Design and optimization of 3D reactor technologies for the production of light olefins

Kevin M. Van Geem

Laboratory for Chemical Technology, Ghent, Belgium

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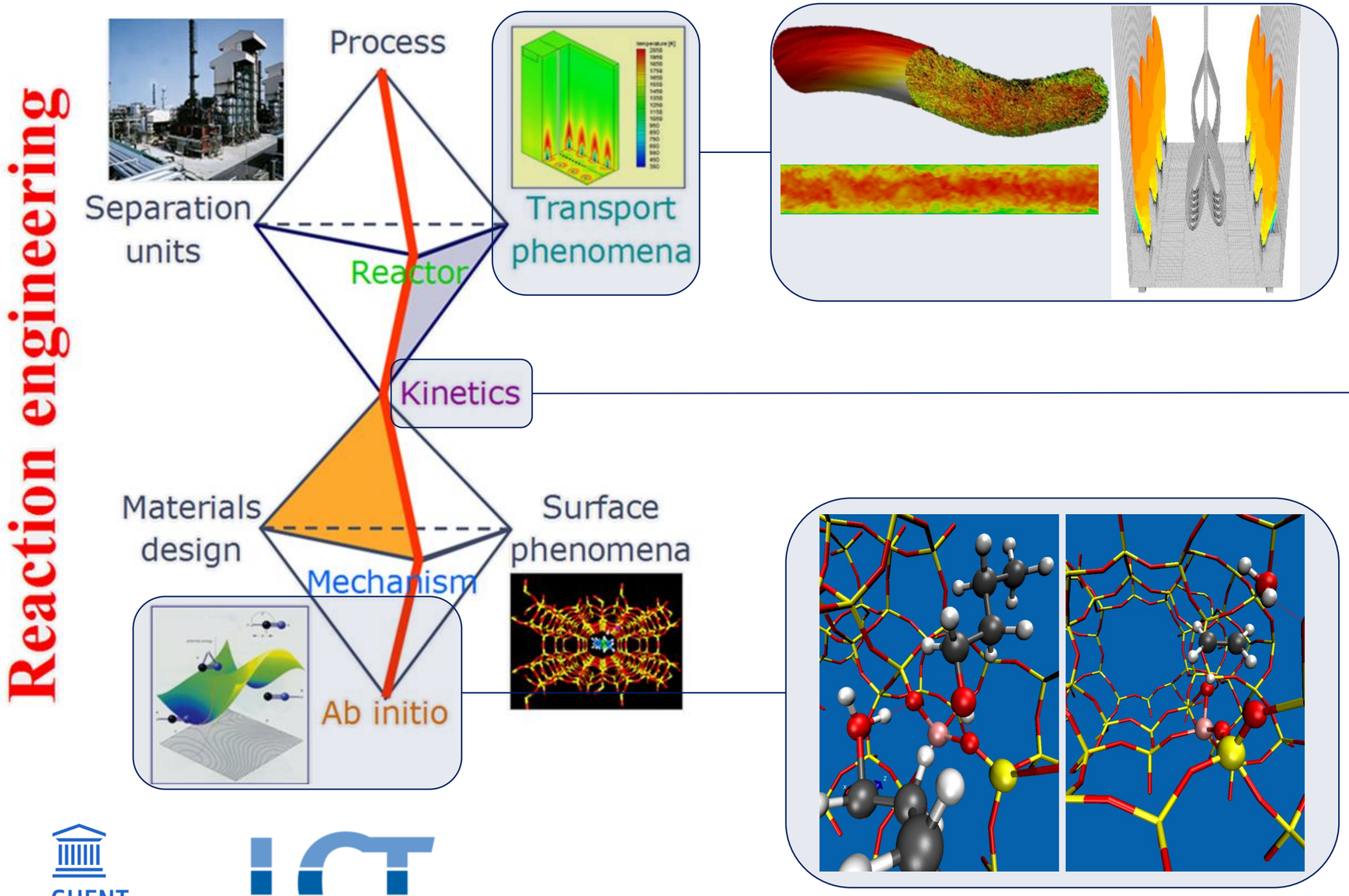
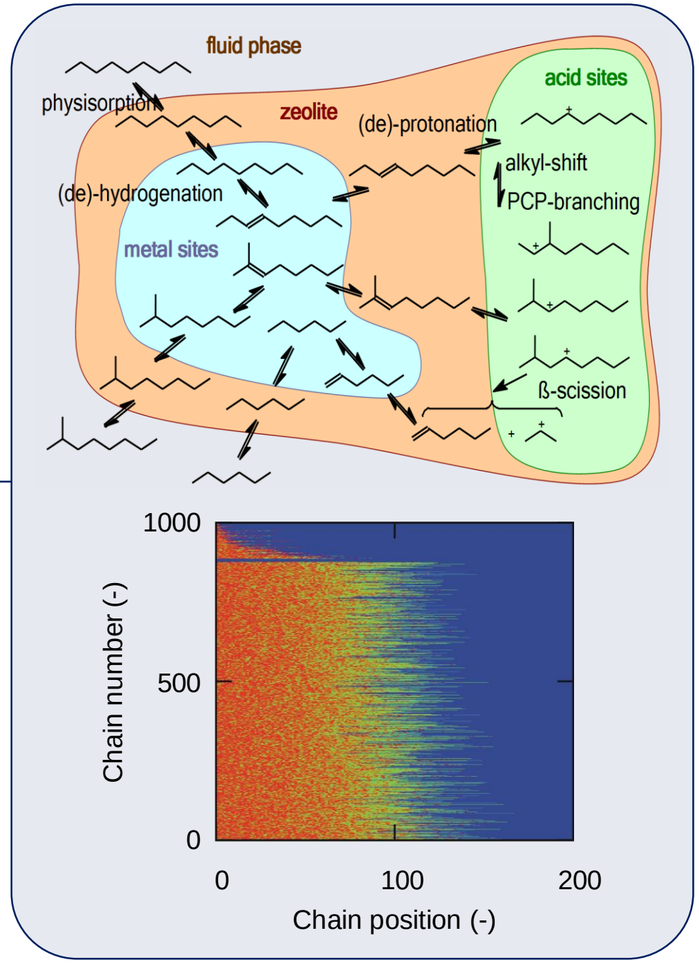
The von Karman Institute for Fluid Dynamics

The “old” LCT





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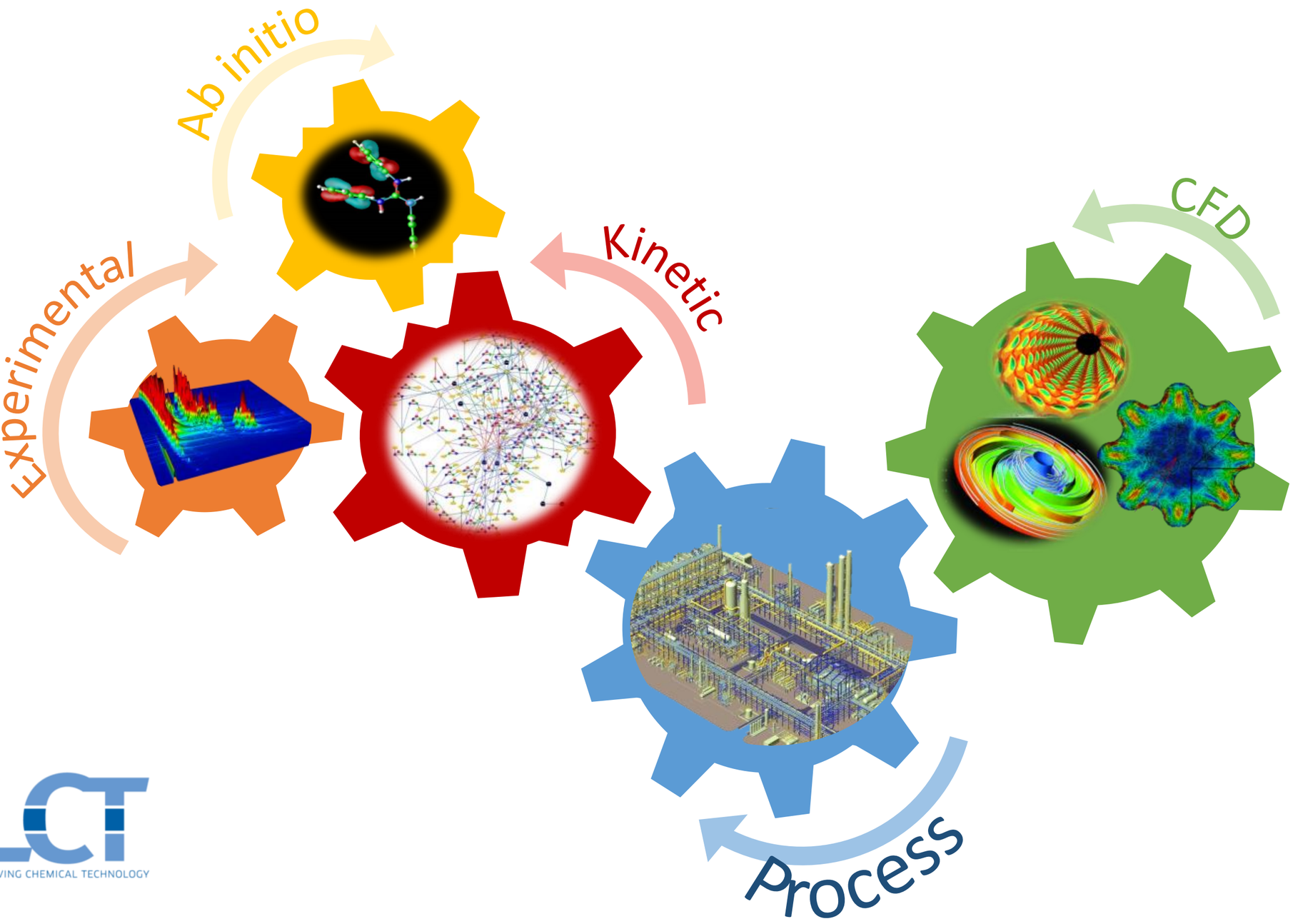
LCT’s new vision



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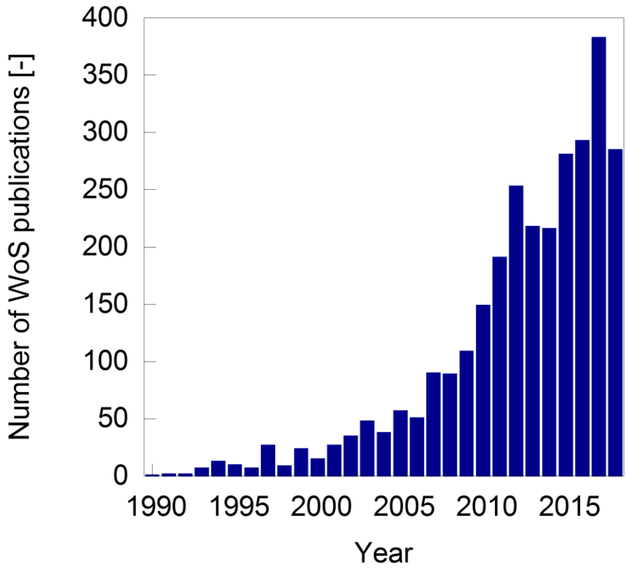
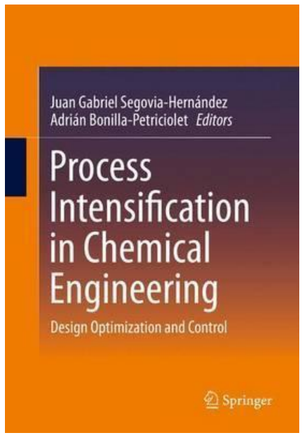
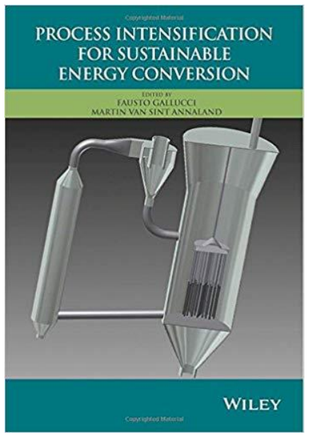
What is Process intensification?

