FACULTY OF ENGINEERING AND ARCHITECTURE

DEPARTMENT OF MATERIALS, TEXTILES AND CHEMICAL ENGINEERING (MATCH)
LABORATORY FOR CHEMICAL TECHNOLOGY

129F

IMPROOF: INTEGRATED MODEL GUIDED PROCESS OPTIMIZATION OF STEAM CRACKING FURNACES

S.H. Symoens, M.R. Djokic, J. Zhang, G. Bellos, D. Jakobi, J. Weigandt, S. Klein, F. Battin-Leclerc, G. Heynderickx, J. Van Thielen, B. Cuenot, T. Faravelli, G. Theis, P. Lenain, A.E. Muñoz, J. Olver, K.M. Van Geem

2018 Spring National Meeting, Orlando, Florida, April, 24, 2018

A SPIRE project

SPIRE PROJECT

IMPROOF

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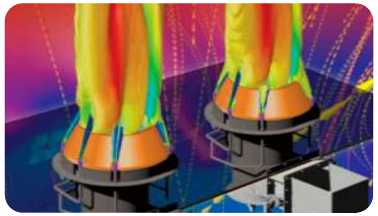
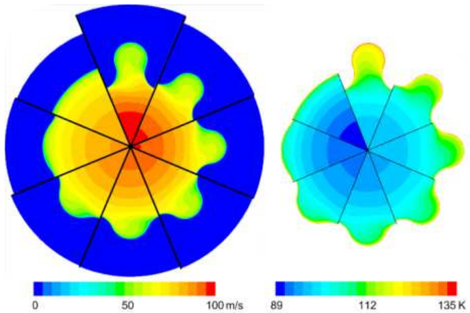
IMPROOF IS ALL ABOUT:

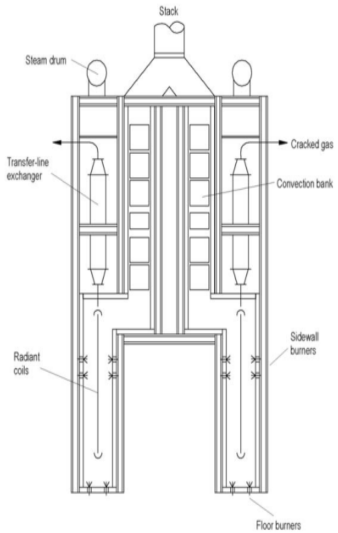
Renewable fuel characterization
- experimental activity
- kinetic mechanisms

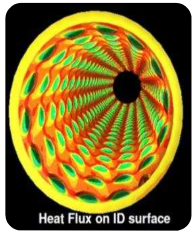


Innovative Furnace System developments and integration
- oxy-fuel combustion
- coke formation
- emissivity coating
- 3D reactor testing



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





Upscaling and Demonstration

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OUTLINE

- Introduction
- Objectives
- Coke formation on high-temperature alloys and 3D reactor technology
- Conclusions

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OUTLINE

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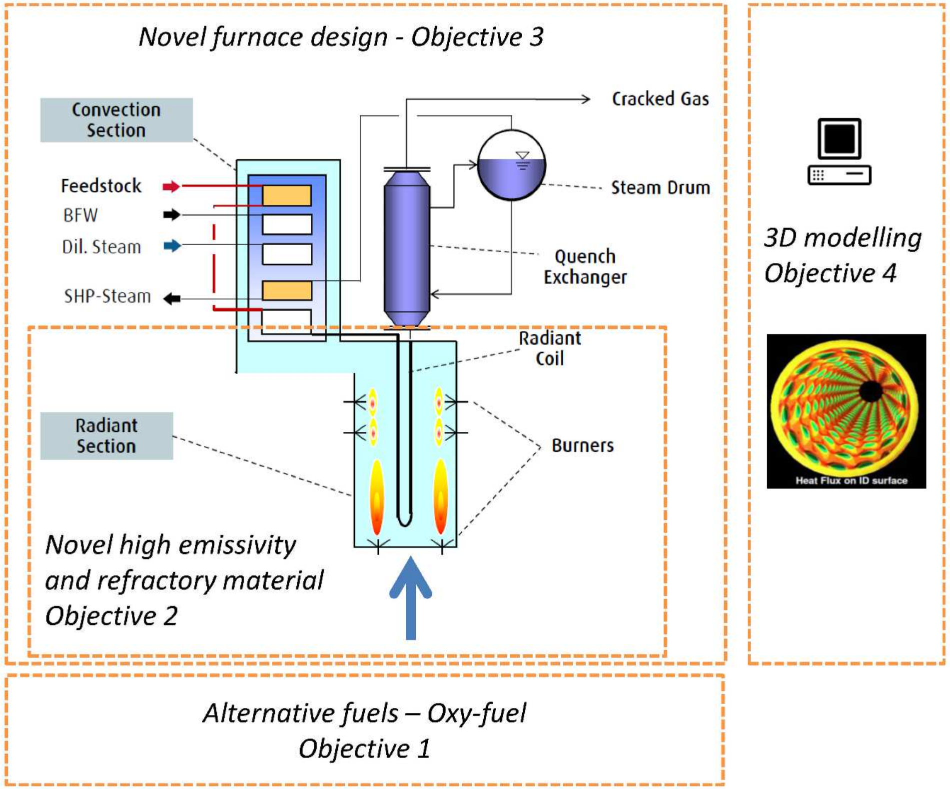
CONCEPT AND OBJECTIVES



1. Novel combustion technology using alternative fuels and oxy-fuel combustion
2. Demonstrate the individual impact of **novel** emissive, **reactor** and refractory materials **on 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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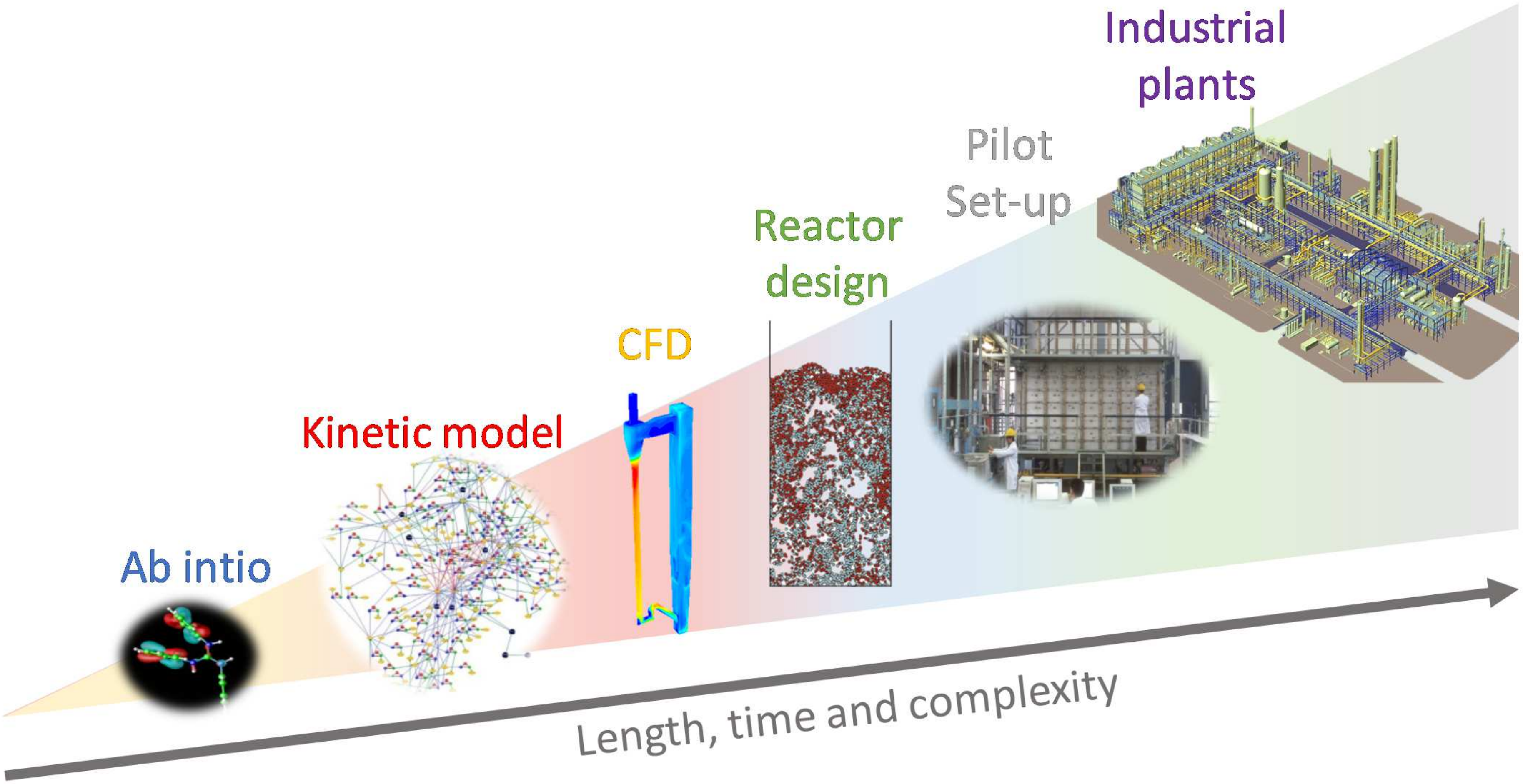
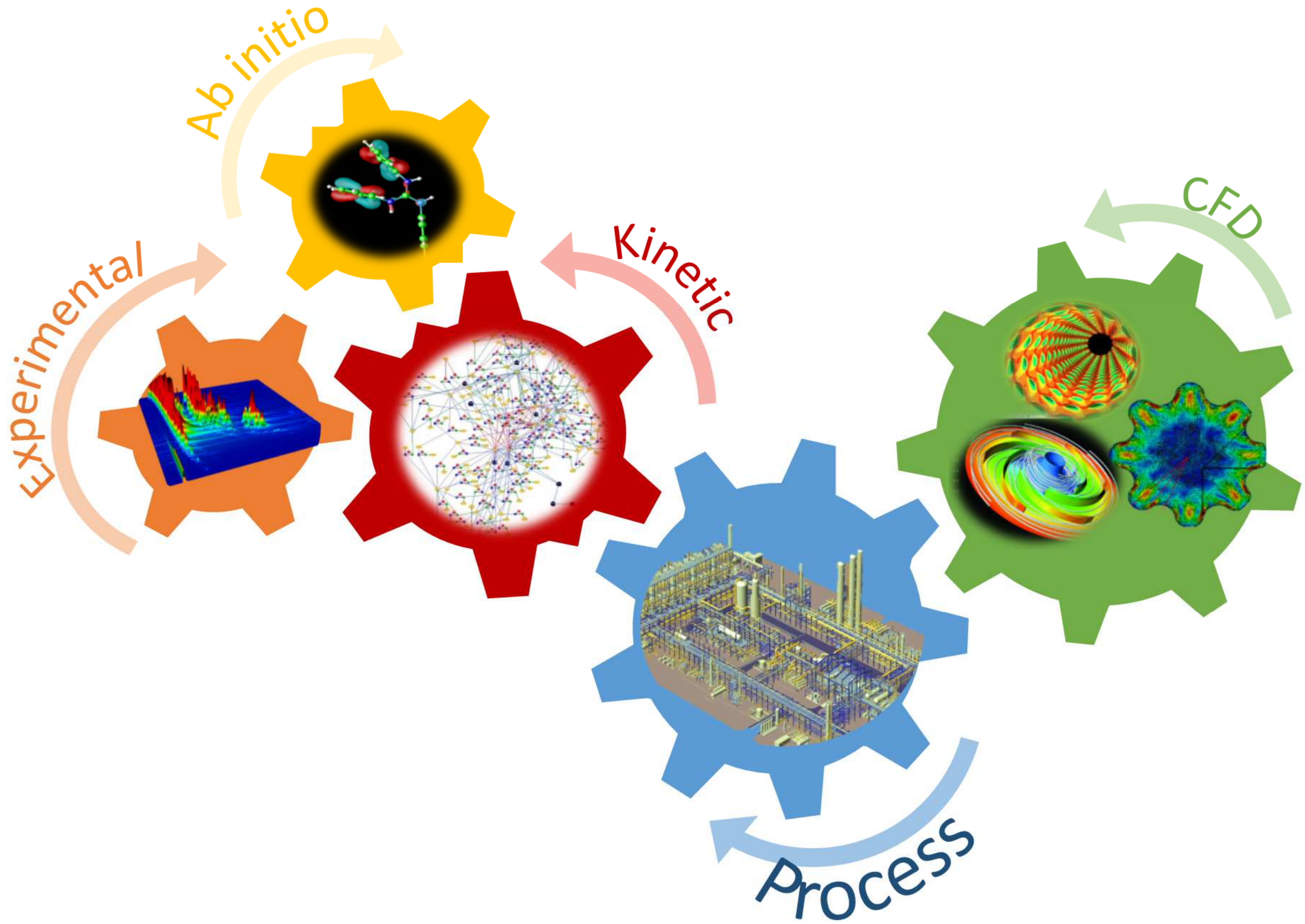
MULTI SCALE APPROACH



