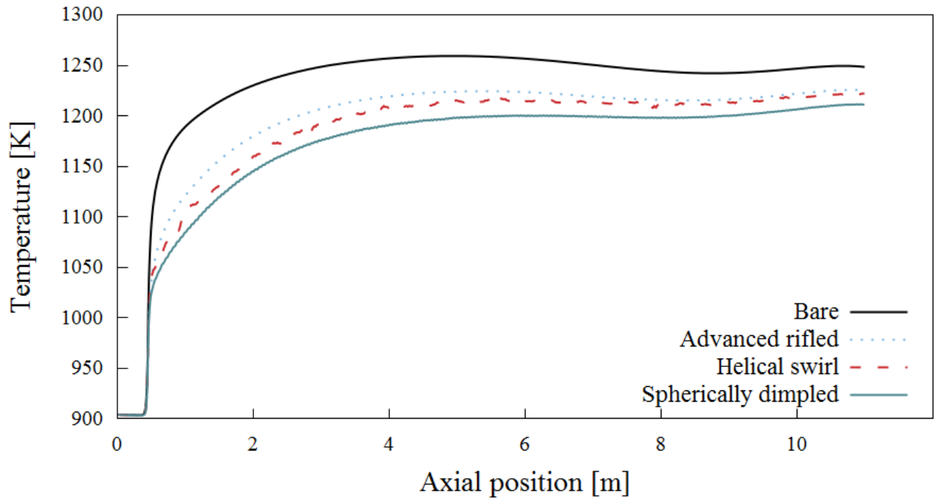
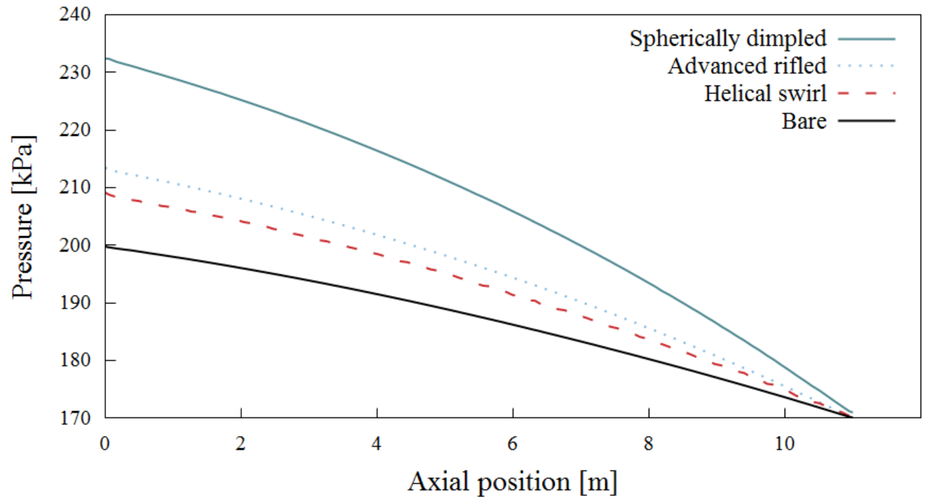
Lower temperatures – higher pressure drop





Yields [wt%]	Bare	SFT	SCOPE	UGent
C3H6	17.41	18.32	17.99	18.33
C2H4	34.02	33.54	33.71	33.55
C4H6	1.66	1.57	1.60	1.58
CH4	19.27	19.21	19.30	19.33
C3H4	0.65	0.65	0.65	0.63
Benzene	1.54	1.45	1.48	1.43
Relative				
C3H6	1.00	1.05	1.03	1.05
C2H4	1.00	0.99	0.99	0.99
C4H6	1.00	0.94	0.96	0.95
CH4	1.00	1.00	1.00	1.00
C3H4	1.00	1.00	0.99	0.96
Benzene	1.00	0.94	0.96	0.93