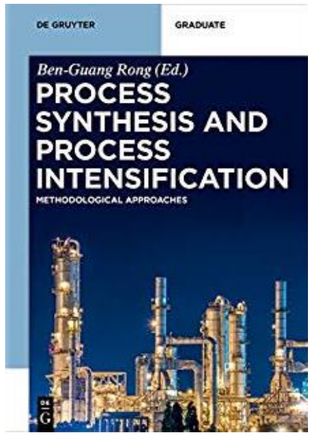
"any chemical engineering development that leads to a substantially smaller, cleaner, and more energy-efficient technology"

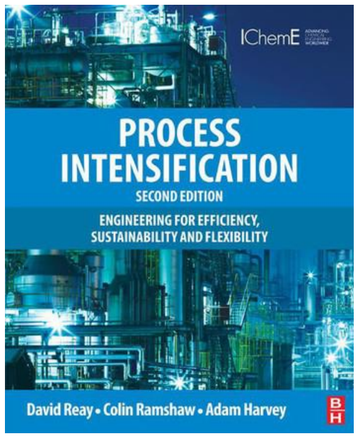
A. Stankiewicz, J. Moulijn

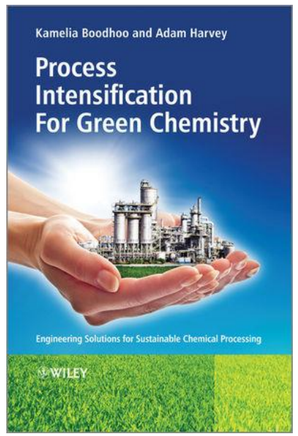


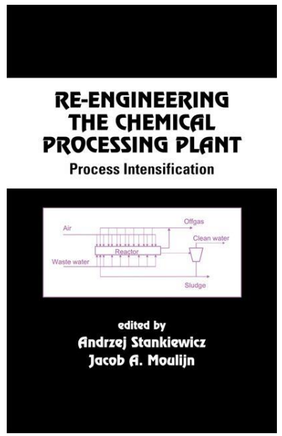


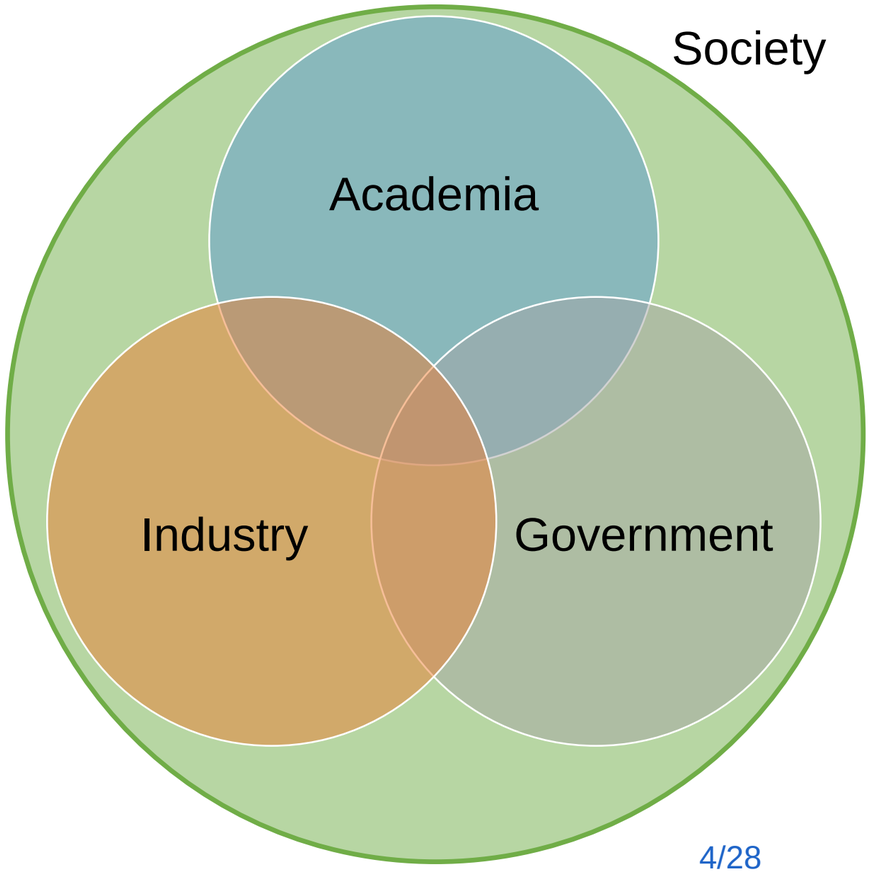












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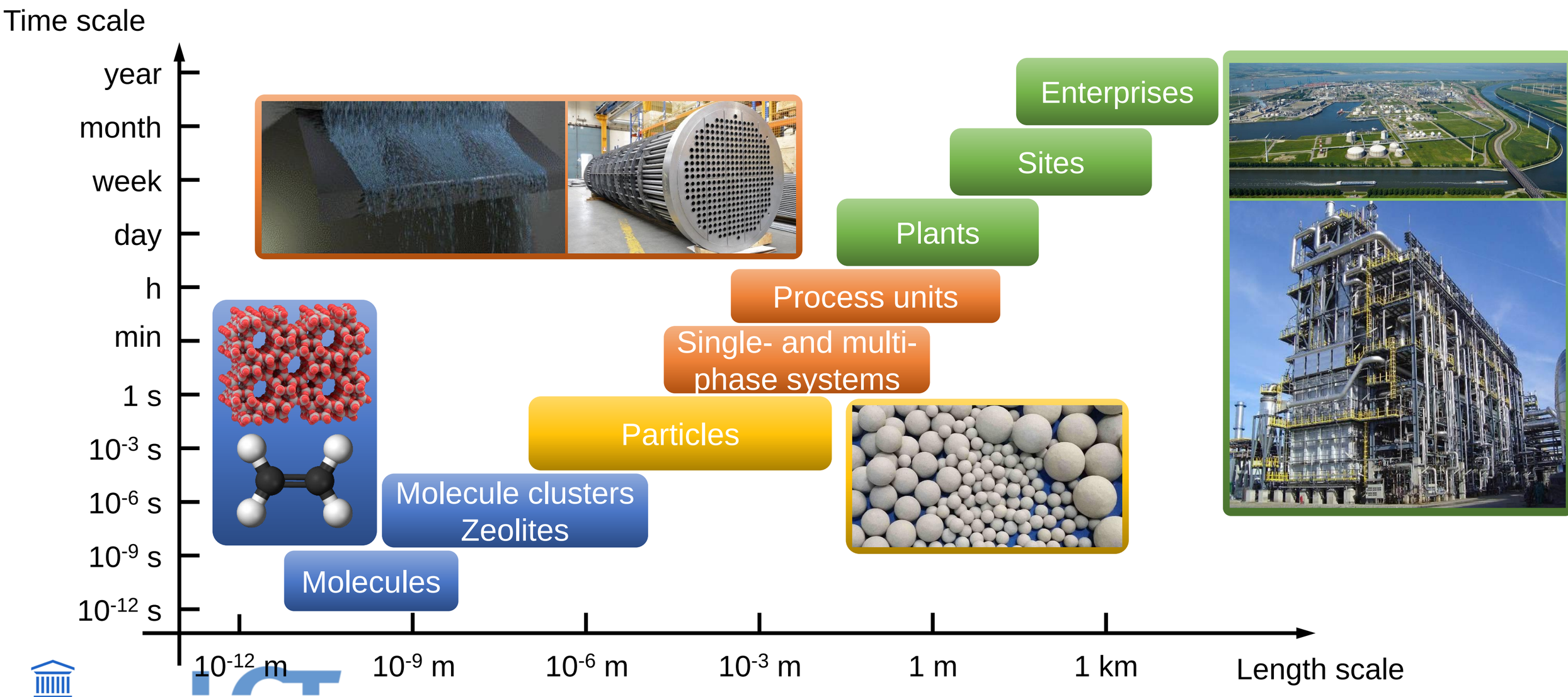
Stankiewicz, A. I.; Moulijn, J. A., Process Intensification: Transforming Chemical Engineering. Chemical Engineering Progress 8500, 22.
https://www.ugent.be/csc/en

Chemical engineering – length and time scales



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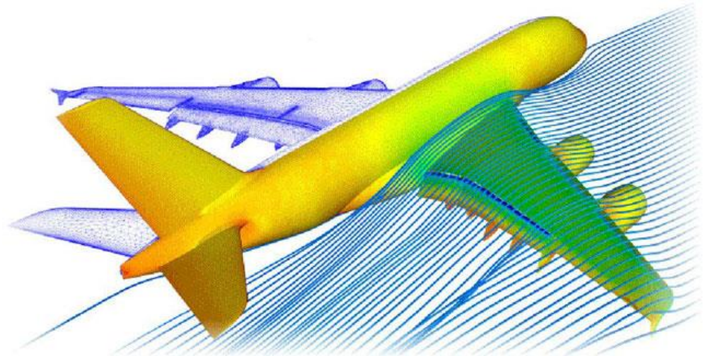
Computational fluid dynamics (CFD)

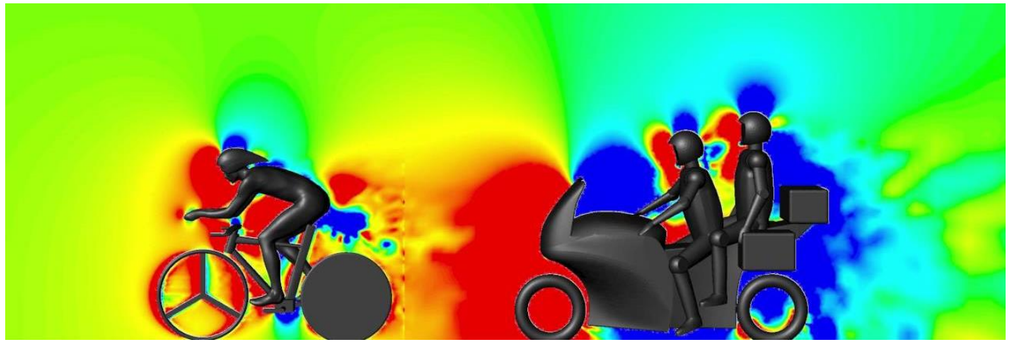
“cleverly forged data”

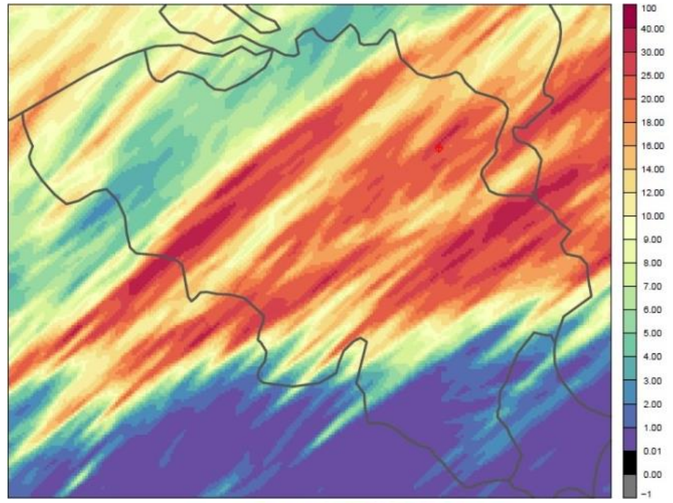
“contract for difference”

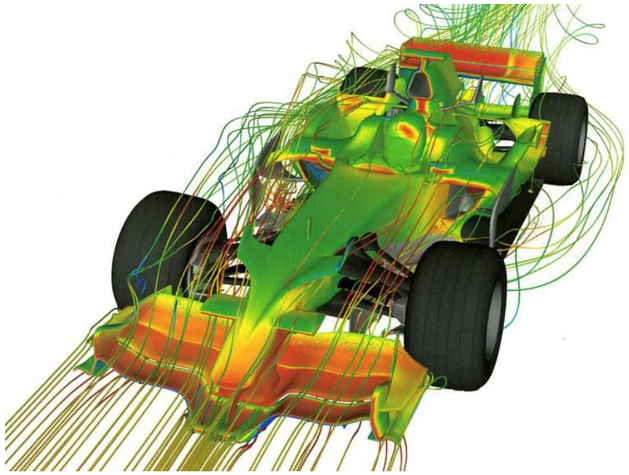
“colors for directors”

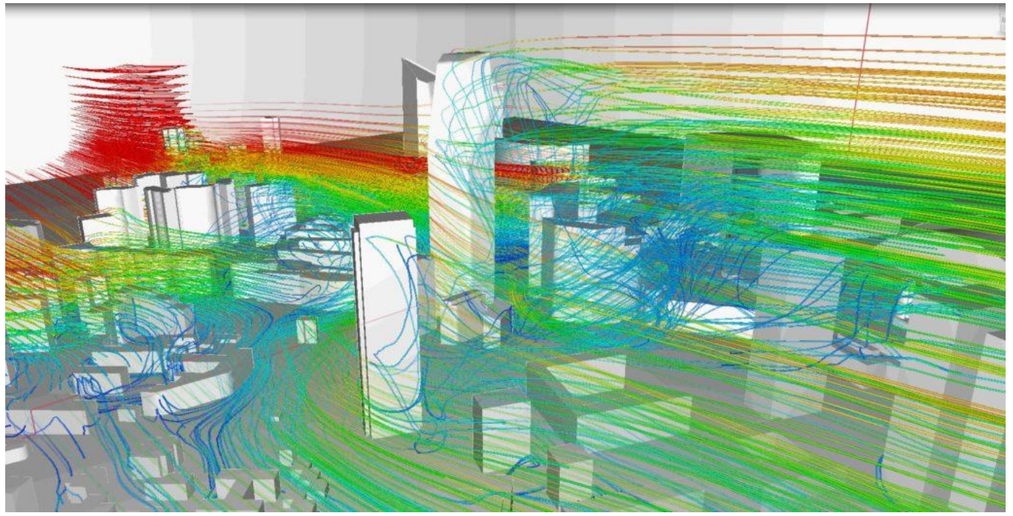
Simulate **fluid flow** based on conservation equations