LCT'S VISION



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COKE FORMATION

Deposition of a carbon layer on the reactor surface

- ☒ Thermal efficiency
- ☒ Product selectivity
- ☒ Decoking procedures

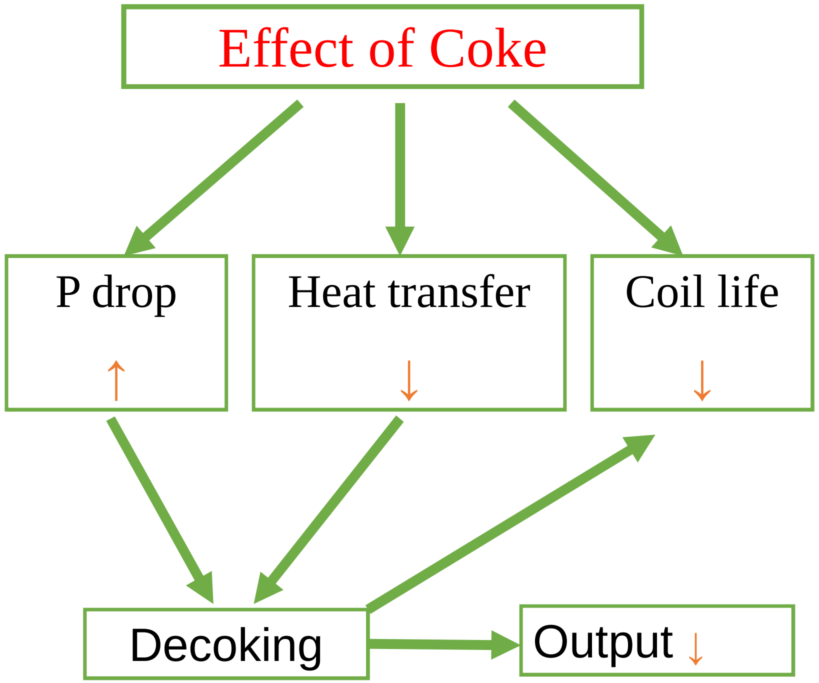
[Muñoz, 2013]

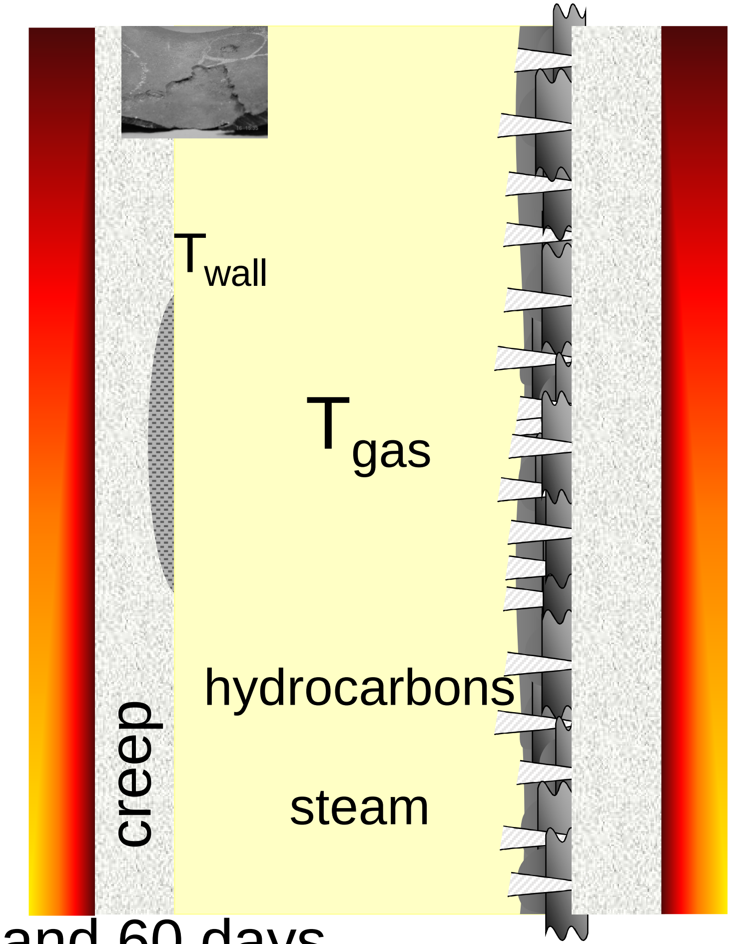
Estimated annual cost to industry: $ 2 billion

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.

COKES FORMATION





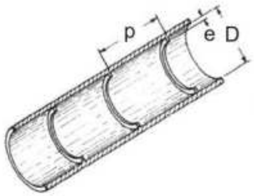
Run length is typically between 20 and 60 days

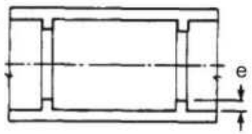
3D REACTOR TECHNOLOGY

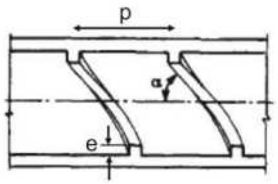
Improve the reactor by decreasing $T_{gas/coke}$

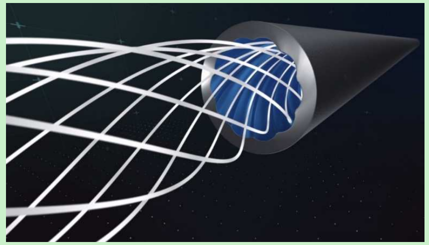
$$Q = U \cdot A \cdot \left(T_{gas/coke} - T_{bulk}\right)$$

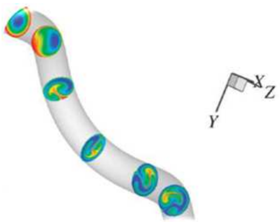
- Increase tube area (A)
- Increase heat transfer coefficient (U)

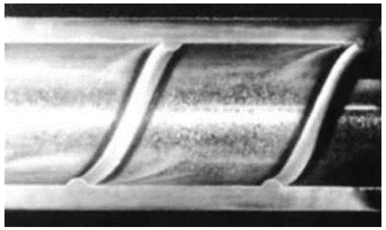






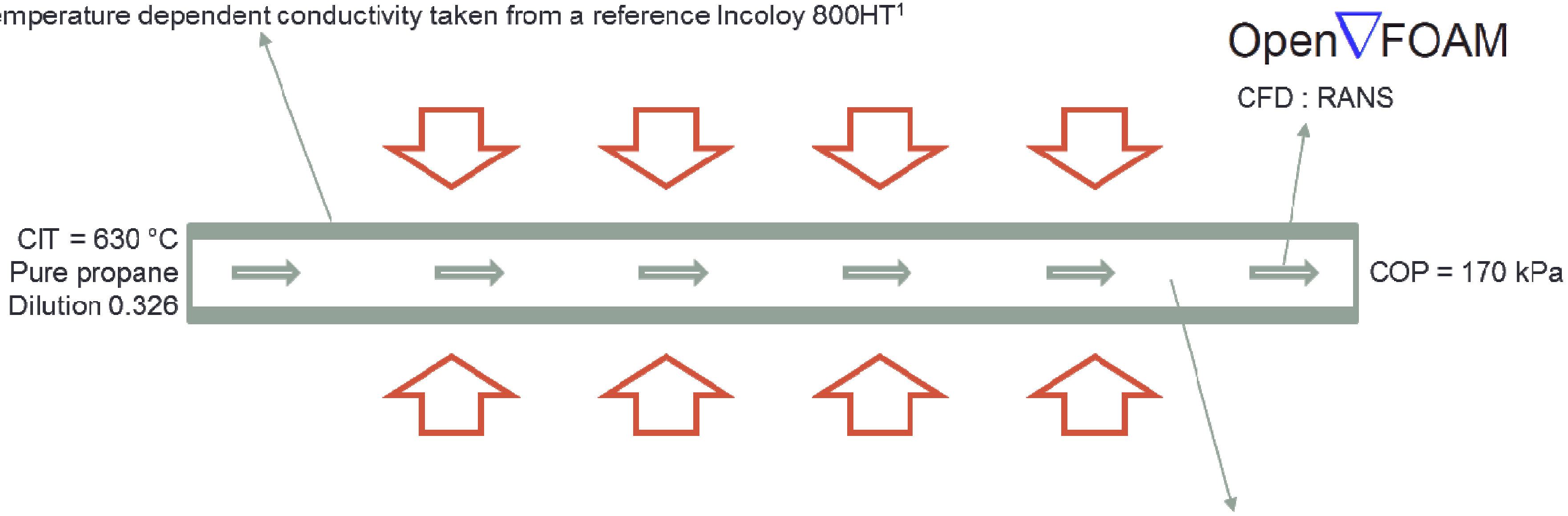




M. Zhu, "Large eddy simulation of thermal cracking in petroleum industry," 2015.

MILLISECOND BENCHMARK SIMULATION

Solving of the conjugated heat transfer: $\nabla \cdot (\lambda_s \nabla T) = 0$

Temperature dependent conductivity taken from a reference Incoloy 800HT[1]



1D heat flux profile from furnace simulations validated with industrial measurements

Linear scaling of heat flux profile to obtain equal conversion for all reactor technologies

CRACKSIM model was reduced to its relevant core for propane cracking.
Final network consists of 151 reactions between 29 species of which 13 radical species.
QSSA applied to reduce stiffness of the model.[3]

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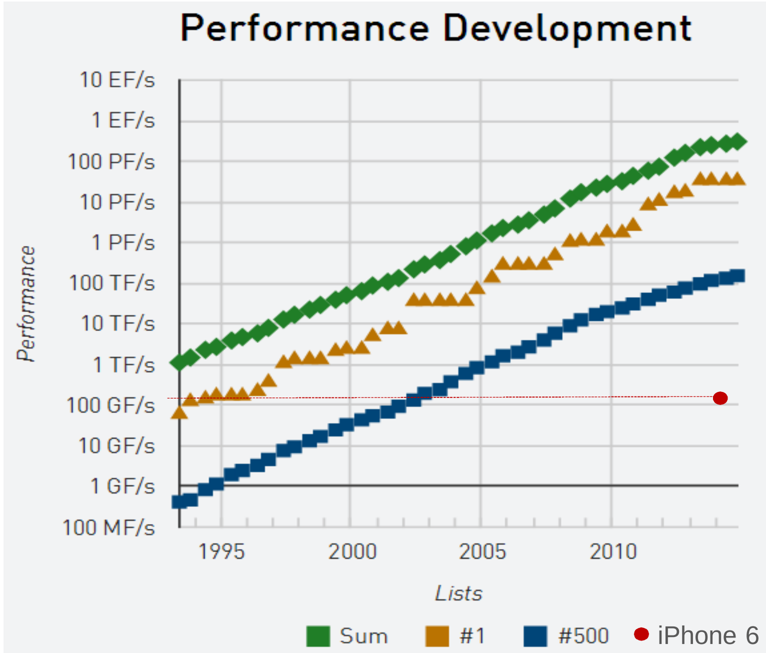
SUPERCOMPUTING INFRASTRUCTURE

Tier-0 supercomputers



From $15M world-record supercomputer to smartphone in 20 years

"SUPER" calculations are possible

But are they useful?