Less ethylene but more other high valuable chemicals

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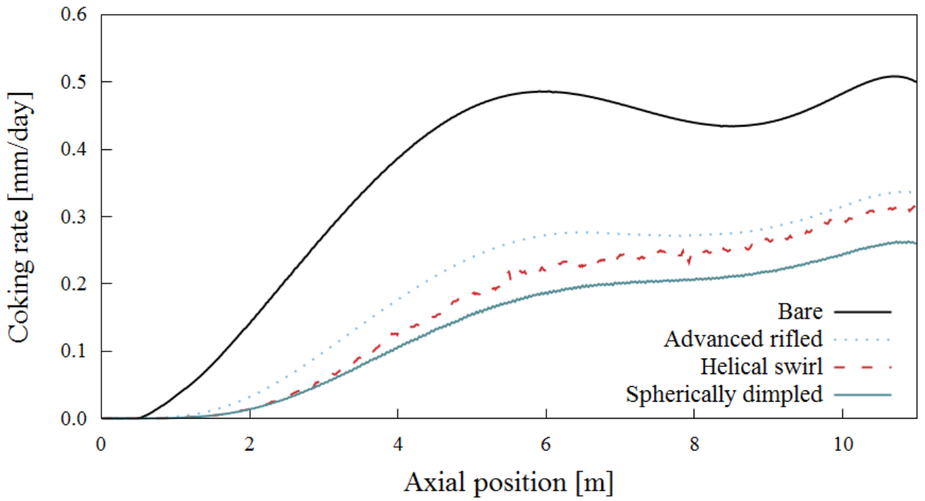
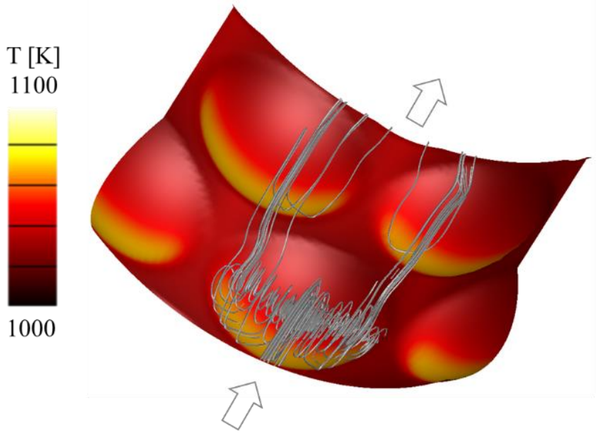
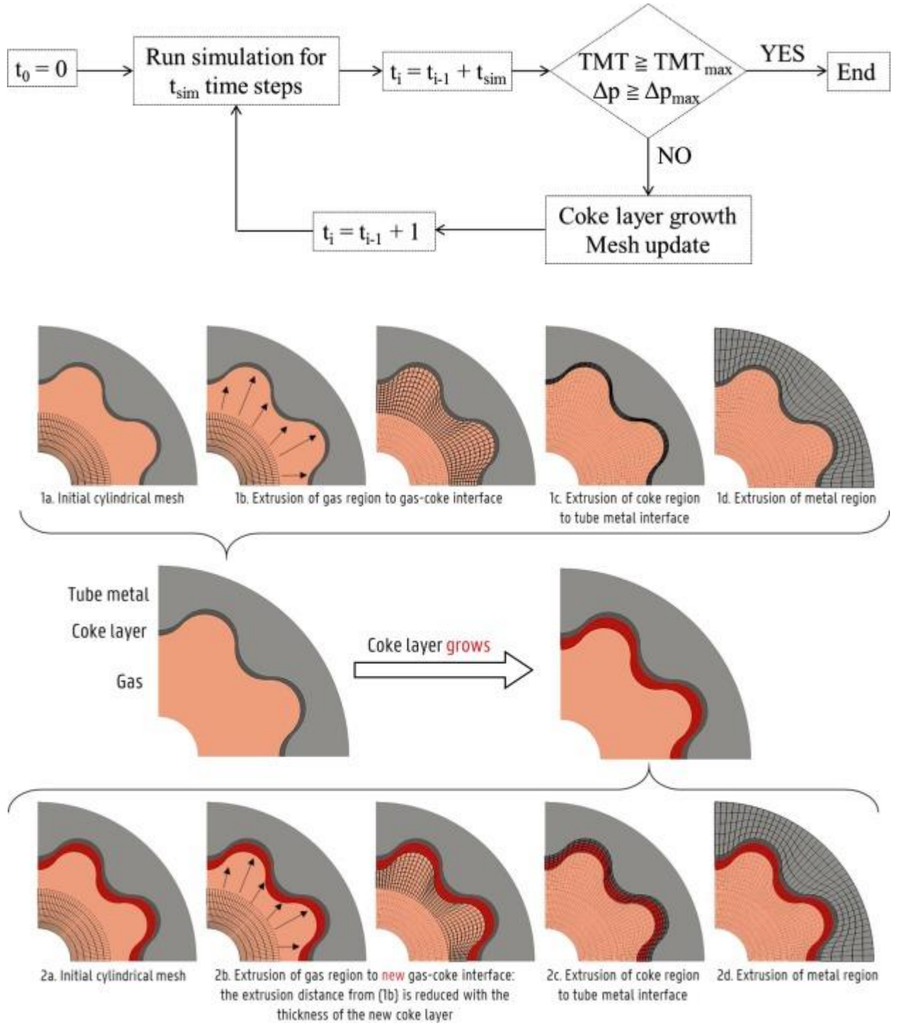
Lower coking rate – non uniform temperature