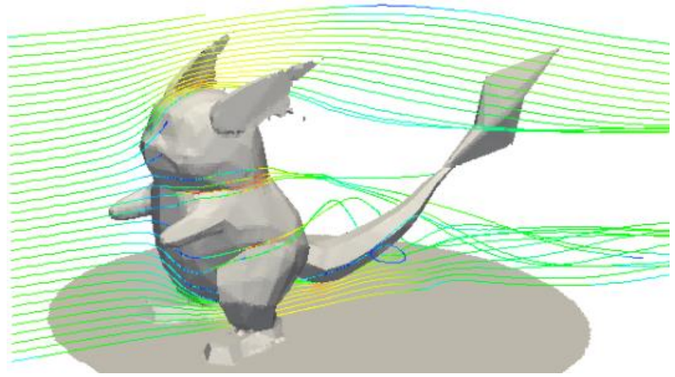








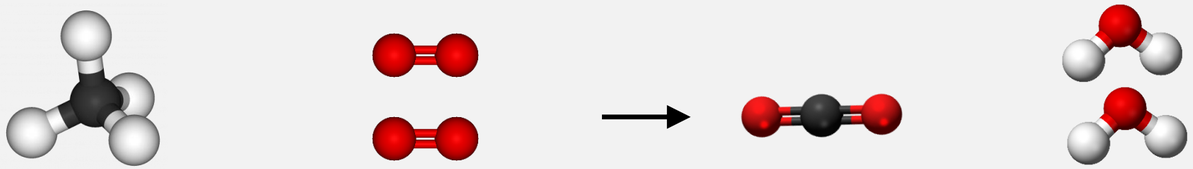




Computational fluid dynamics (CFD)

Simulate **fluid flow** based on conservation equations

Species and global mass (~composition)

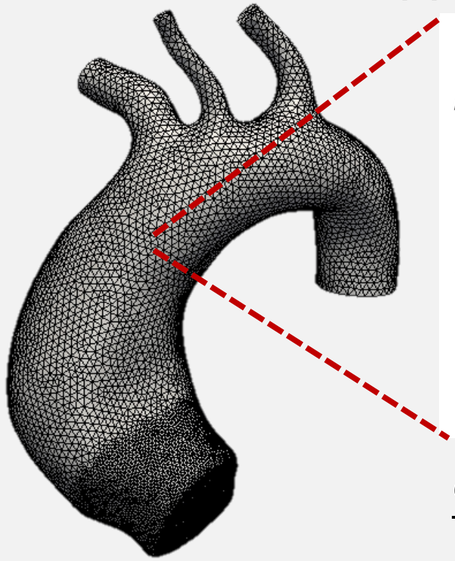


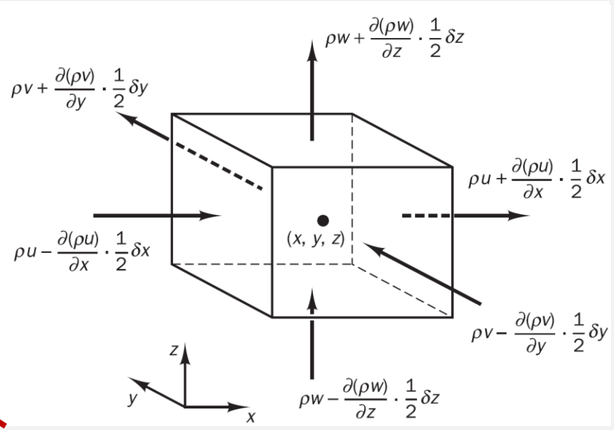
$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$

Enthalpy (~temperature)

Momentum (~velocity)

Control volume approach





$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$$

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LCT: Innovation through Supercomputing

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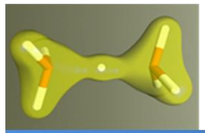
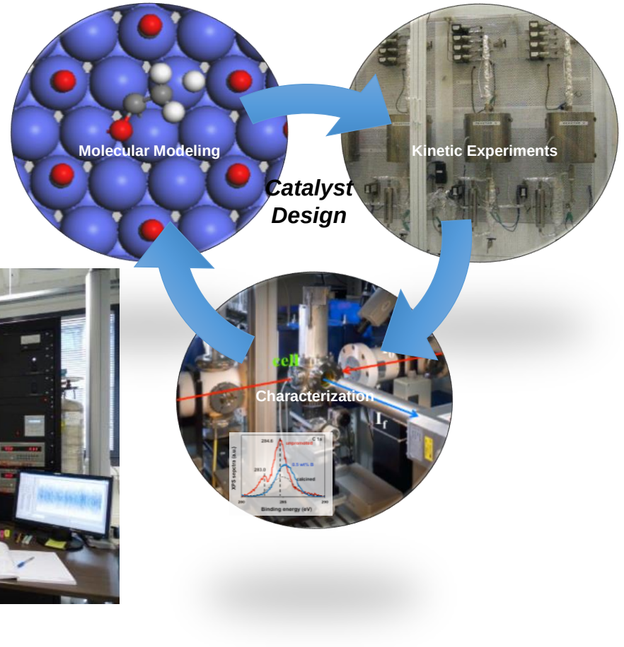
Laboratory for Chemical Technology

Design and **optimization** of sustainable products and processes



COILSIM1D

The advanced simulation and optimization software for the ethylene industry



[Circular process design](#)

[Low carbon technology](#)

[Renewable chemicals and technology](#)

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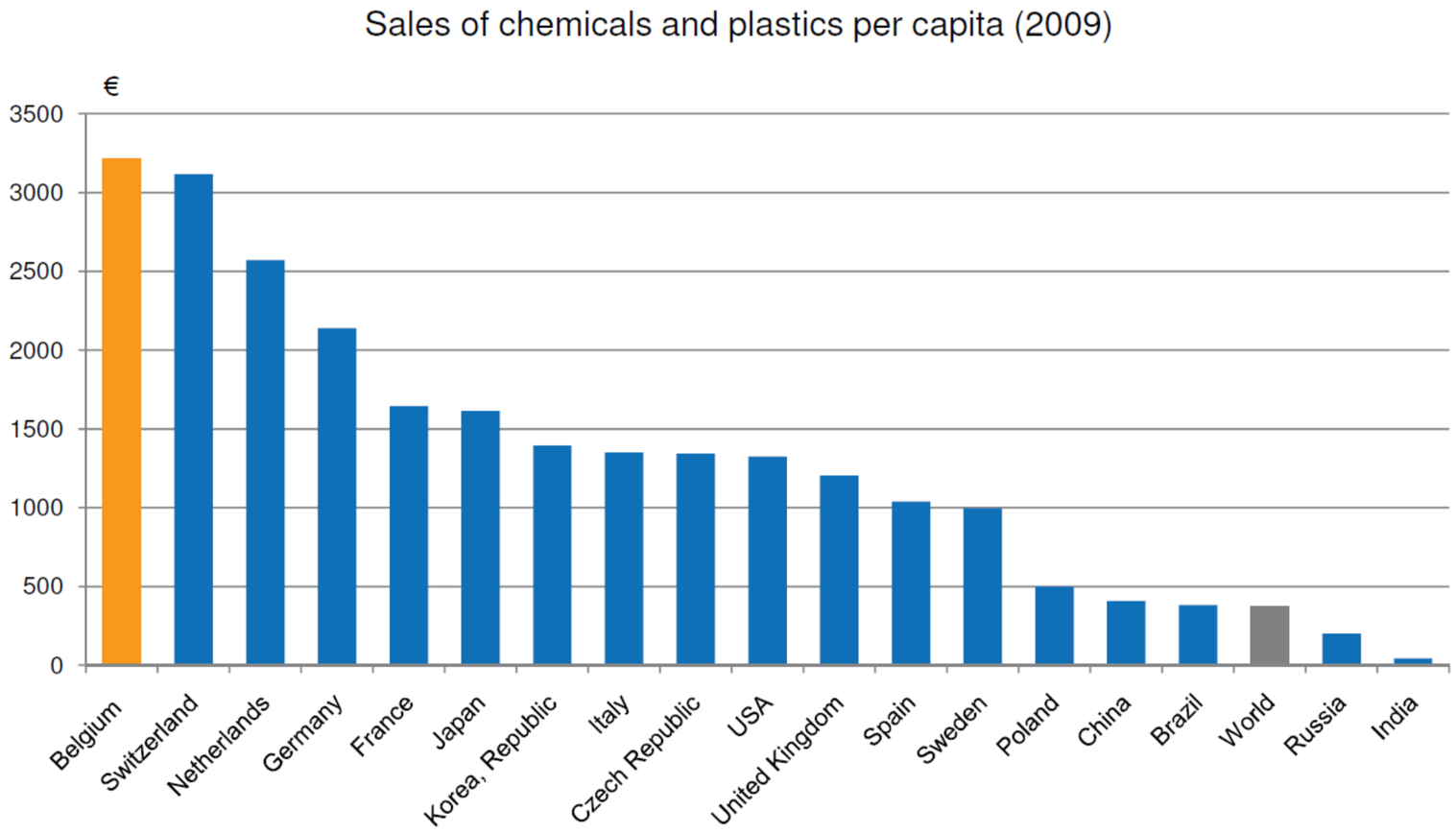
The chemical industry is the enemy

Chemical industry

- Belgium is the N°1 chemical country in the world (per capita basis)



Source: Feri, NIS
2009 Figures

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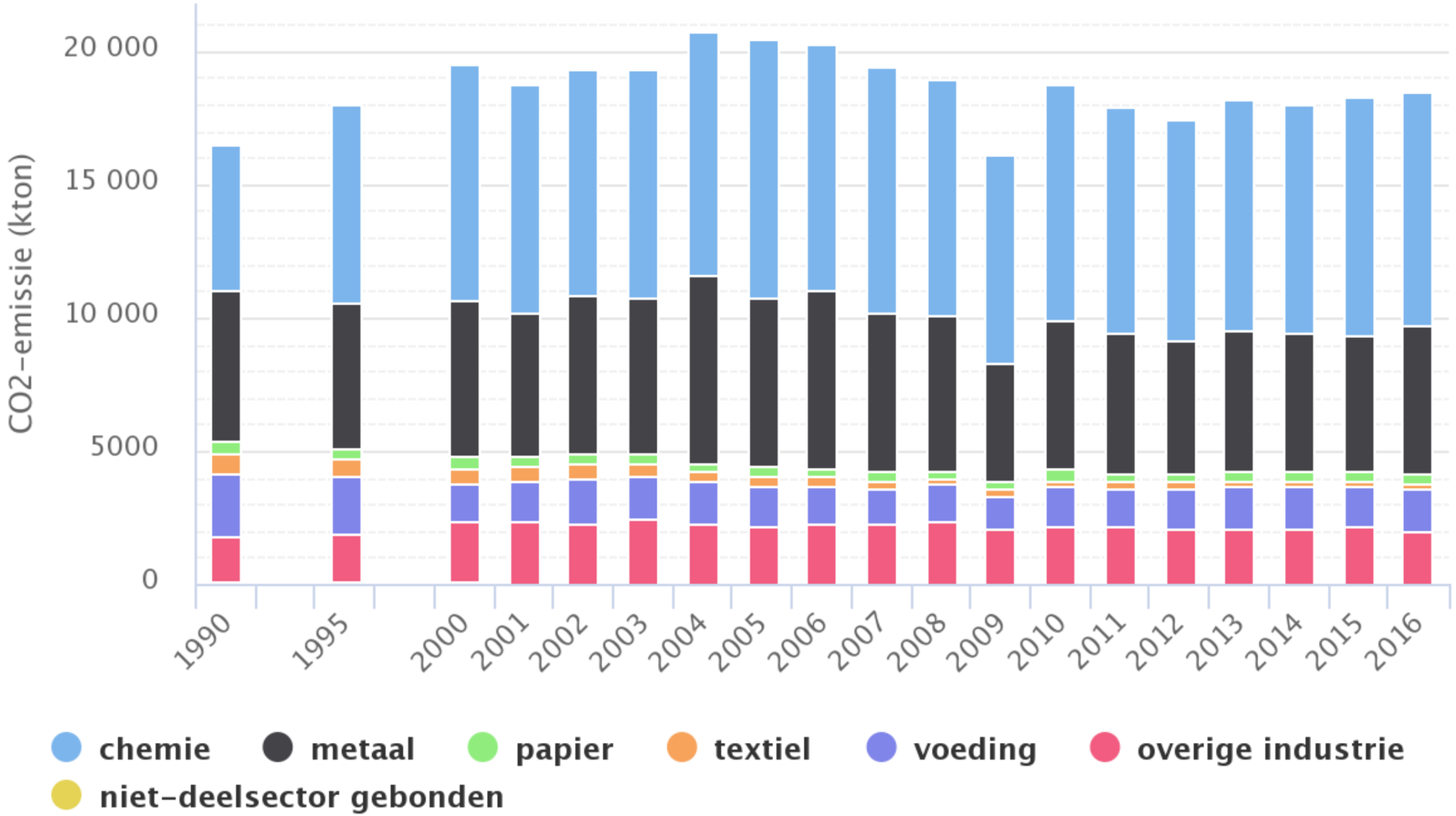
Process transformation