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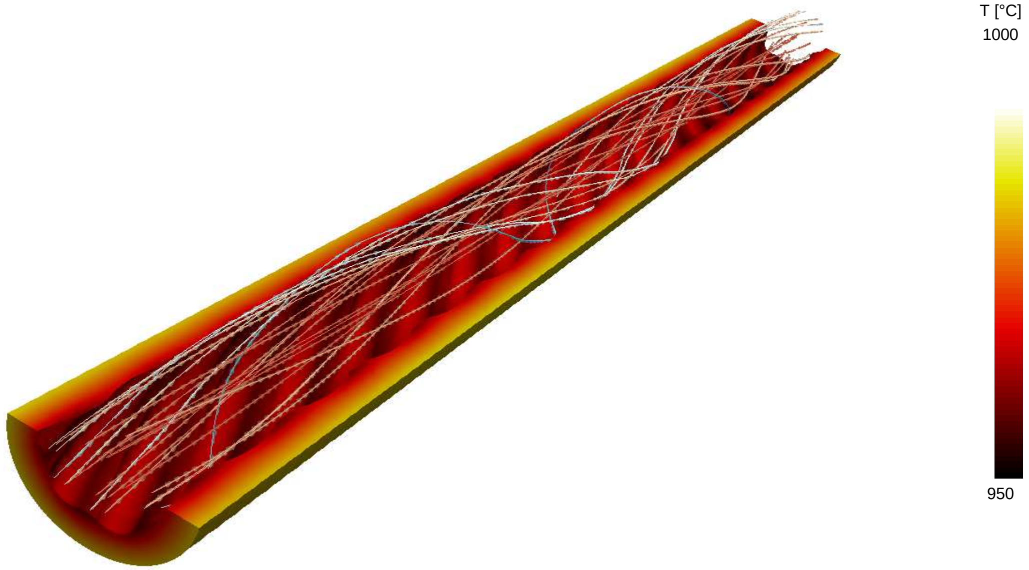
COMPARISON TO BARE REACTOR



SCOPE	
976.7	TMT_{max} [°C]
1.40	$\Delta p/\Delta p_0$ [-]
1.006	$(P+E)/(P+E)_0$ [-]
0.536	P/E [-]

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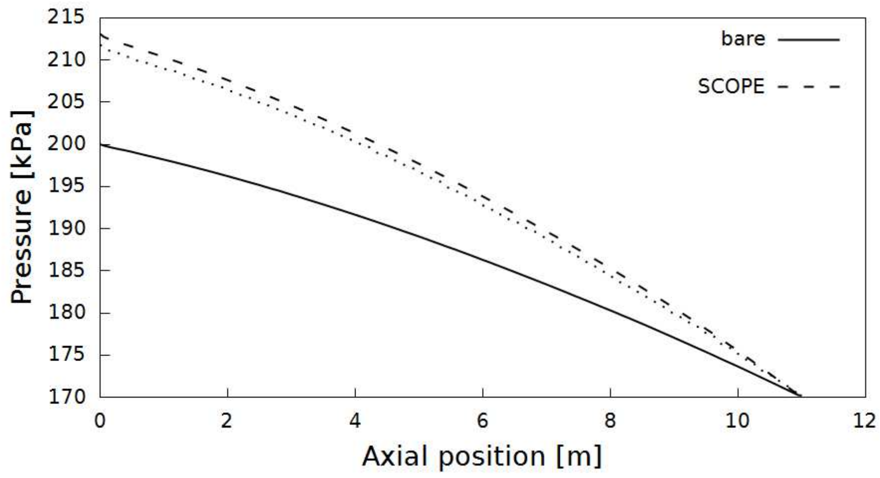
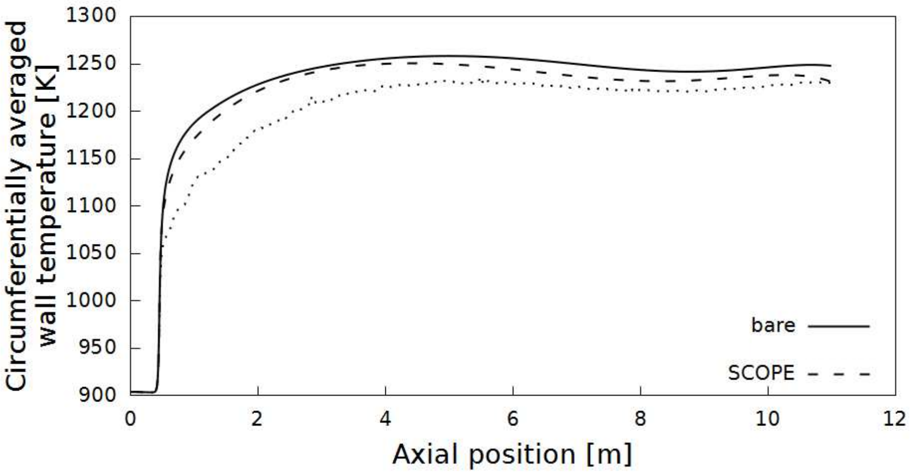
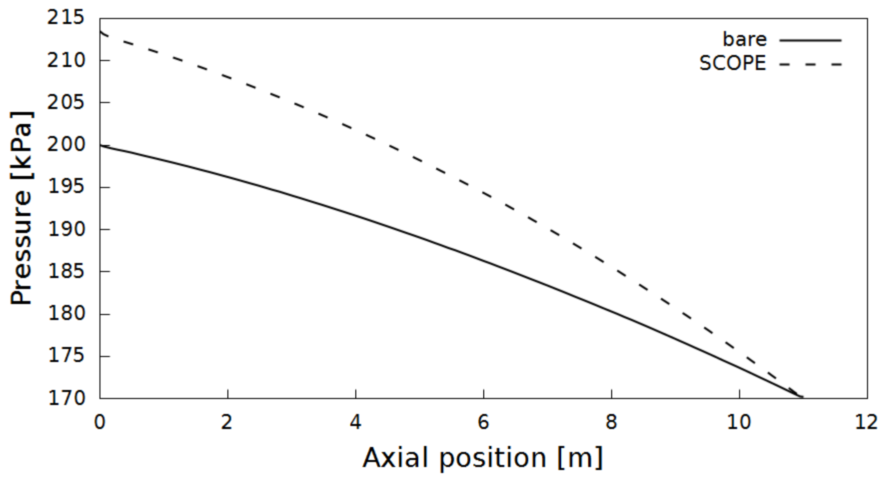
COMPARISON OF TECHNOLOGIES

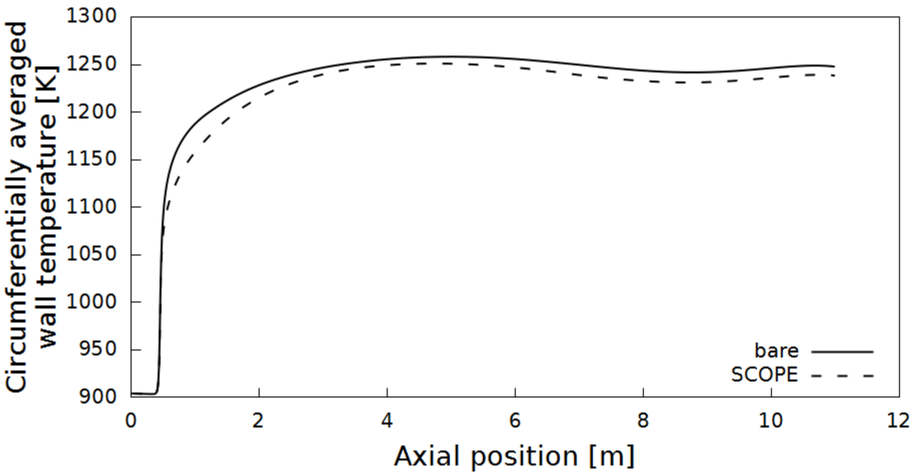




		SCOPE
X	[%]	80.6
P/E	[-]	0.536
C_2H_4	[wt%/wt$_{\%0}$]	0.987
C_3H_6	[wt%/wt$_{\%0}$]	1.033
1-3.C_4H_6	[wt%/wt$_{\%0}$]	0.958
C_2H_6	[wt%/wt$_{\%0}$]	0.955
CH_4	[wt%/wt$_{\%0}$]	1.002
C_2H_4	[wt%]	33.77
C_3H_6	[wt%]	17.96
1-3.C_4H_6	[wt%]	1.61
C_2H_6	[wt%]	1.55
CH_4	[wt%]	19.34

COMPARISON OF TECHNOLOGIES





		SCOPE
X	[%]	80.6
P/E	[-]	0.534
C_2H_4	[wt%/wt%$_0$]	0.985
C_3H_6	[wt%/wt%$_0$]	1.034
1-3.C_4H_6	[wt%/wt%$_0$]	0.953
C_2H_6	[wt%/wt%$_0$]	0.950
CH_4	[wt%/wt%$_0$]	1.000
C_2H_4	[wt%]	33.70
C_3H_6	[wt%]	17.99
1-3.C_4H_6	[wt%]	1.60
C_2H_6	[wt%]	1.54
CH_4	[wt%]	19.30

SIMULATION ACCURACY GOOD ENOUGH?



- **Burner geometry detail?**
- **Gas radiative properties?**
- **Furnace – Reactor coupling?**

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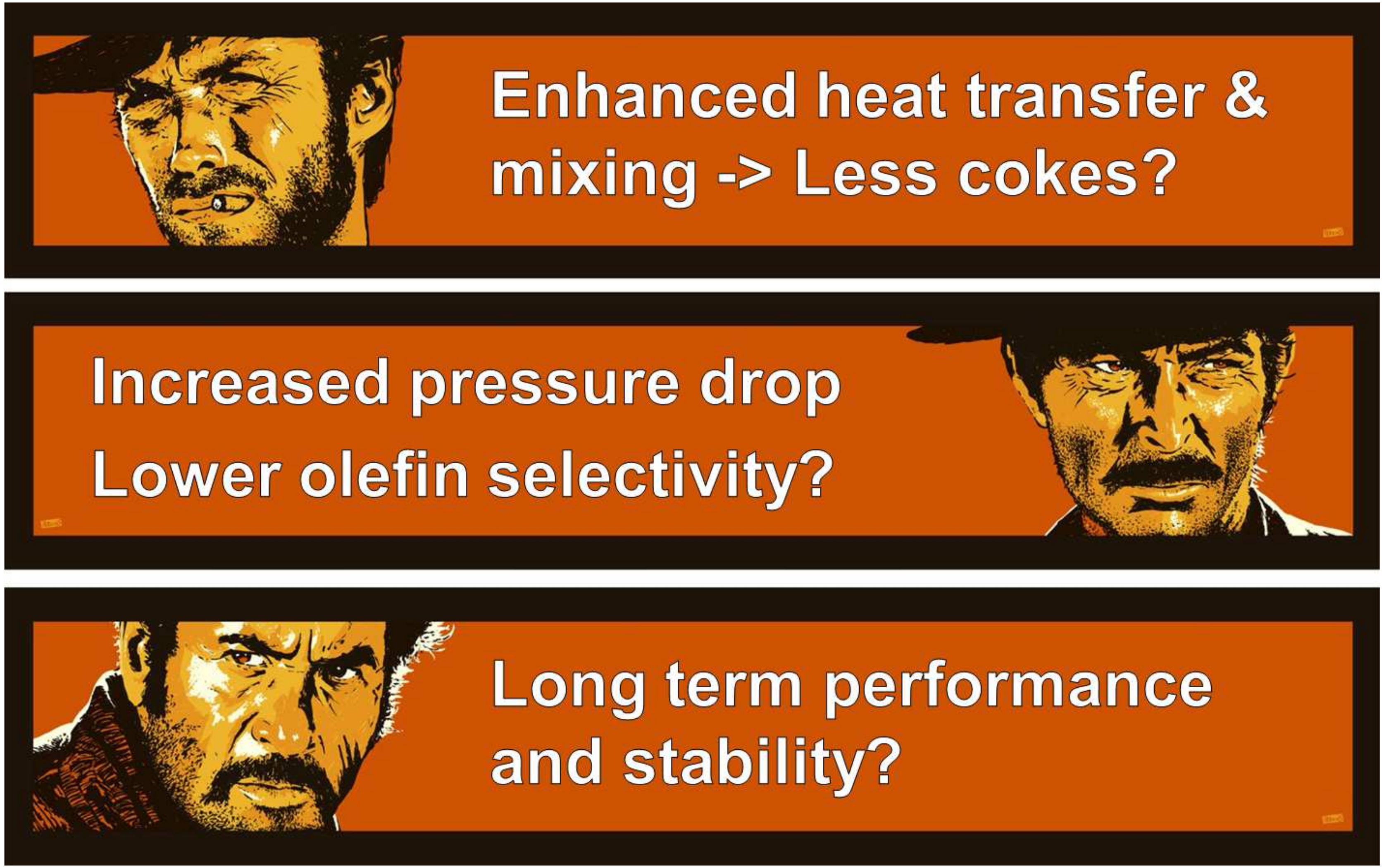
3D REACTOR TECHNOLOGY