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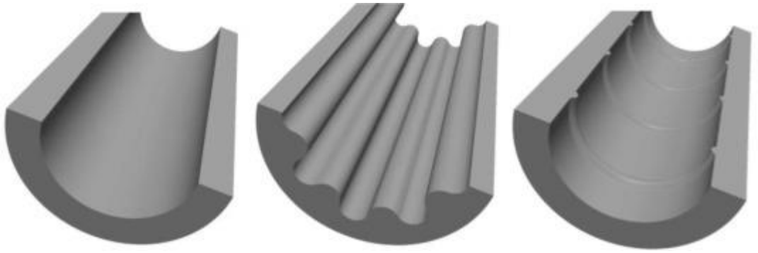
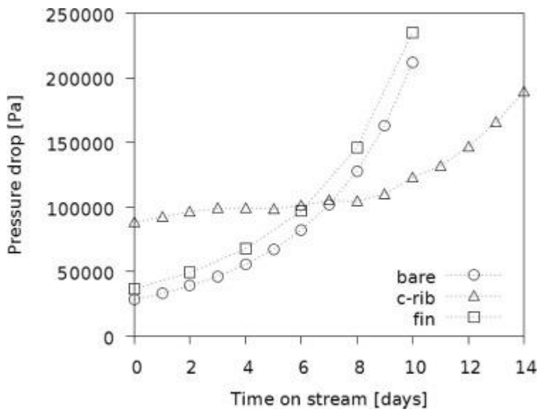
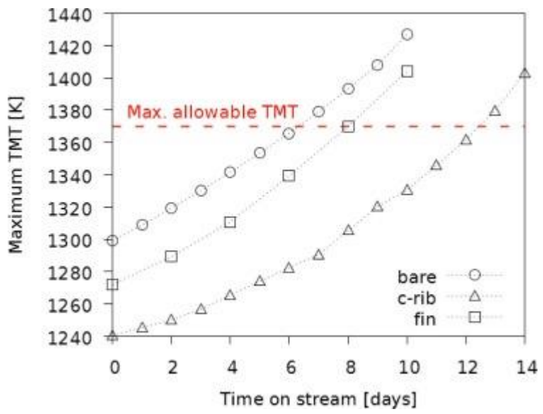
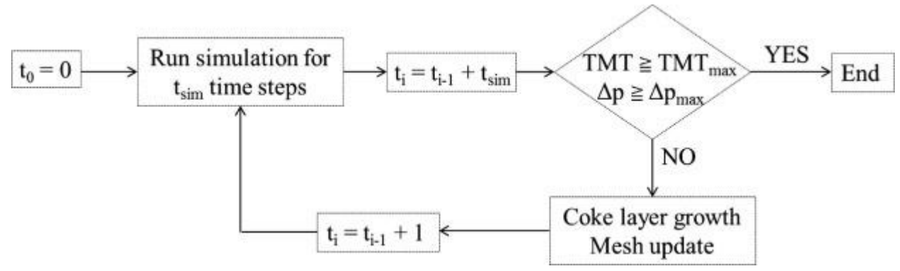
Impact of coke growth on run length behavior