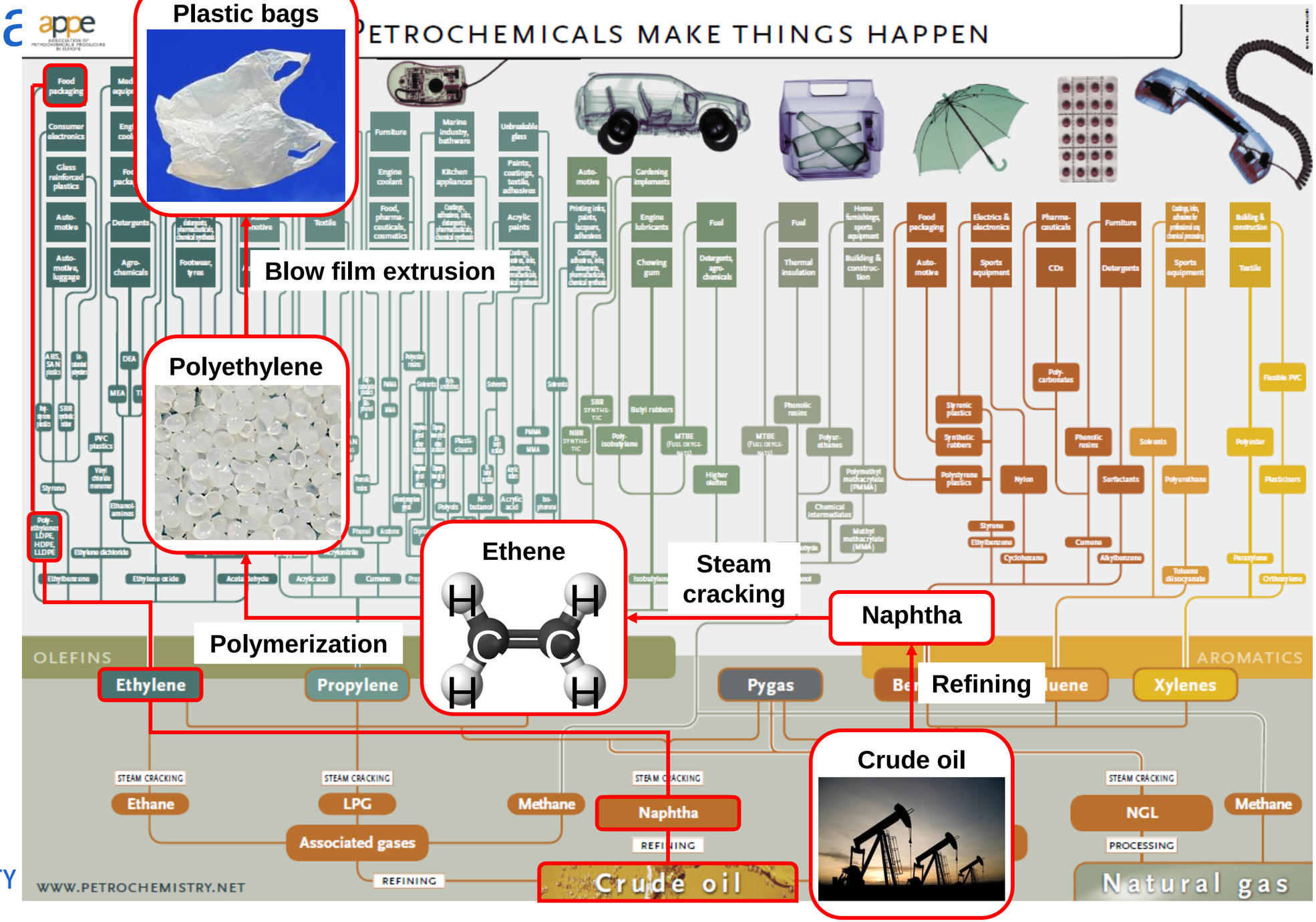
Industrial CO_2 emissions (Flanders, 85120)



- 18,4 Mton/y
  - ✓ 27,6% of total
- Chemical industry
  - ✓ 47,4%
  - ✓ 8,72 Mton/y

Source: *MIRA op basis van EIL (VMM)*

Stea



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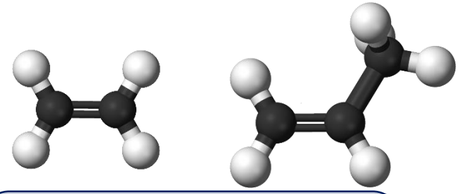
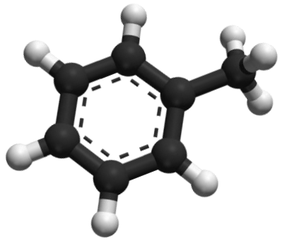
Steam cracking





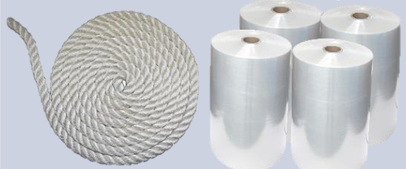
Crude oil

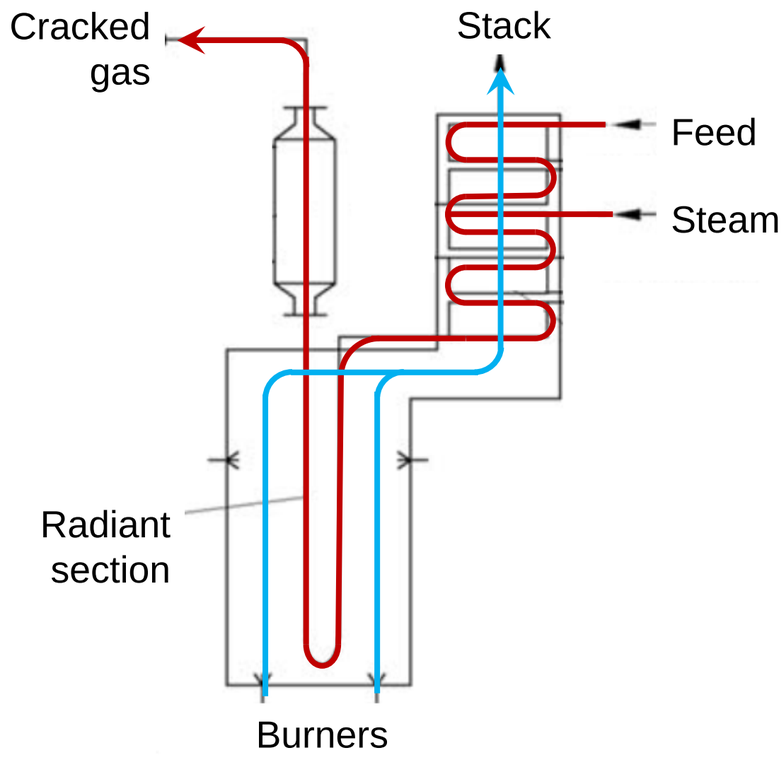
Natural gas

Bio-based feeds

Steam cracking

Consumer goods from chemical industry





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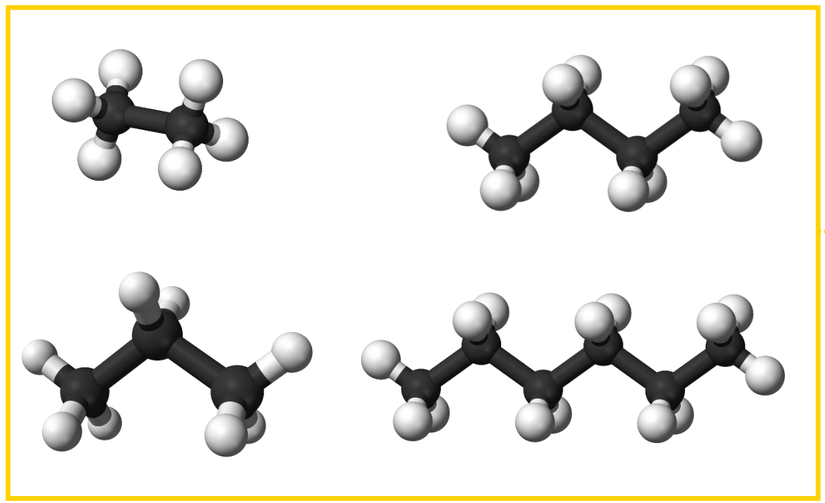
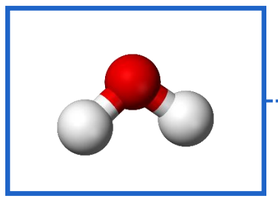
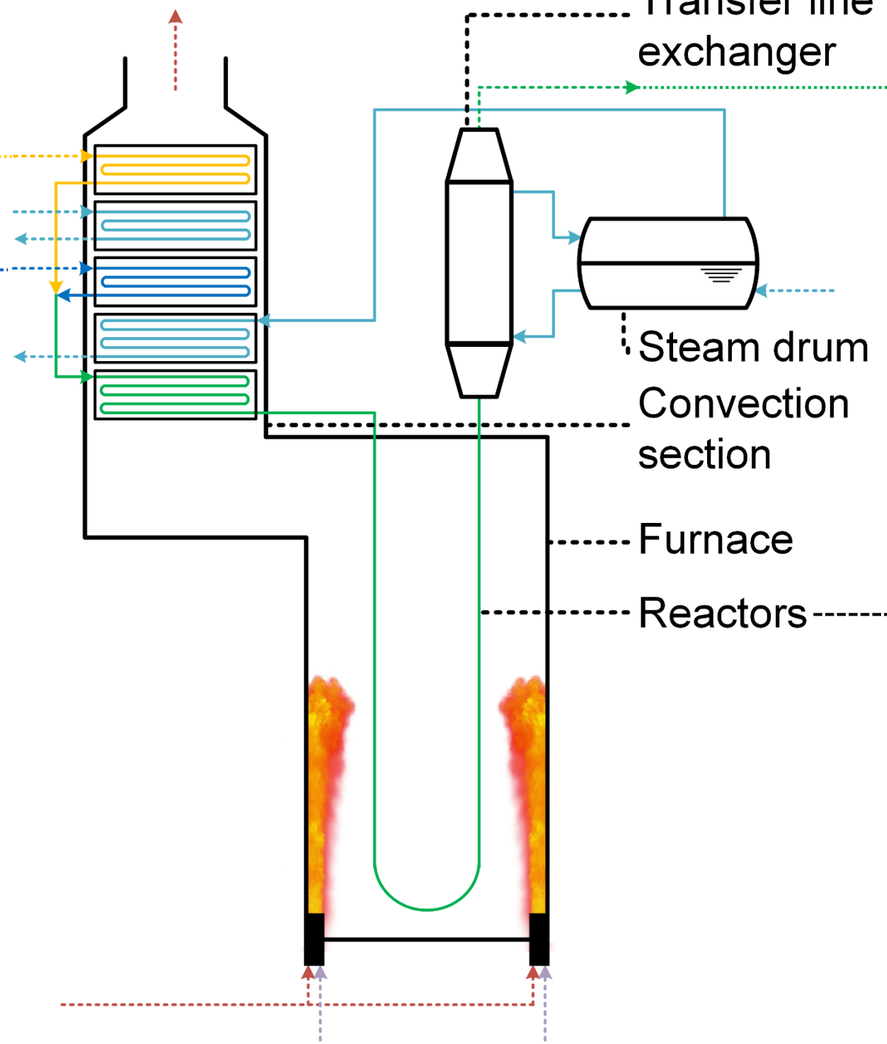
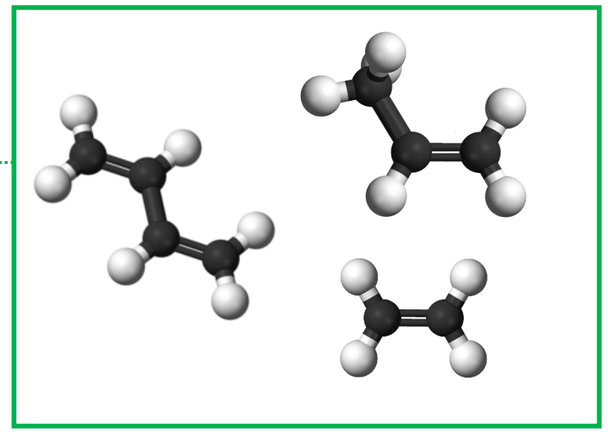
atozforex.com; pnnl.org; districtenergy.org; scade.fr; schmidt-clemens.de; Linde Group; IHS Chemical Insight