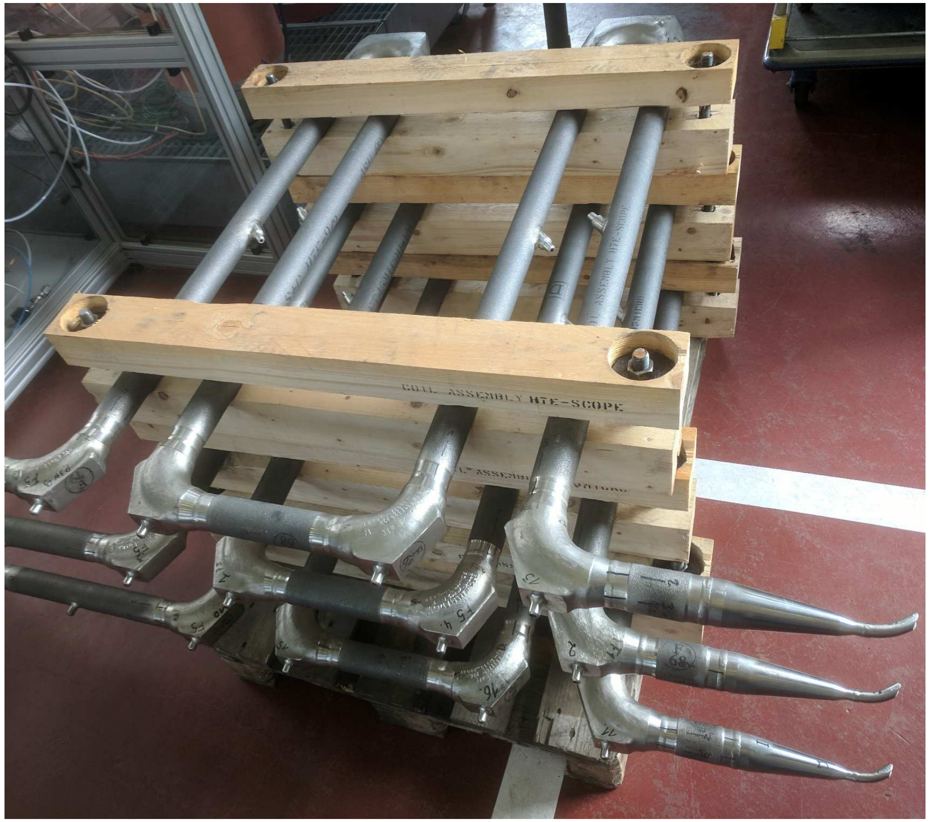


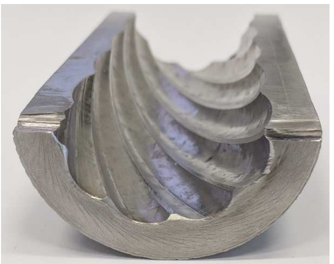
REACTORS

Centralloy® ET 45 Micro

Centralloy® HT E

Centralloy® HT E + SCOPE®





Alloy	Composition [wt %]								
	C	Si	Mn	Cr	Fe	Ni	Al	Nb	Additions
ET 45 Micro	0.45	1.6	1.0	35	bal.	45	-	1.0	MAE, RE
HT E	0.45	-	-	30	bal.	45	4.0	0.5	MAE, RE

RE: reactive elements; MAE: micro-alloying elements

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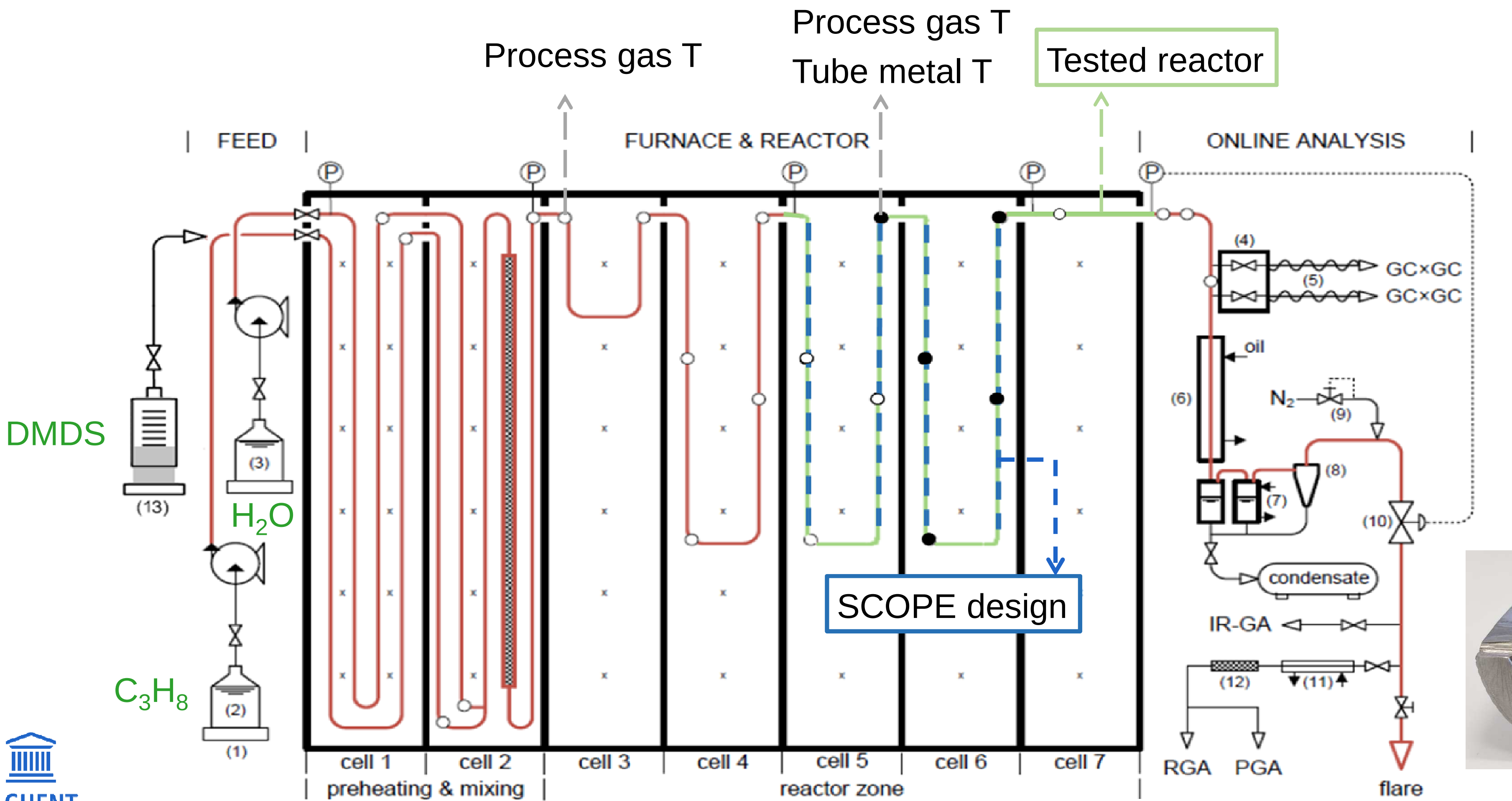
PILOT PLANT


Process gas T
Process gas T
Tube metal T
Tested reactor
FEED
FURNACE & REACTOR
ONLINE ANALYSIS
DMDS
(13)
(3)
H_2O
C_3H_8
(2)
(1)
SCOPE design
cell 1
cell 2
cell 3
cell 4
cell 5
cell 6
cell 7
preheating & mixing
reactor zone
(4)
(5)
GC×GC
GC×GC
oil
(6)
N_2
(9)
(8)
(7)
(10)
condensate
IR-GA
(12)
(11)
RGA
PGA
flare

EXPERIMENTAL PROGRAM

- Steam treatment for 10 hours
- 1CC: COT = base; 6 hours
- 2CC: COT = base; 2 hours
- 3CC: COT = base; 6 hours
- 4CC: COT = base + 110 °C/ + 160 °C*; 1.67 hours
- 5CC: COT = base; 12 hours

*SCOPE®

✓ Decoking was performed after every Cracking Cycle (CC)
✓ Prior to each CC a pre-sulfiding step was performed

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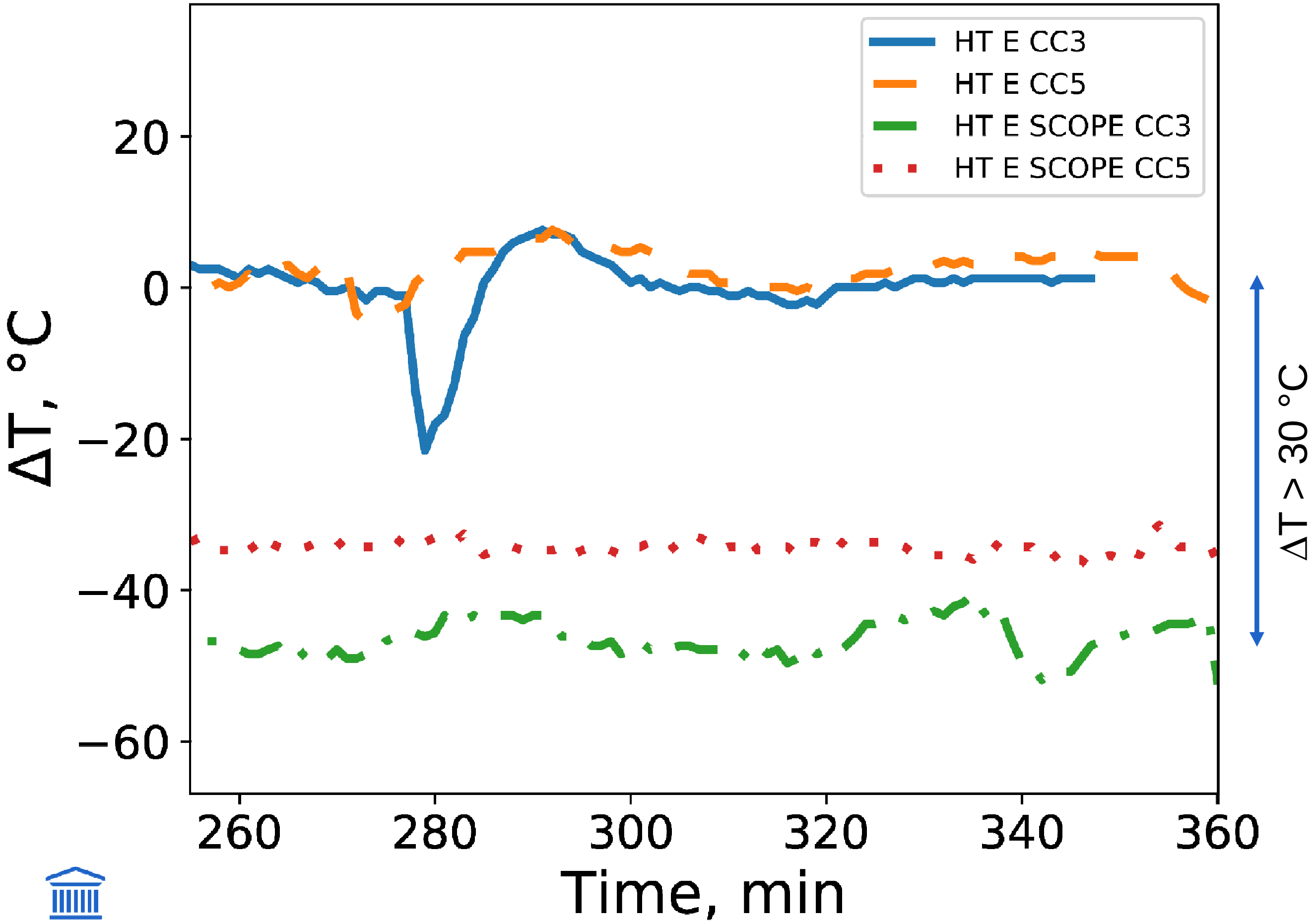
TUBE METAL TEMPERATURES