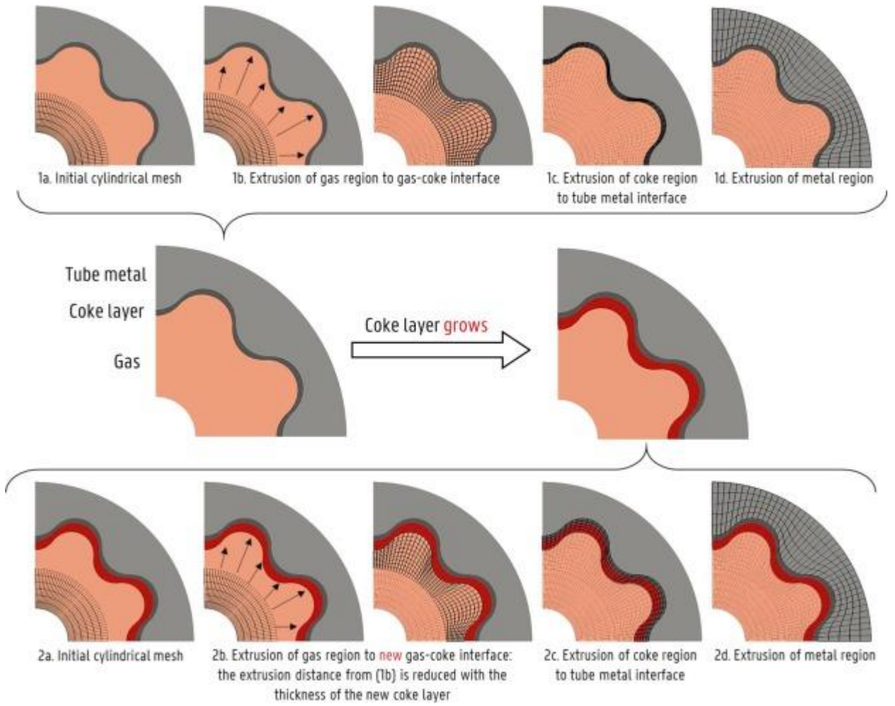


bare fin c-rib









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IMPROOF workshop
27-28 January 2020 at Ghent University

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IMPROOF project

IMPROOF is a European Union H2020 project* which aims to improve the energy efficiency of steam cracking furnaces, while reducing emissions of greenhouse gases and NO_x.

The strongly industrially oriented consortium is composed of the following partners:

AVGI, Ayming, CERFACS,

LRGP-CNRS, CRESS, Dow,

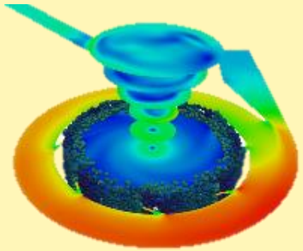
Ghent University, John Zink,

POLIMI, Schmidt & Clemens and TechnipFMC

Computational Fluid Dynamics assisted Process Intensification (27 January)

Speakers:

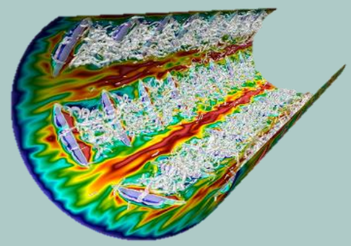
prof. T. Poinsot	CERFACS
prof. H. Kuipers	TU Eindhoven
prof. T. Arts	von Karman Institute
prof. A. Cuoci	POLIMI
prof. V. Francia	Heriot-Watt University
prof. K. Van Geem	Ghent University



Novel Technologies in Steam Cracking Furnaces (28 January)

Speakers:

dr. M. van Goethem	TechnipFMC
dr. J. Olver	Emisshield
G. Theis	John Zink
dr. J. Weigandt	Schmidt & Clemens
dr. D. Van Cauwenberge	BASF
dr. D. Brown	AVGI



Practical information:

- This workshop will be organized by the IMPROOF consortium but registration is open for all stakeholders from both industry and academia.
- The two-day workshop will take place at Ghent (Laboratory for Chemical Technology) 27 and 28 January 2020.
- Attendance is free of charge, but registration is required: eventmanager.ugent.be/improofWorkshop (additional information on improof.cerfacs.fr)
- Due to the limited capacity of the event (90 participants), participants who register but fail to attend, will be charged with a no show fee of € 50 (except for valid reasons)

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