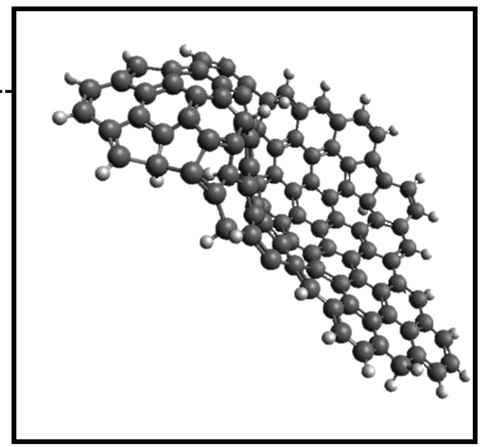
Steam cracking furnace 101











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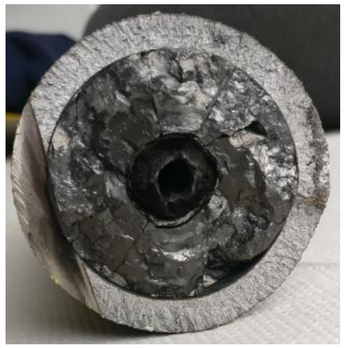
S. Vangaever, P. A. Reyniers, C. Visser, D. Jakobi, G. J. Heynderickx, G. B. Marin, *et al.*, "Computational Fluid Dynamics-Based Study of a High Emissivity Coil Coating in an Industrial Steam Cracker," *Industrial & Engineering Chemistry Research,* vol. 57, pp. 120782-120794, 12018.

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

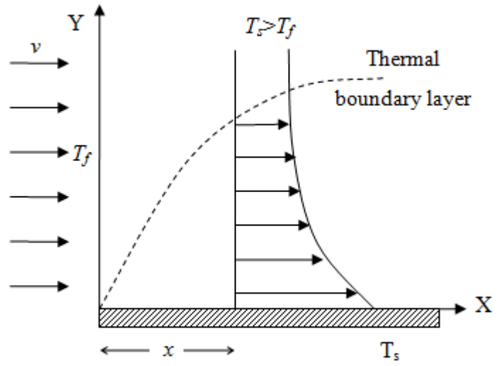


Fig.4.3: Thermal boundary layer flow past a flat surface

- ☑ Disrupt the boundary layer

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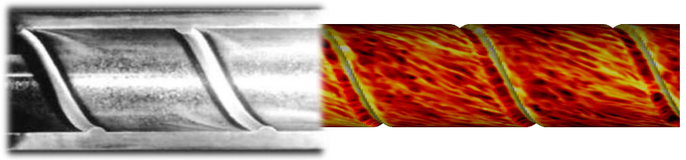
3D reactor technologies for flow modulation

Bumps or dents throughout the reactor wall

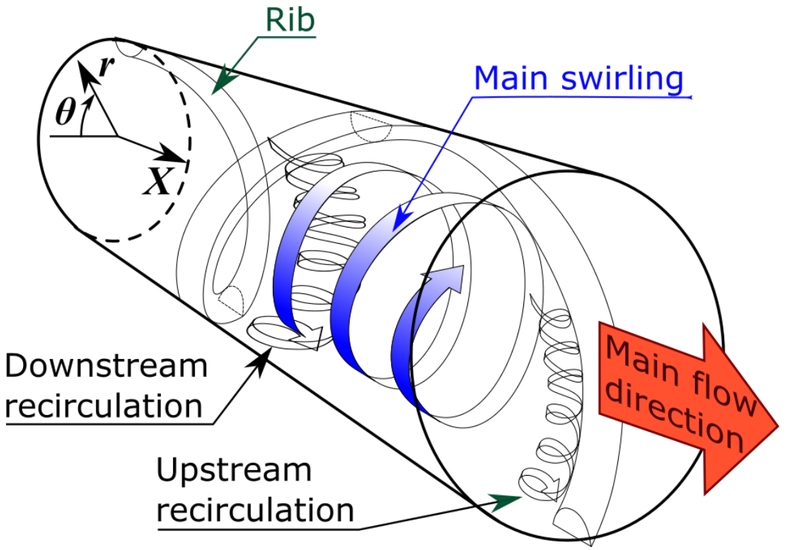


MERT

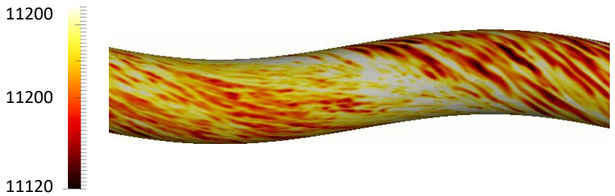
Finned tube

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, 120120, Vol 5b,* Proceedings Paper p. 11, 120120.

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.

This sounds easy but reality is different

What do you need:

1. Accurate experimental data
2. A kinetic model
3. Accurate boundary conditions
4. Properly accounting for turbulence
5. Automated geometry optimsation

LCT's Steam cracking setups

Detailed Feedstock Characterization

- ✓ Elemental analysis
- ✓ D2887 SimDist
- ✓ D11200 distillation
- ✓ GC×GC-FID/TOF-MS

- ✓ GC×GC-FID/SCD
- ✓ GC×GC-FID/NCD

Process Conditions

- ✓ High temperature on-line product sampling
- ✓ Internal standard based product quantification
- ✓ On-line GC×GC-FID/TOF-MS analyses
- ✓ On-line GC×GC-SCD/NCD analyses
- ✓ Computer controlled process conditions

Detailed Product Characterization

Pilot Plant

Bench Scale Setup

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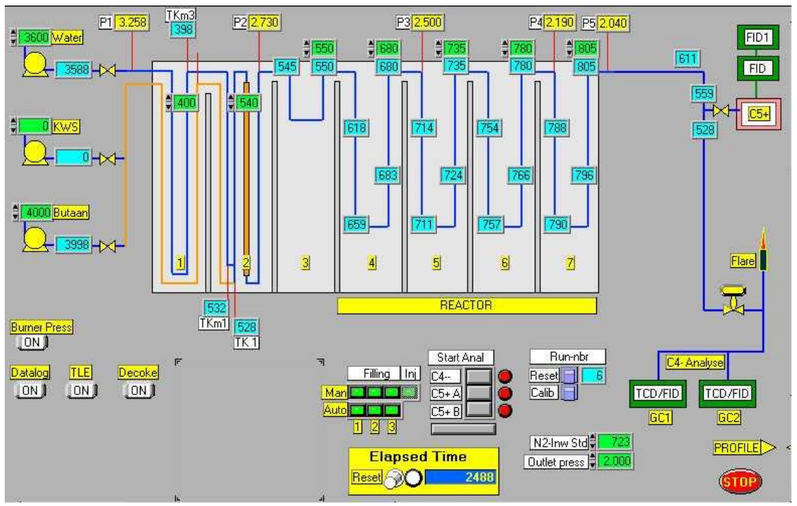
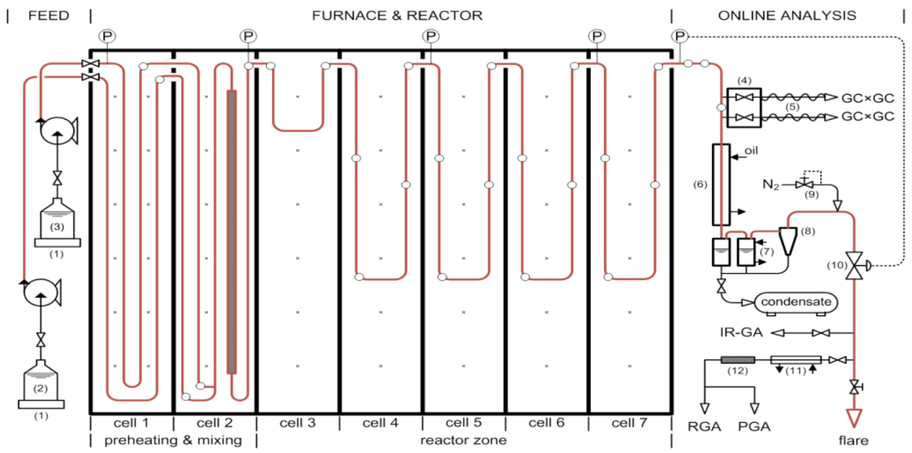
History of Pilot Plant

- Furnace is originally built in 1968
- Continuous improvement:
  - 12008: new RGA (GC)
  - 12009: first GC×GC
  - 12010: improved flow regulation
  - 12011: new TLE design
  - 12012: automation and feed section
  - upgrade
  - 12013: Online sulfur speciation
  - 12014: Online nitrogen speciation
  - 12018: new refractory/coatings and 3D coils





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LCT's Pilot plant

Extreme flexibility - the major advantage of the pilot plant

For operating companies or engineering contractors:

- To explore ...
  - **Wide range of feedstock**
    - hydrocarbons ranging from gases to heavy crude oils
  - **Wide range of operating conditions**
    - COT, dilution, COP, temperature profile, residence time ...
  - **Inhibition of coke deposition by additives**
    - in the radiant coil
    - in the transfer line heat exchanger
- To get information about
  - **expected product spectrum**
  - **optimal operating conditions**
  - **coke deposition (run length)**

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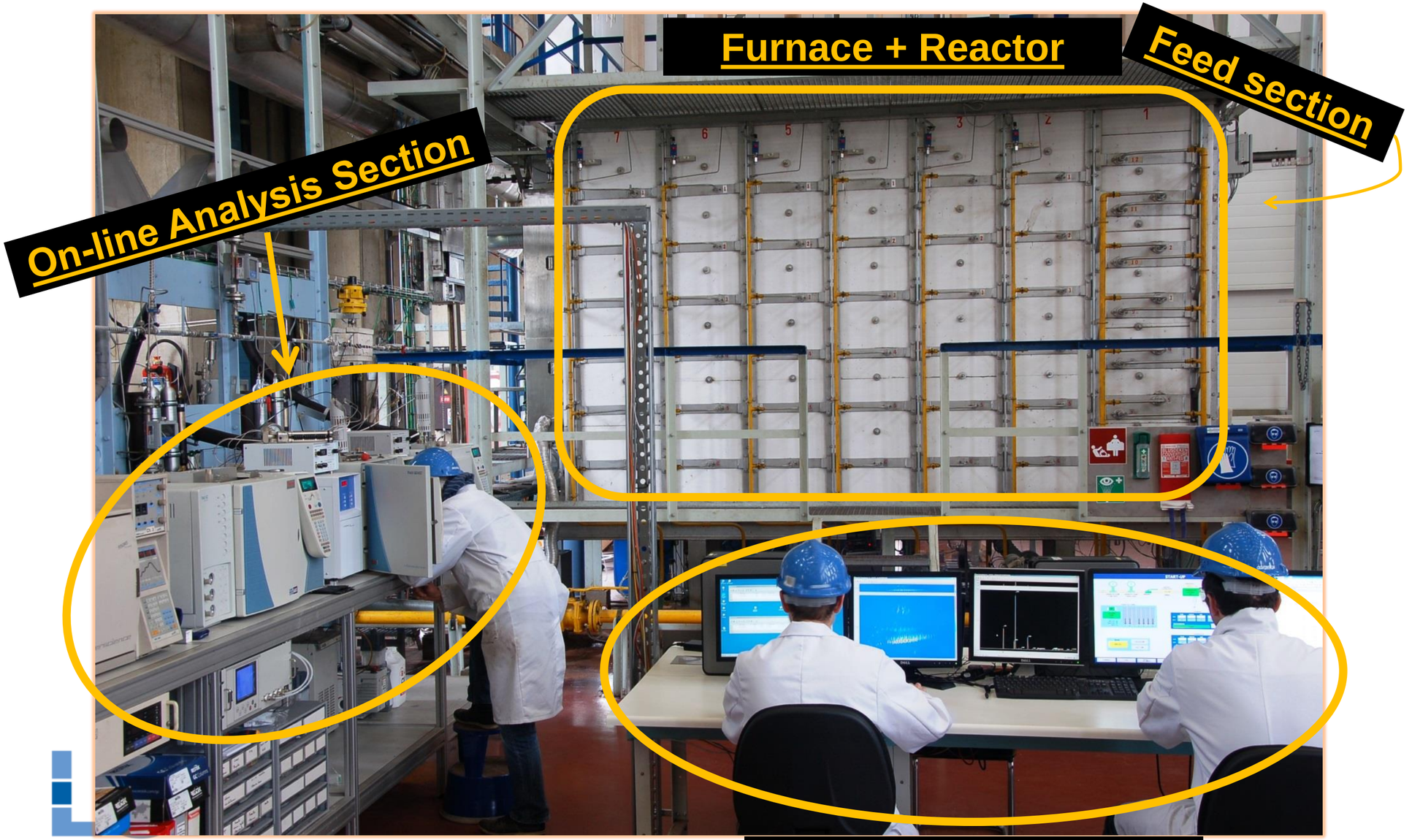
Pilot plant steam cracking setup