Pyrometer

Manual T

Weld-on TC's

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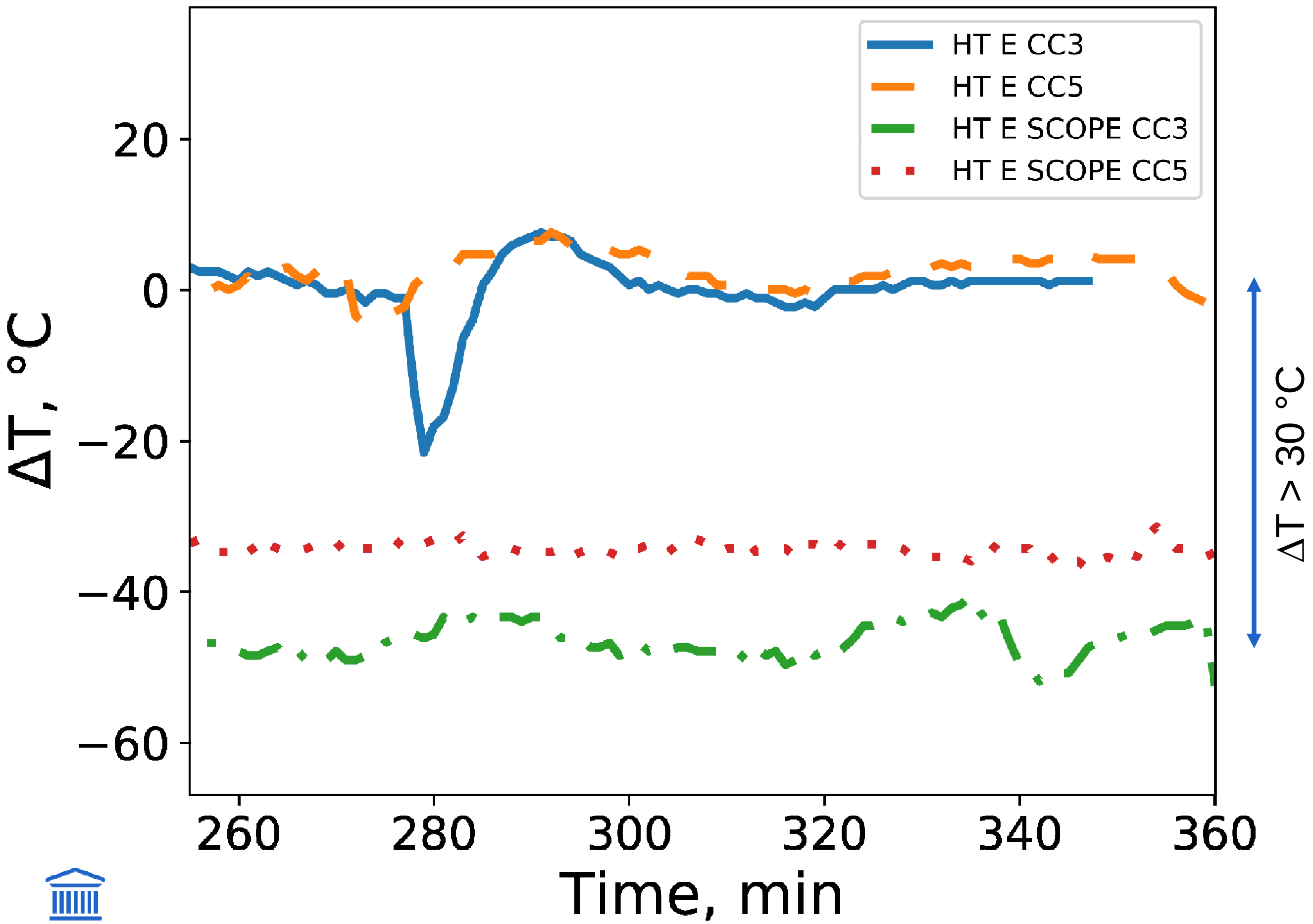
TUBE METAL TEMPERATURES

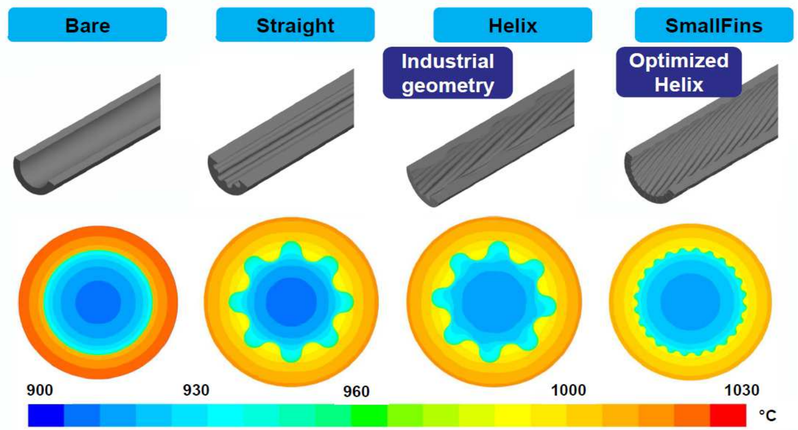


Gas consumption

Result

~10 % lower

Fuel gas consumption



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Schietekat, et al., "Computationally efficient CFD simulations with detailed free-radical mechanisms", in AIChE Annual Meeting, San Francisco, CA, 2013.

TUBE METAL TEMPERATURES

30°C lower tube metal temperature reduces fuel consumption by ~10%

q is constant → $T_{gas/coke}$ decreases

$U\ A$ increases → $T_{gas/coke}$ decreases

↓

$T_{wall,in}$ decreases

↓

$T_{wall,out}$ decreases

↓

q_{emit} decreases

↓

q_{inci}, q_{conv} can decrease

↓

T_{refr}, T_{flue} can decrease

↓

$\dot{m}_{fuel}$ can decrease

Convection on inner wall $q = U\ A\ (T_{gas/coke} - T_{bulk})$

Conduction through coke $q = k_c\ A\ (T_{wall,in} - T_{gas/coke})/d_c$

Conduction through metal $q = k_m\ A\ (T_{wall,out} - T_{wall,in})/d_m$

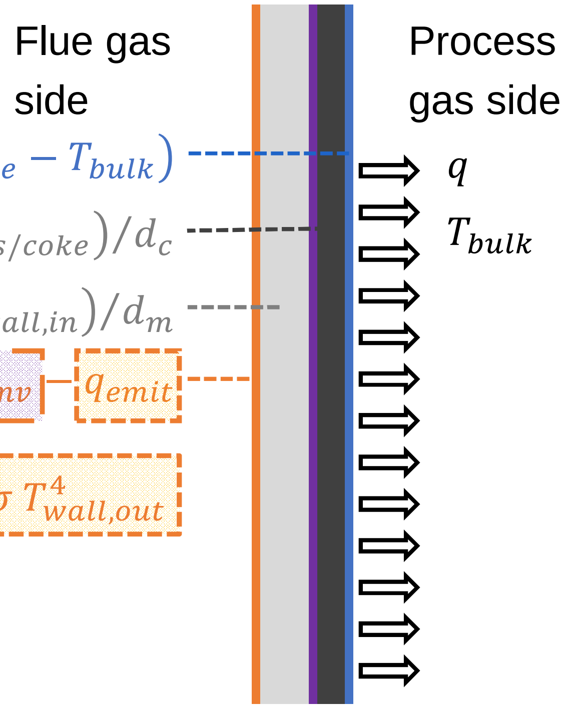
Heat balance on outer wall $q = q_{inci} - q_{re} + q_{conv} - q_{emit}$

$\varepsilon_w\ q_{inci} + q_{conv}$

$\varepsilon_w\ \sigma\ T_{wall,out}^4$

$\sim T_{refr}, T_{flue}$

$\sim \dot{m}_{fuel}$



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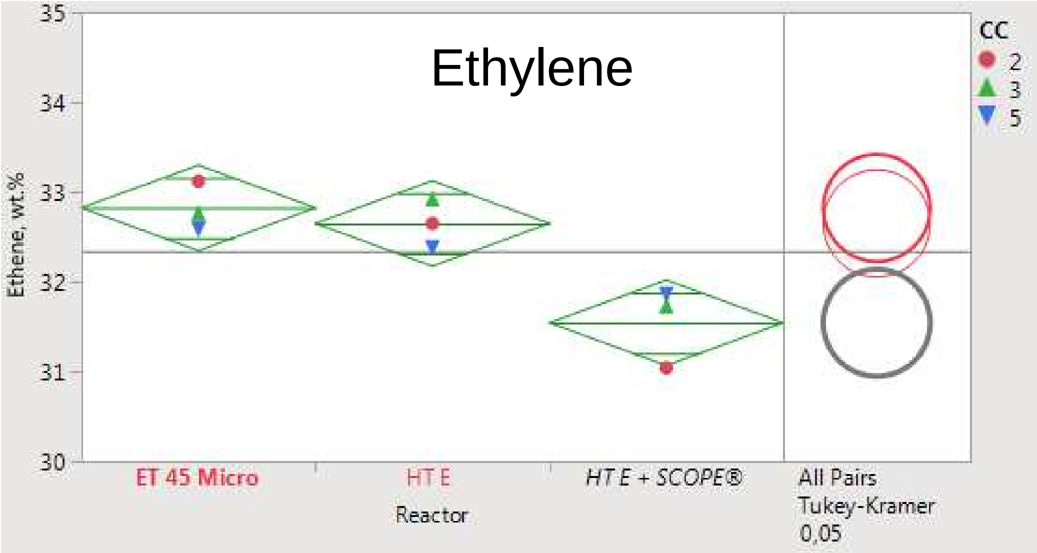
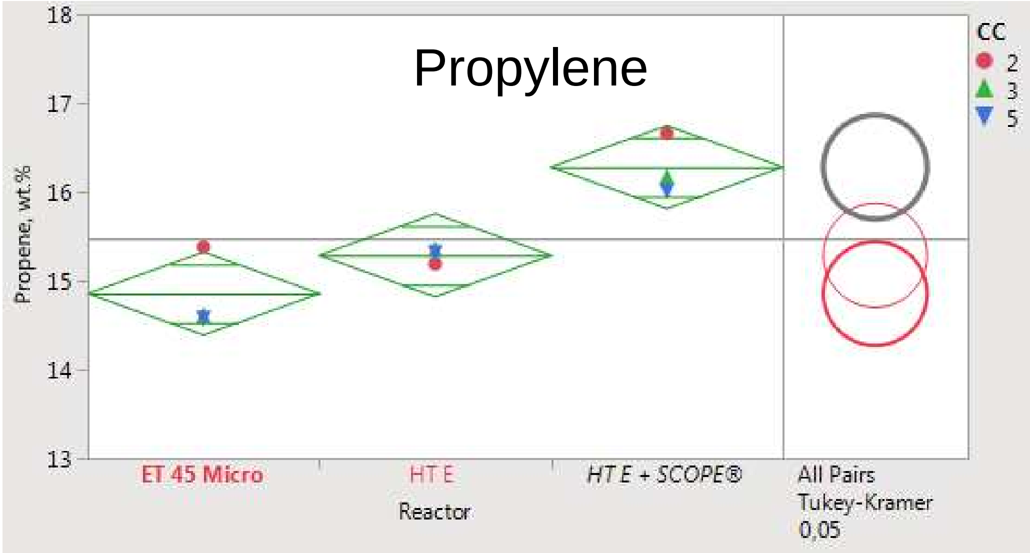
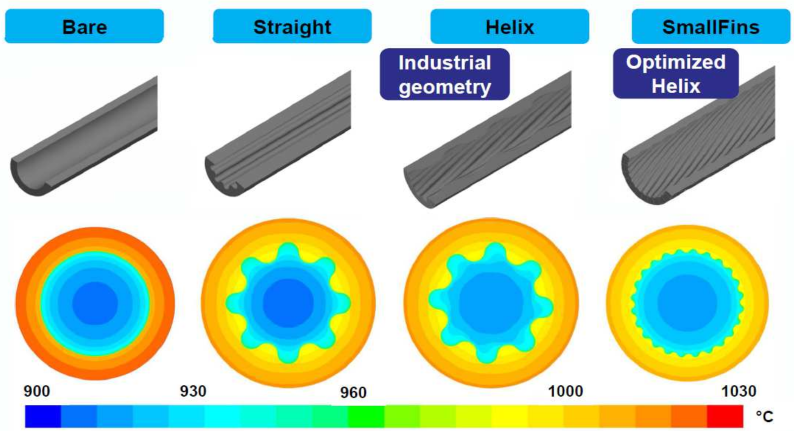
Zhang, Y. et al., Incident Radiative Heat Flux Based Method for the Coupled Run Length Simulation of Steam Cracking Furnaces. Ind. Eng. Chem. Res. 2017, 56, 4156-4172.

PRODUCT YIELDS

2 (CC2), 6 (CC3) and 12 h (CC5) cracking cycles







Reduced over-cracking near wall

Schietekat, et al., "Computationally efficient CFD simulations with detailed free-radical mechanisms", in AIChE Annual Meeting, San Francisco, CA, 2013.