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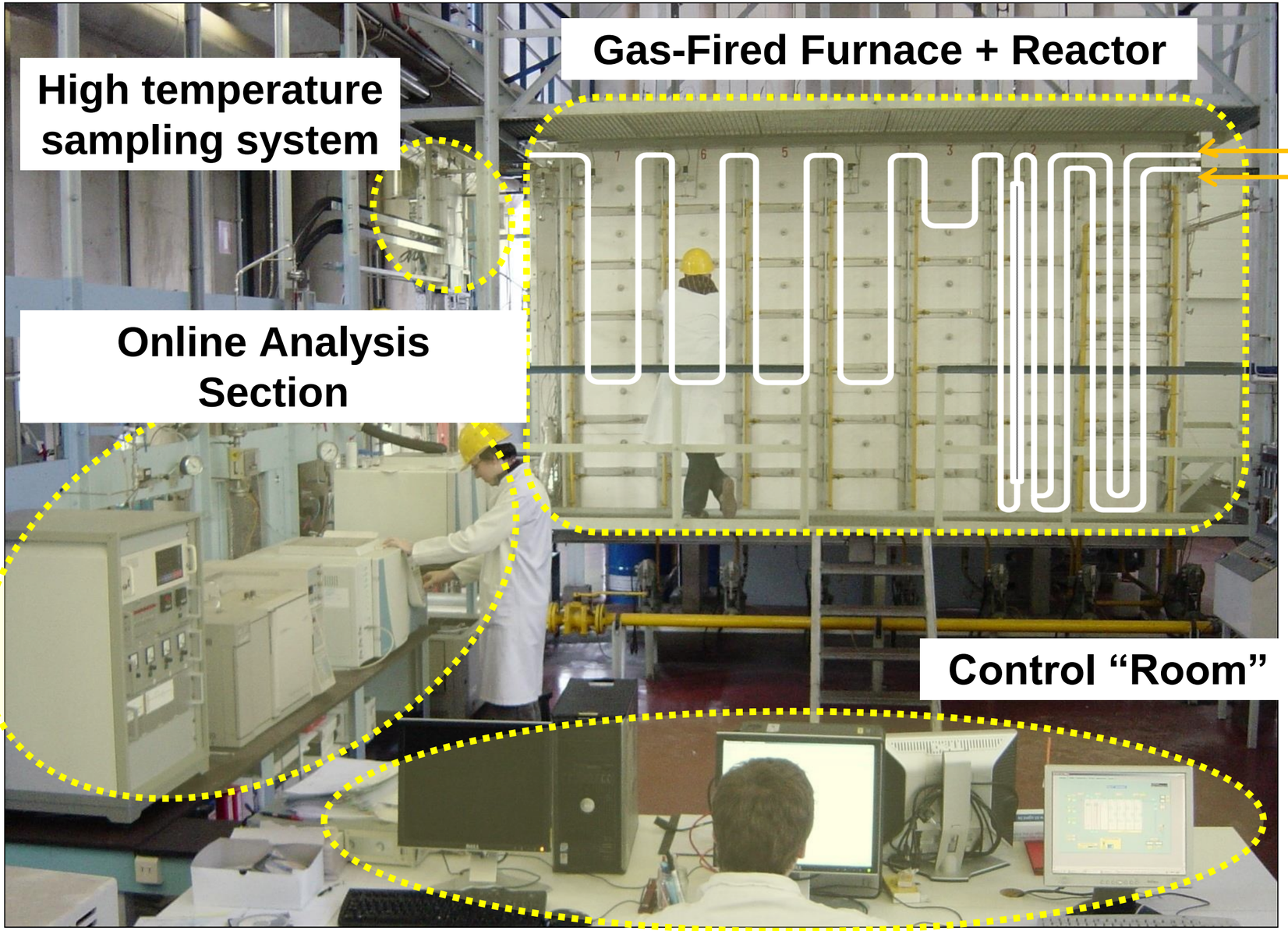
Steam cracking pilot plant



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The LCT's Pilot plant

Feed section

- compressed gases
- liquefied gases
- liquids
- waxes
- additives
- water

Features
- Coriolis based controllers
- co-cracking
- coke inhibition

Reactor section

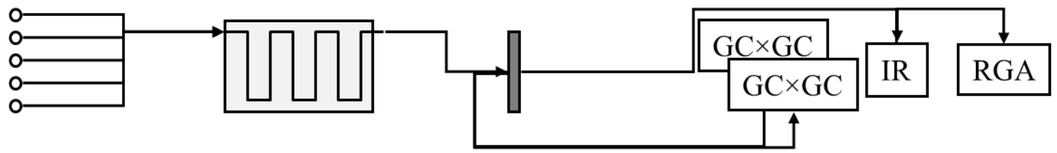
- gas fired furnace
- coil - preheating
  - mixing
  - cracking
- TLE

Features
- ...

Analysis section

- on-line sampling
- powerful analytics
  - ✓ 2 GC×GC's
    FID, SCD, NCD
  - ✓ RGA for C_{4min}
  - ✓ IR-CO/CO_2 meter

Features
- ...



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Universal On-line quantification

Nitrogen = Internal Standard

RGA (TCD) H_2 CO_2 C_2H_4 C_2H_6 C_2H_2 N_2 CH_4 CO

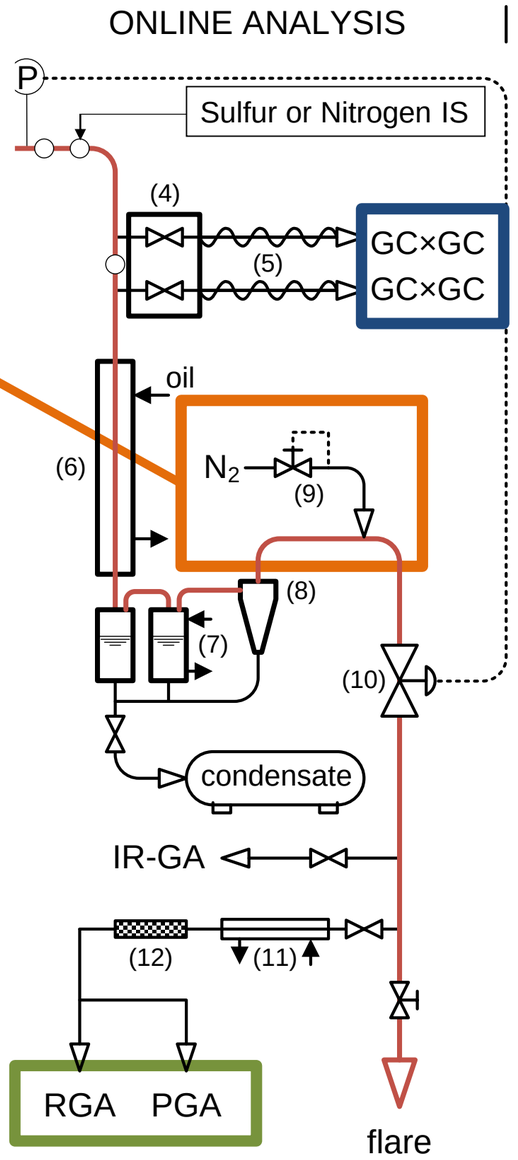
RGA (FID) CH_4 C_2 C_3 C_4

check

PGA (TCD) CO_2 C_2H_4 C_2H_6 C_2H_2 N_2 CO CH_4

GC×GC (FID) CH_4 C_2 C_3 C_4 C_5 C_6 ... C_{16}

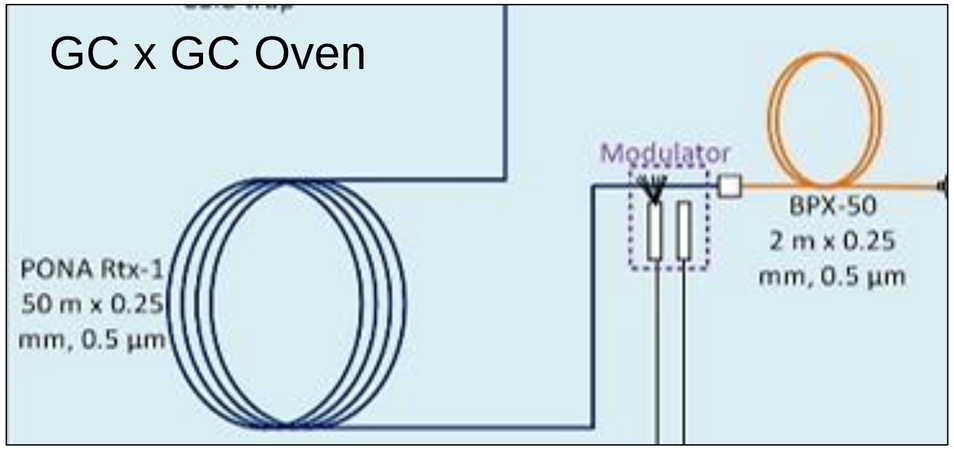
GC×GC (FID) CH_4 ... C_{25}



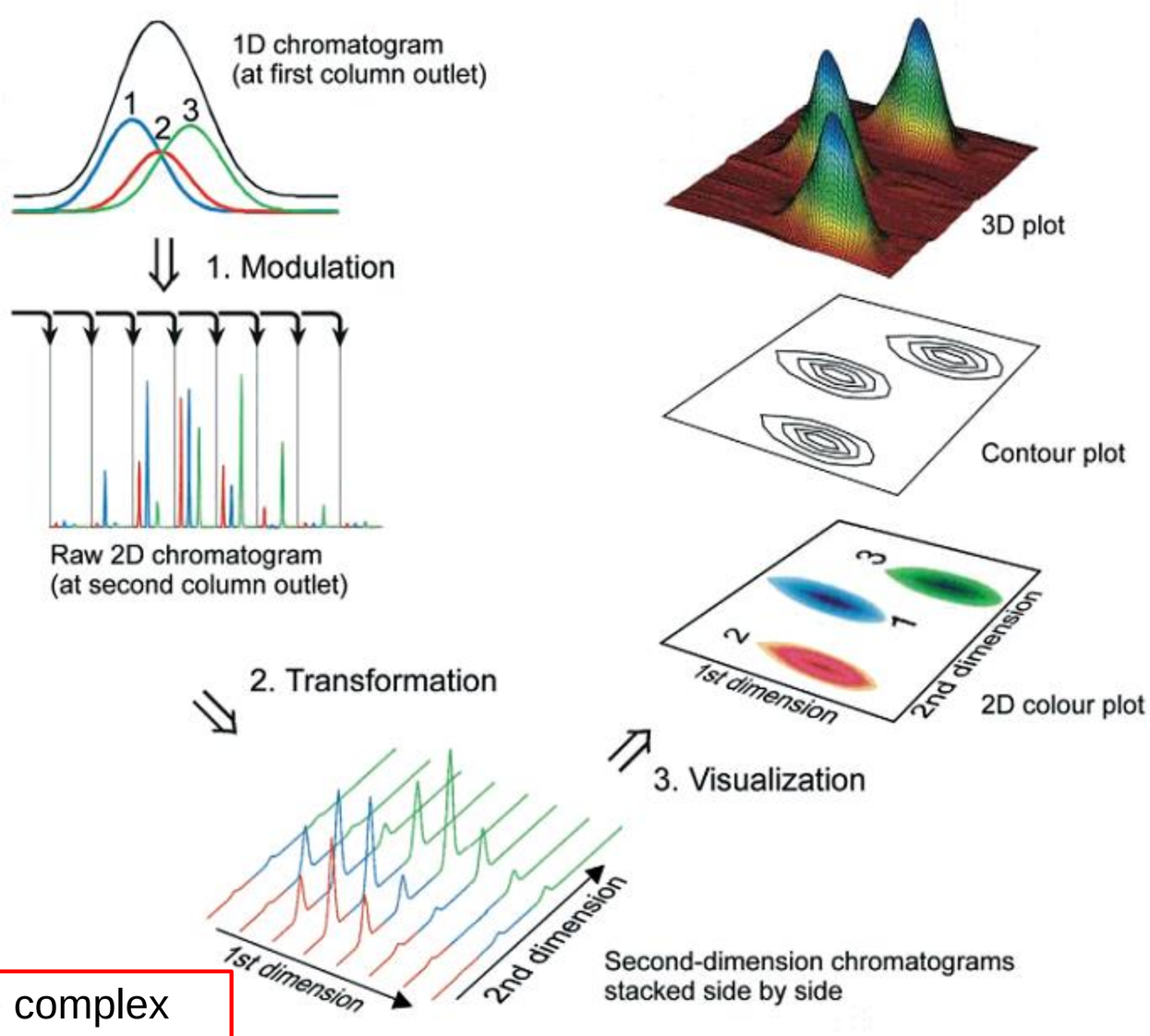
Methane = Reference Component

GC×GC temperature program: -40°C → 300°C

GC x GC Principle



Liquid CO_2



- Analytes are separated using two different columns with two different stationary phases.
- The modulator quickly traps, then "injects" the analytes from the first dimension column onto the second dimension.
- This process creates a retention plane of the 1st dimension separation x 2nd dimension separation.

Highly beneficial to analyze complex samples

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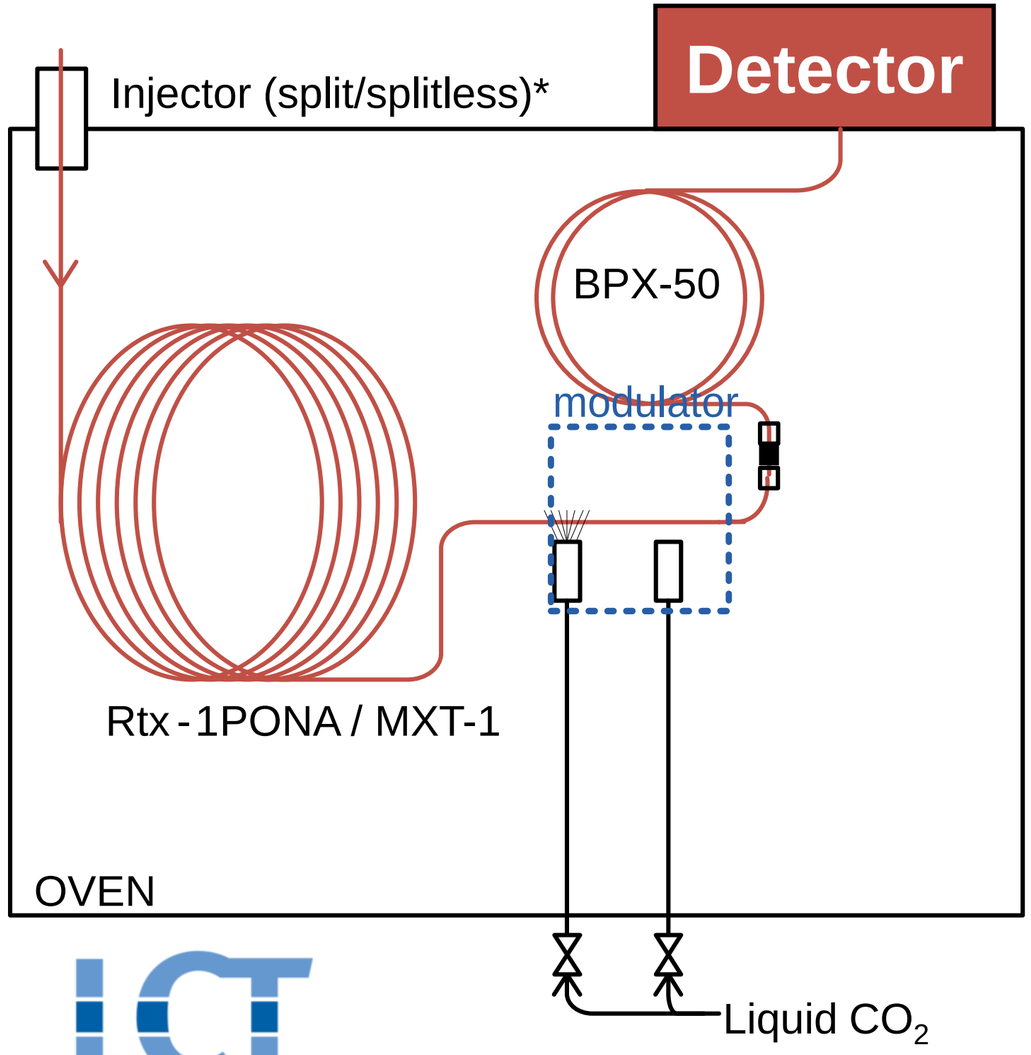
Dalluge, Beens, & Brinkman (12003), Comprehensive two-dimensional gas chromatography: a powerful and versatile analytical tool. Journal of Chromatography A. 69-108

GC×GC-TOF-MS/NCD/SCD setups



Detectors:

TOF-MS:

- Qualitative analysis

NCD:

- Quantitative analysis
- Selective to N- compounds

SCD:

- Quantitative analysis
- Selective to S- compounds

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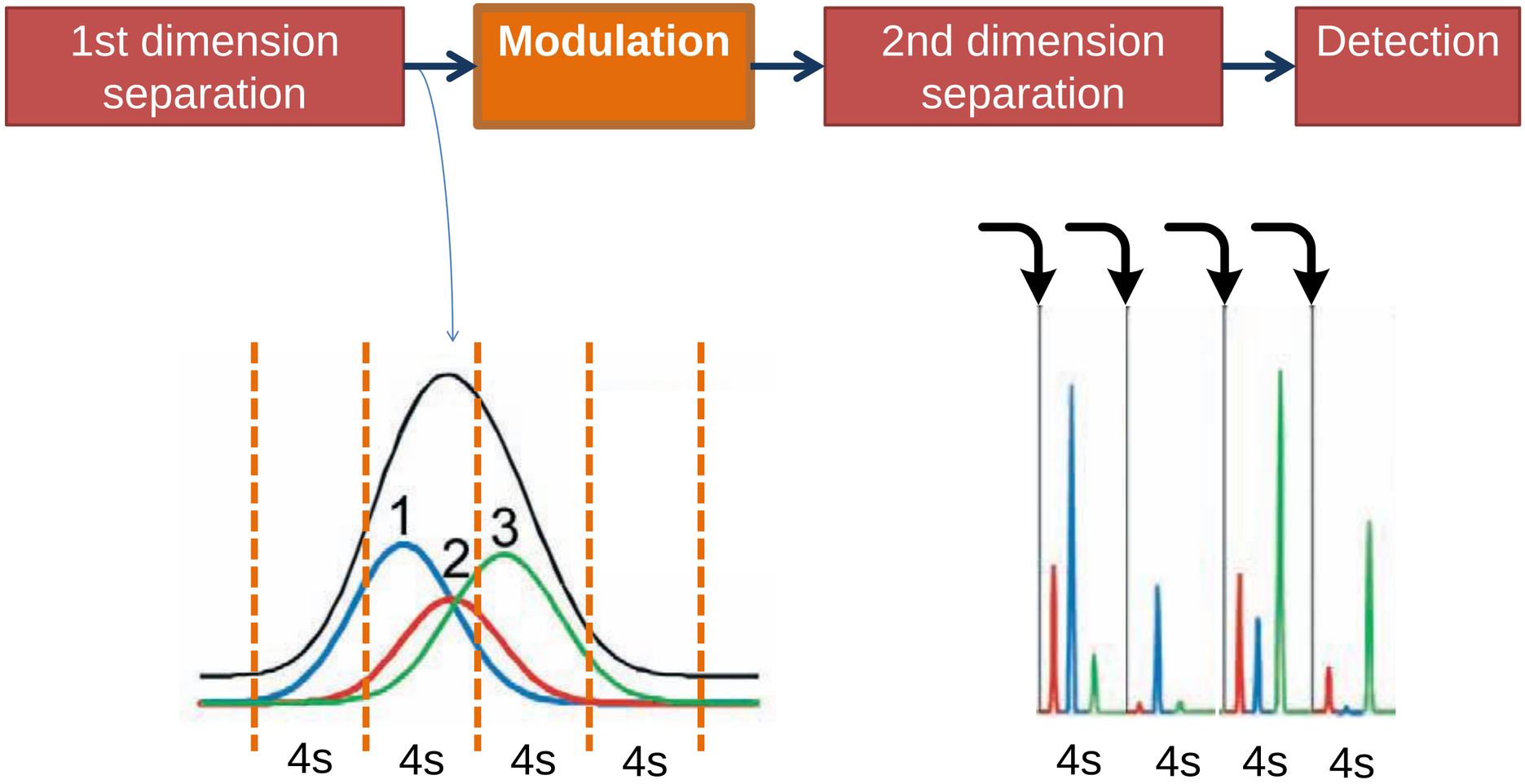
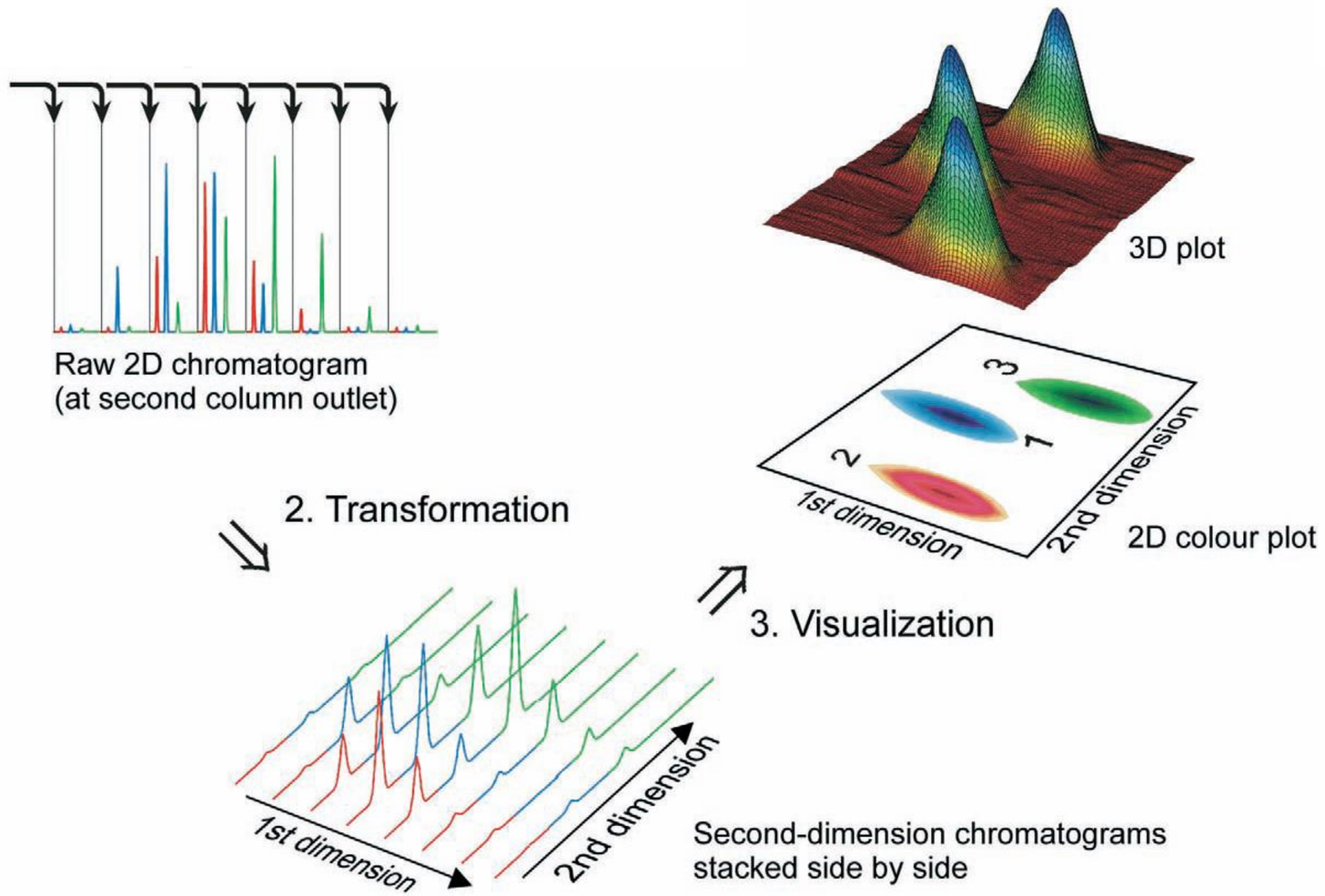
* Injector (PTV) for GCxGC-NCD