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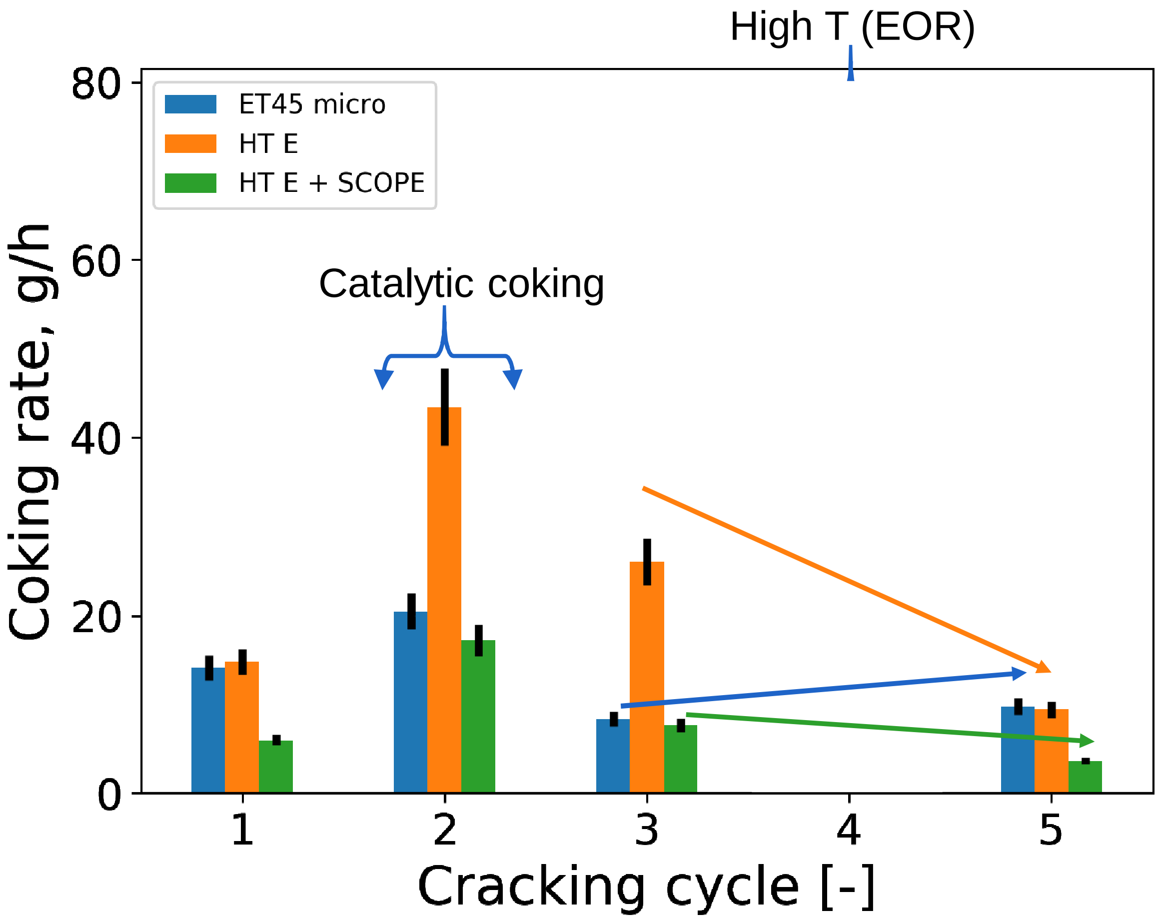
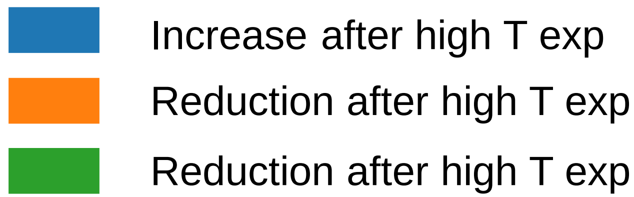
COKING RATES



1CC: COT; 6 hours
2CC: COT; 2 hours
3CC: COT; 6 hours
4CC: COT+110 °C/+160 °C*;
1.67 hours
5CC: COT = base; 12 hours
*SCOPE



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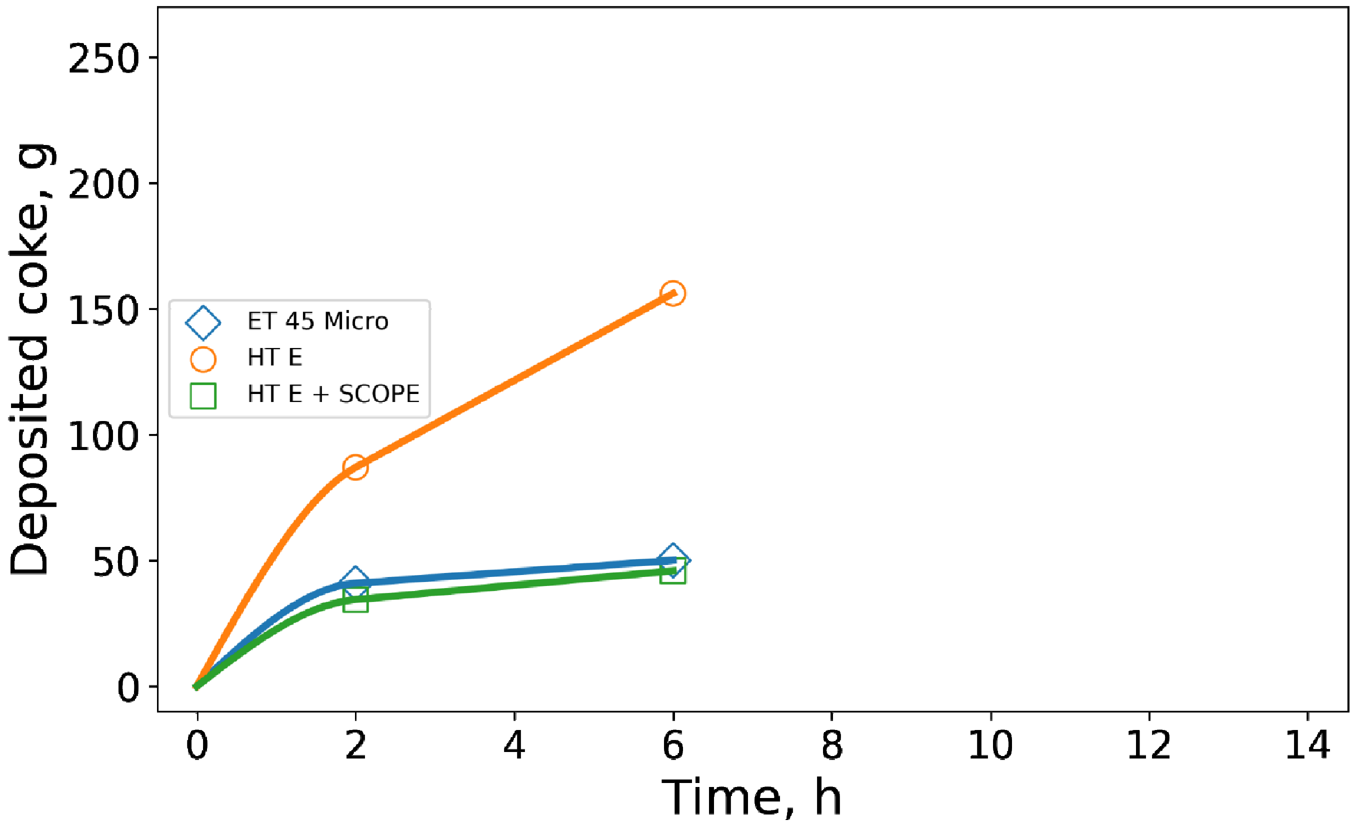
COKE DEPOSITION



Coke after 2 (CC2) and 6h (CC3)

ET 45 Micro and HT E + SCOPE comparable

HT E significantly worse

Line: estimated coking curve

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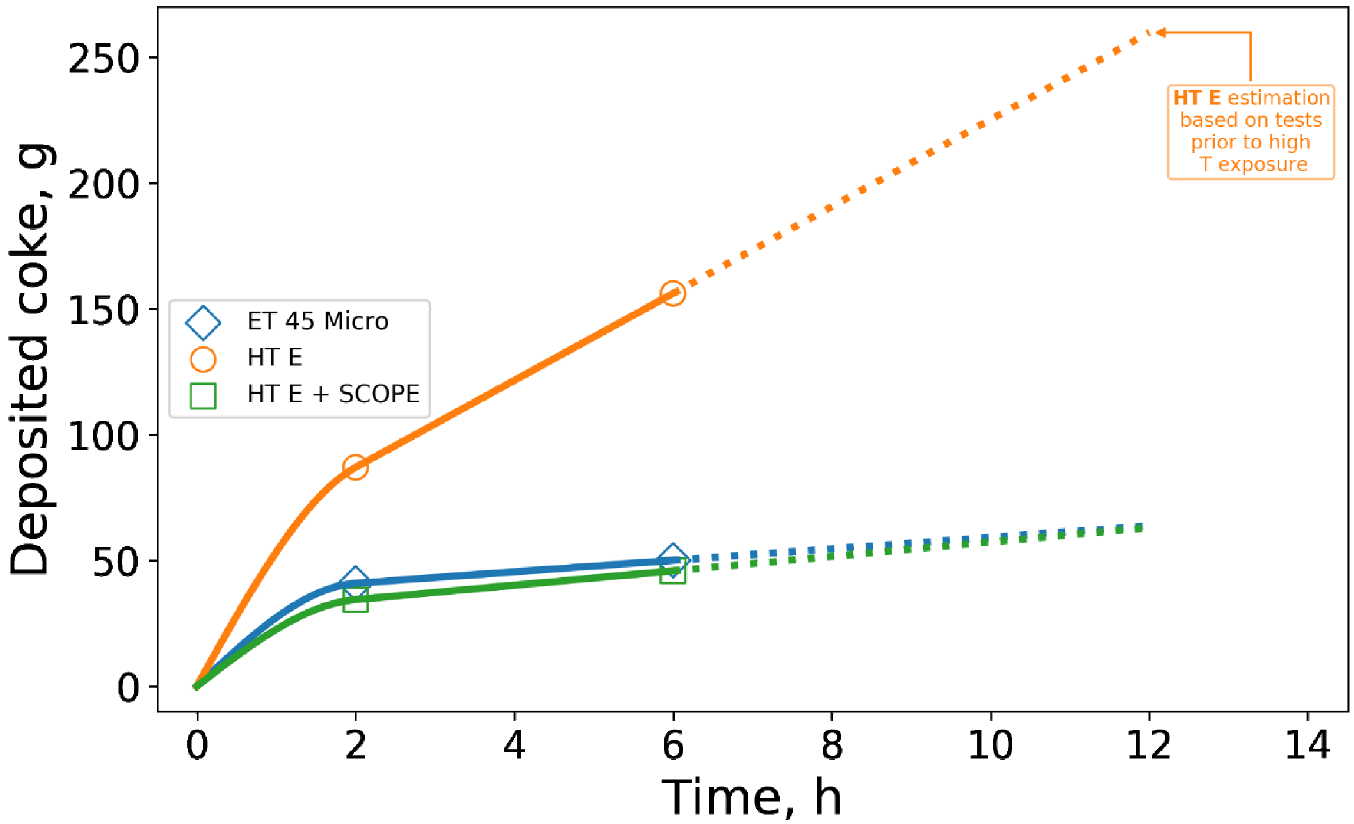
COKE DEPOSITION



Extrapolation for 12 h coke

Assumptions:

2 h (CC2) = Catalytic

6 h (CC3) = asymptotic

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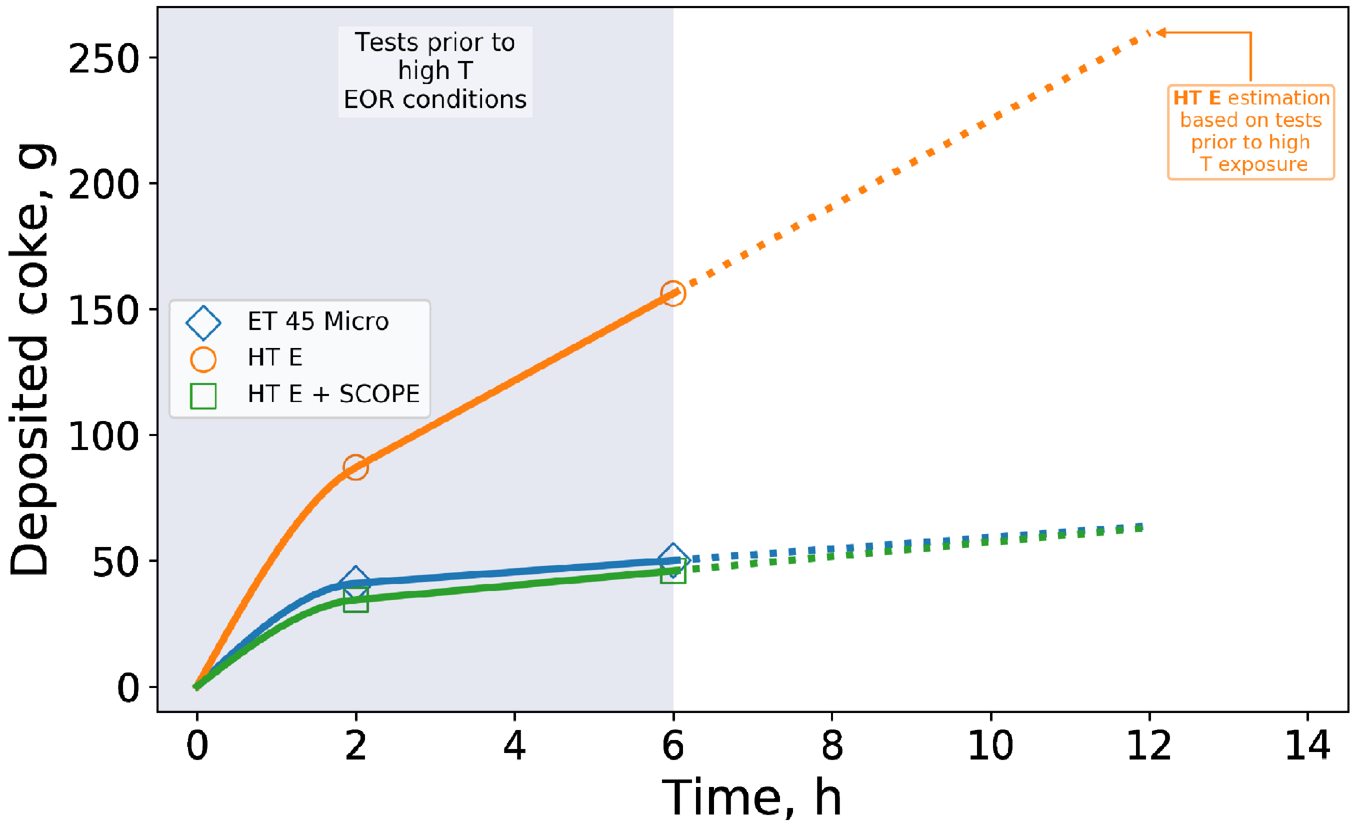
COKE DEPOSITION



Extrapolation based on tests prior to high T (EOR) exposure

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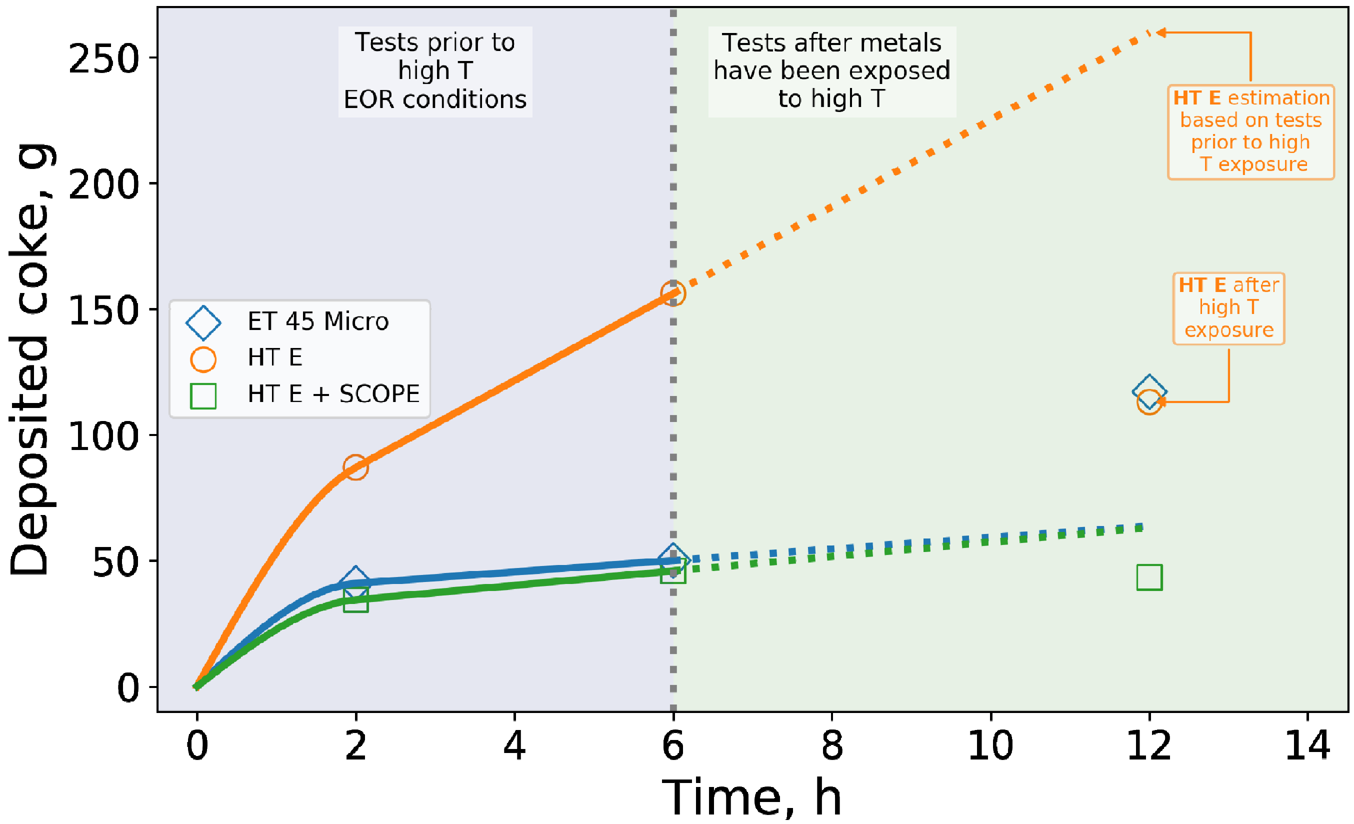
COKE DEPOSITION



Coke after high T exposure

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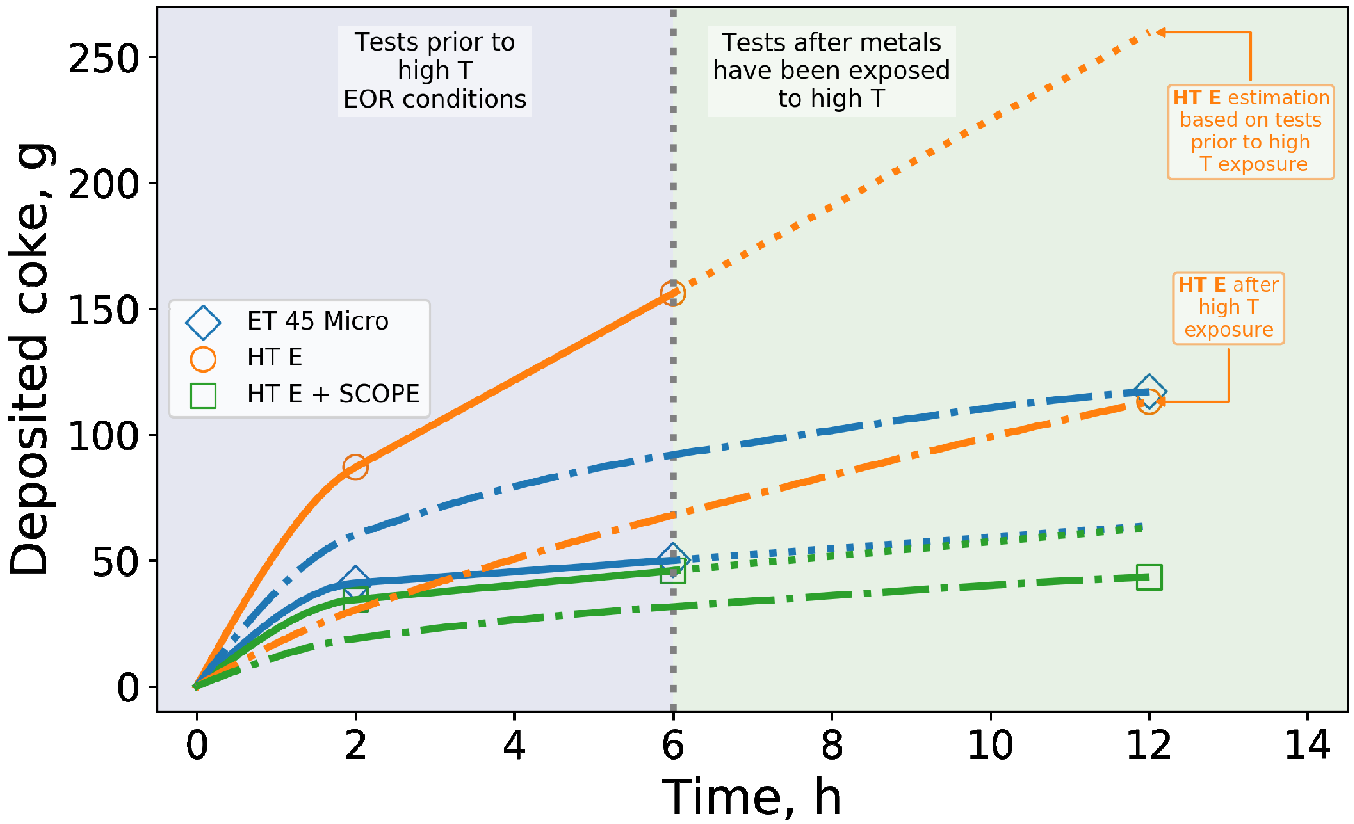
COKE DEPOSITION



Estimation coking curve

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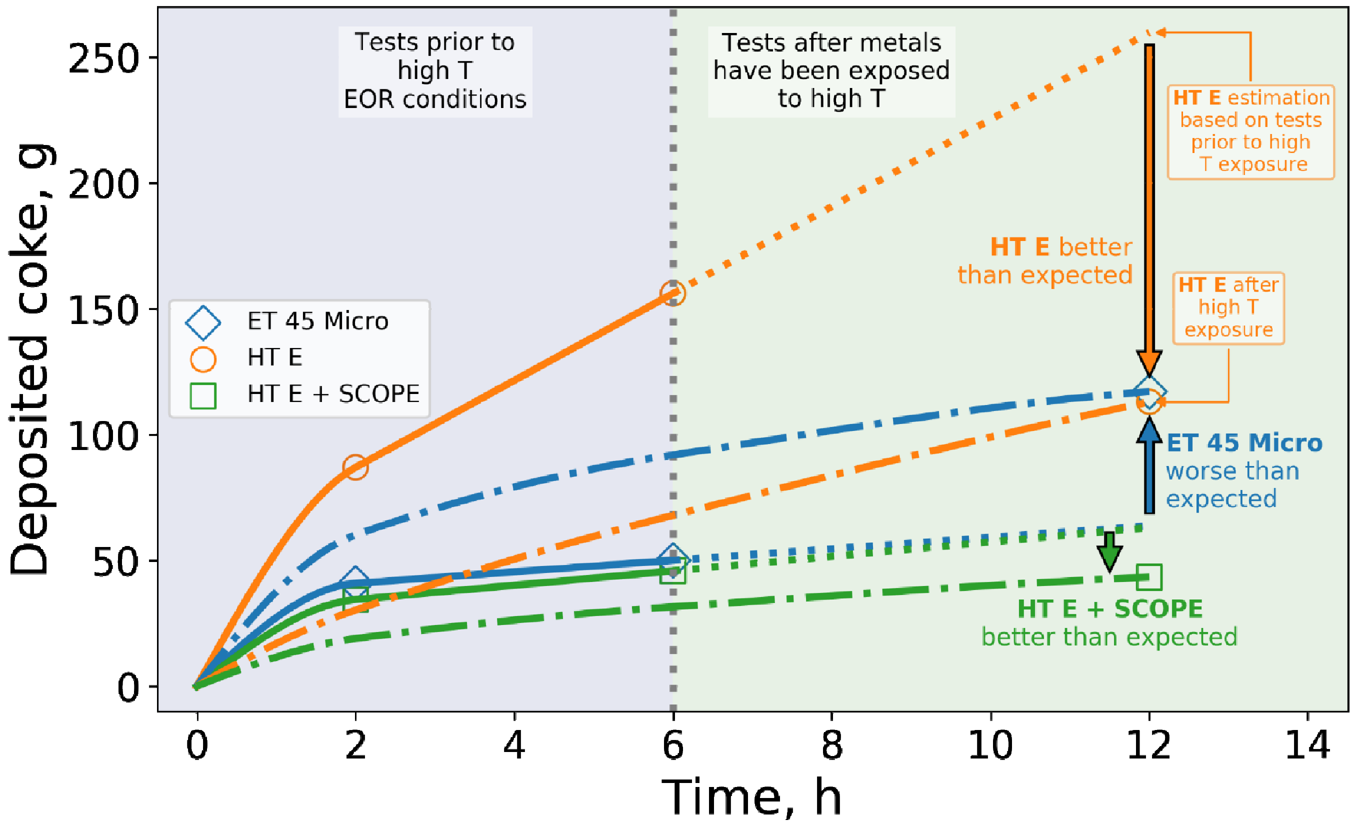
COKE DEPOSITION



HT E better than expected

ET 45 Micro worse than expected

SCOPE design →

Lower temperatures

Lower influence high T excursion

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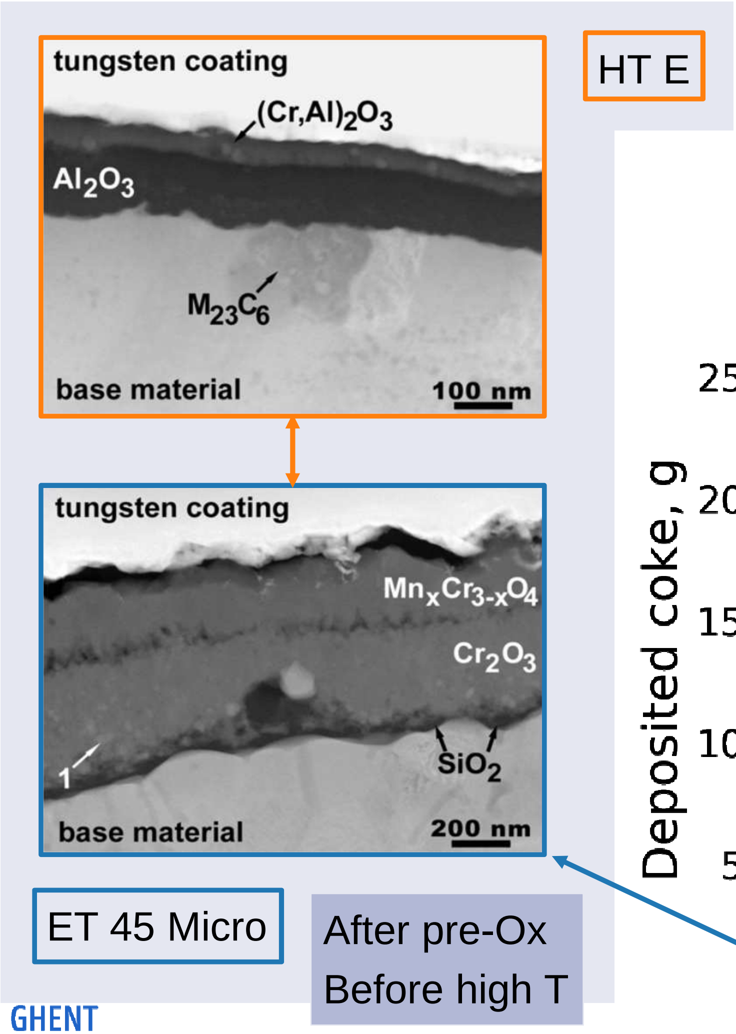
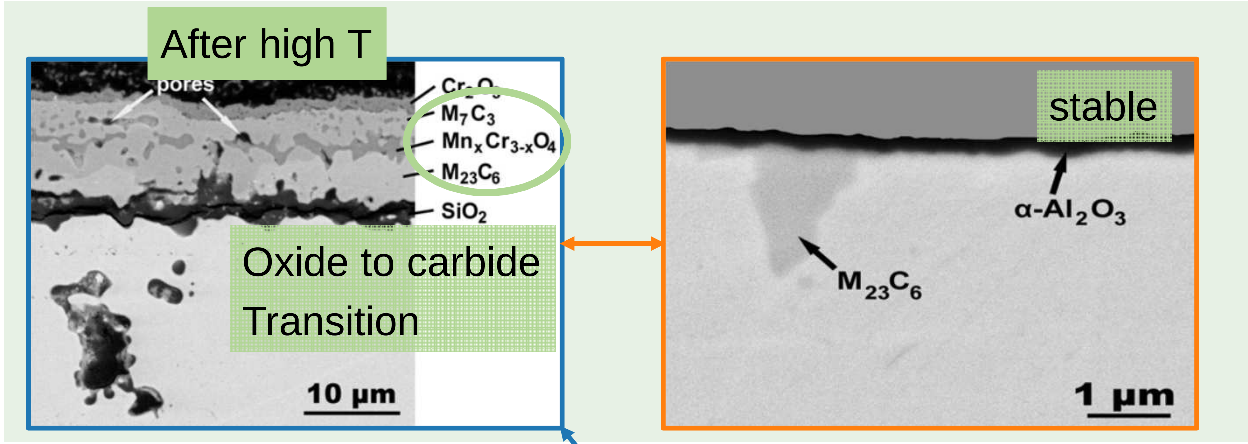
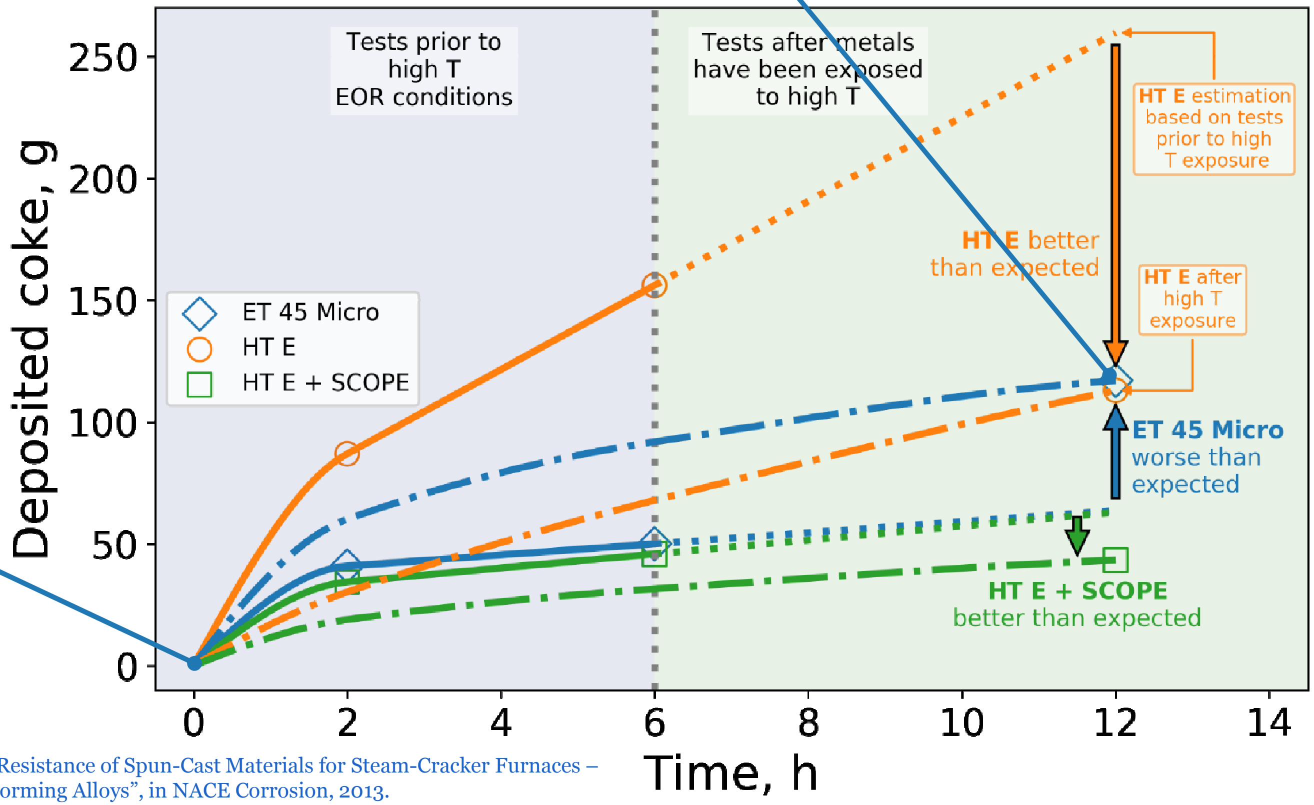
COKE DEPOSITION







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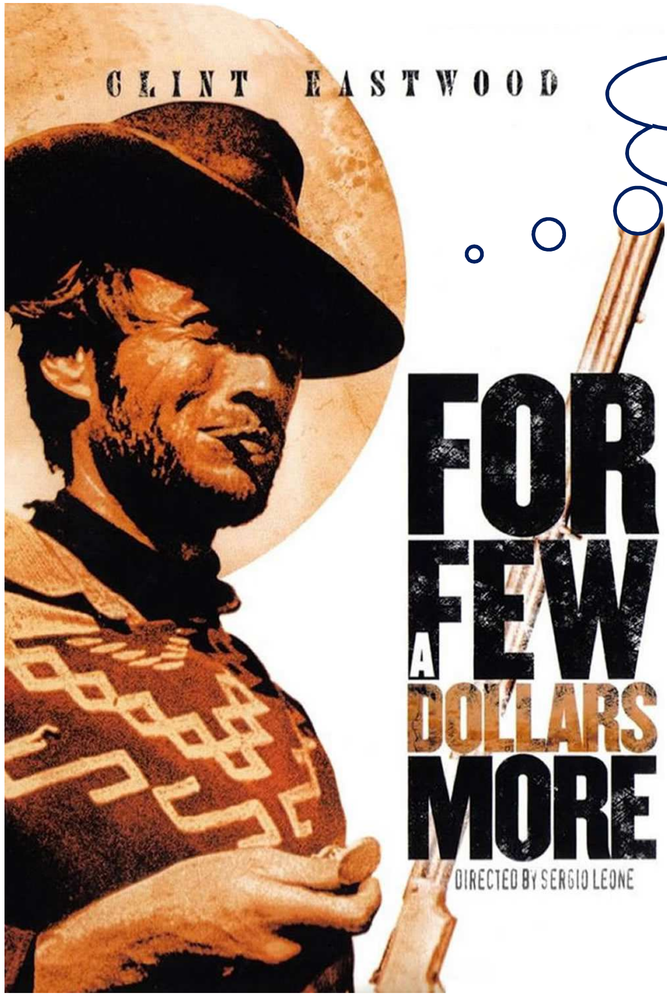
Jakobi, et al., "The high-Temperature Corrosion Resistance of Spun-Cast Materials for Steam-Cracker Furnaces – A Comparative Study of Alumina- and Chromia-Forming Alloys", in NACE Corrosion, 2013.

FOR A FEW DOLLARS MORE



Cracking furnace under
optimal operating
conditions

- Safety
- Production
- Emission
- Energy efficiency
- Run length

NEXT STEPS

- Testing high emissivity coating's performance in the **pilot plant** furnace/cracker at UGent at TRL5 level
  - benchmark to **uncoated** ethylene furnace by calculating the thermal efficiency of the **improved** furnace
- Comparison SCOPE® vs bare in reactive 3D CFD simulations

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OUTLINE

- Introduction
- Objectives
- Coke formation on high-temperature alloys and 3D reactor technology
- Conclusions

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CONCLUSIONS

- After high Temperature (EOR) exposure HT E performs better, while the performance of ET 45 Micro drops
- ET 45 Micro → Oxide to carbide transition
- HT E → Formation stable α-Al_2O_3 scale
- Combining the advanced coil material (HT E) and novel 3D reactor design (SCOPE®) leads to
  - Increased run lengths
  - Improved product selectivities
  - Longer lifetime of the reactor coils
  - Higher energy efficiency of the furnace

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Thank you for your attention!

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GLOSSARY

– CC: Cracking cycle
– DMDS: dimethyl disulfide
– CFD: computational fluid dynamics
– RE: reactive elements
– MAE: micro-alloying elements
– RGA: refinery gas analyzer
– IR GA: infrared analyzer
– PGA: permanent gas analyzer
– COT: coil outlet temperature
– TMT: Tube metal temperature

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