GC × GC modulation



- ✓ Enhanced Resolution
- ✓ Enhanced Signal/Noise Ratio

GC × GC data processing

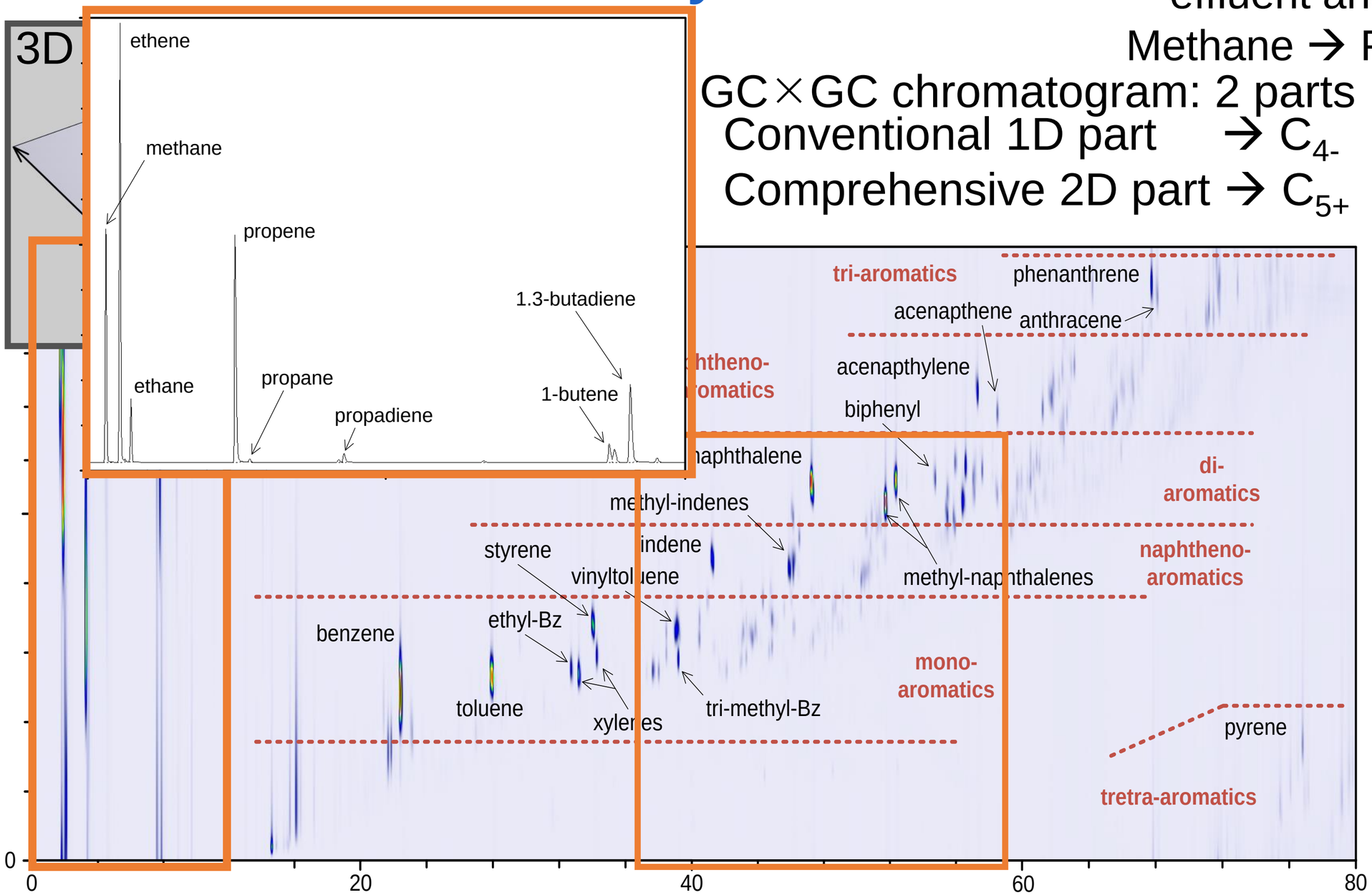


Dallüge et al., *J. Chrom. A* 12003

On line GC×GC-FID analysis

ON-LINE
effluent analysis
Methane → Pyrene+

GC×GC chromatogram: 2 parts
Conventional 1D part → C_{4-}
Comprehensive 2D part → C_{5+}



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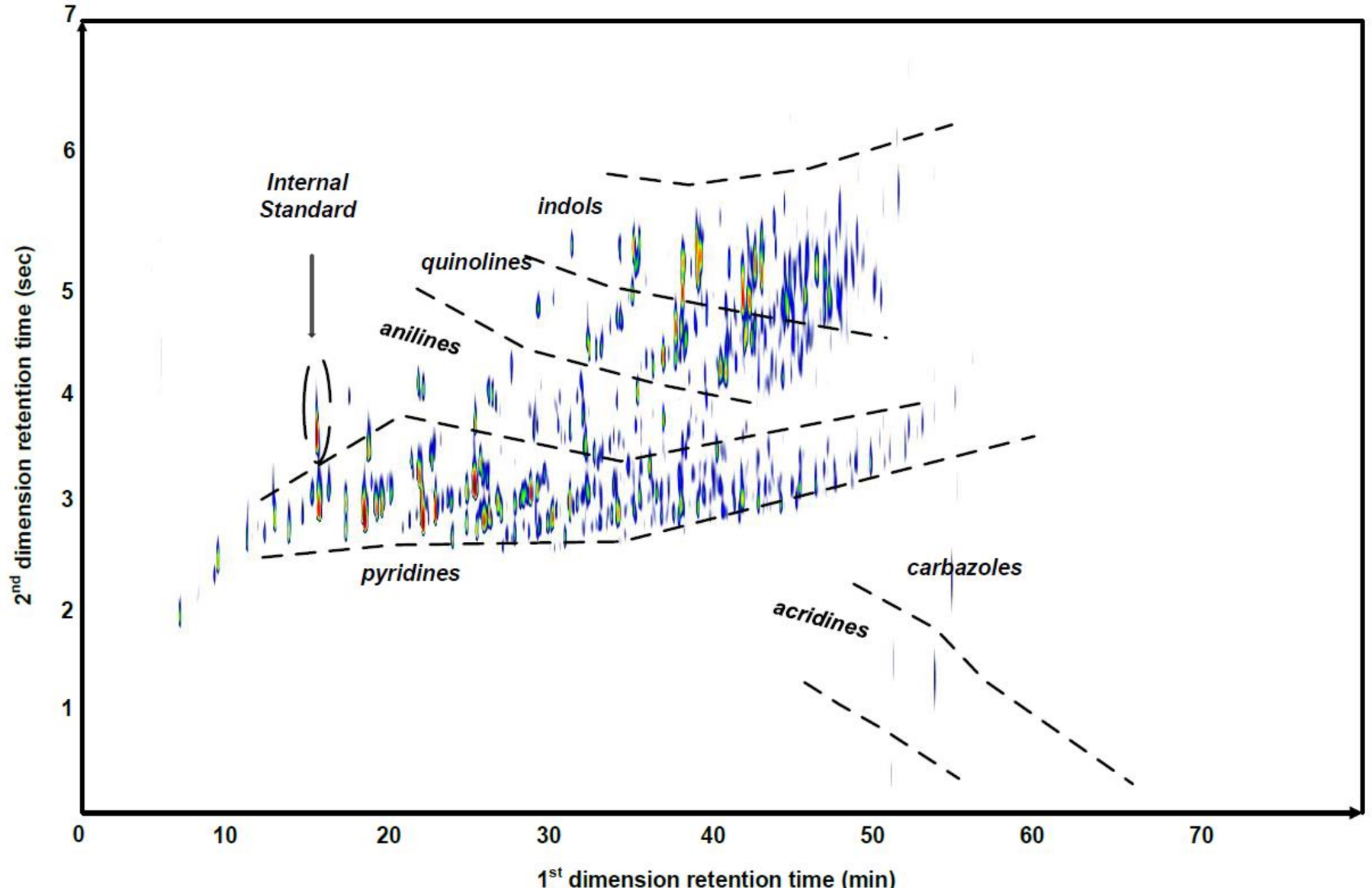
Nitrogen compounds



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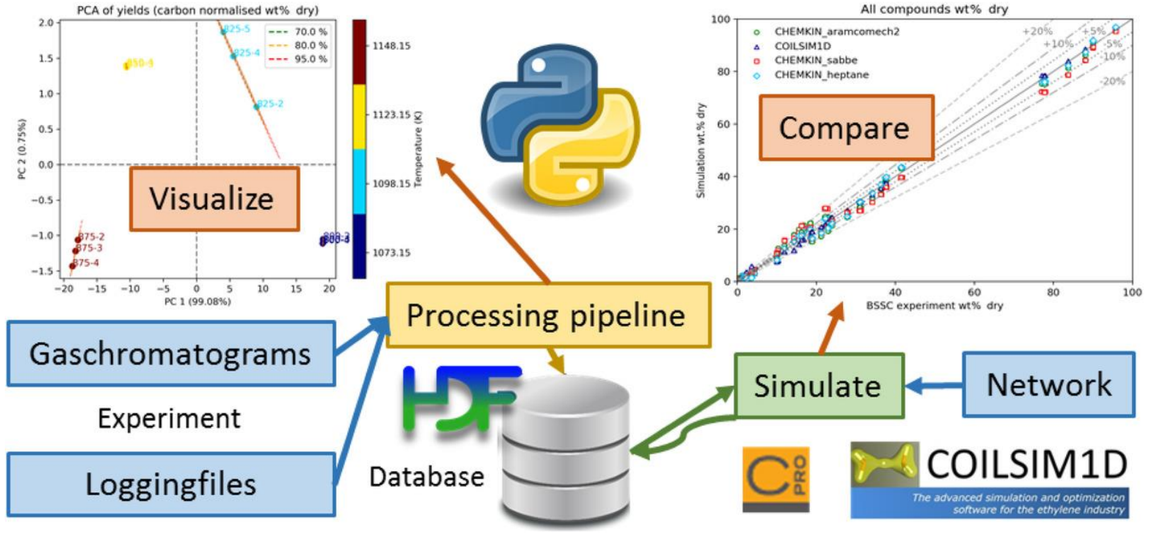
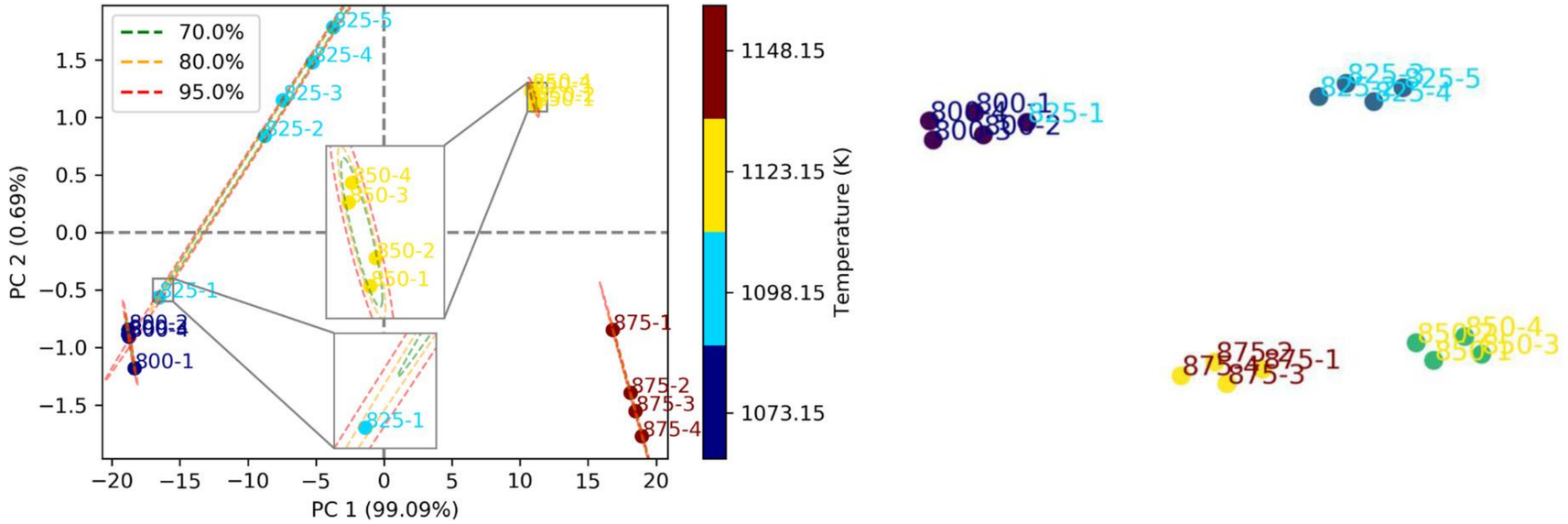
AI in Experimental Analysis – QUANTIS

- Analysis of experimental consistency
- Analysis/detection of outliers
- Improvement of experimental datasets



- PCA: consistency of experiments, outliers
- t-SNE: clustering visualization

Different colors represent datapoints from different experimental runs

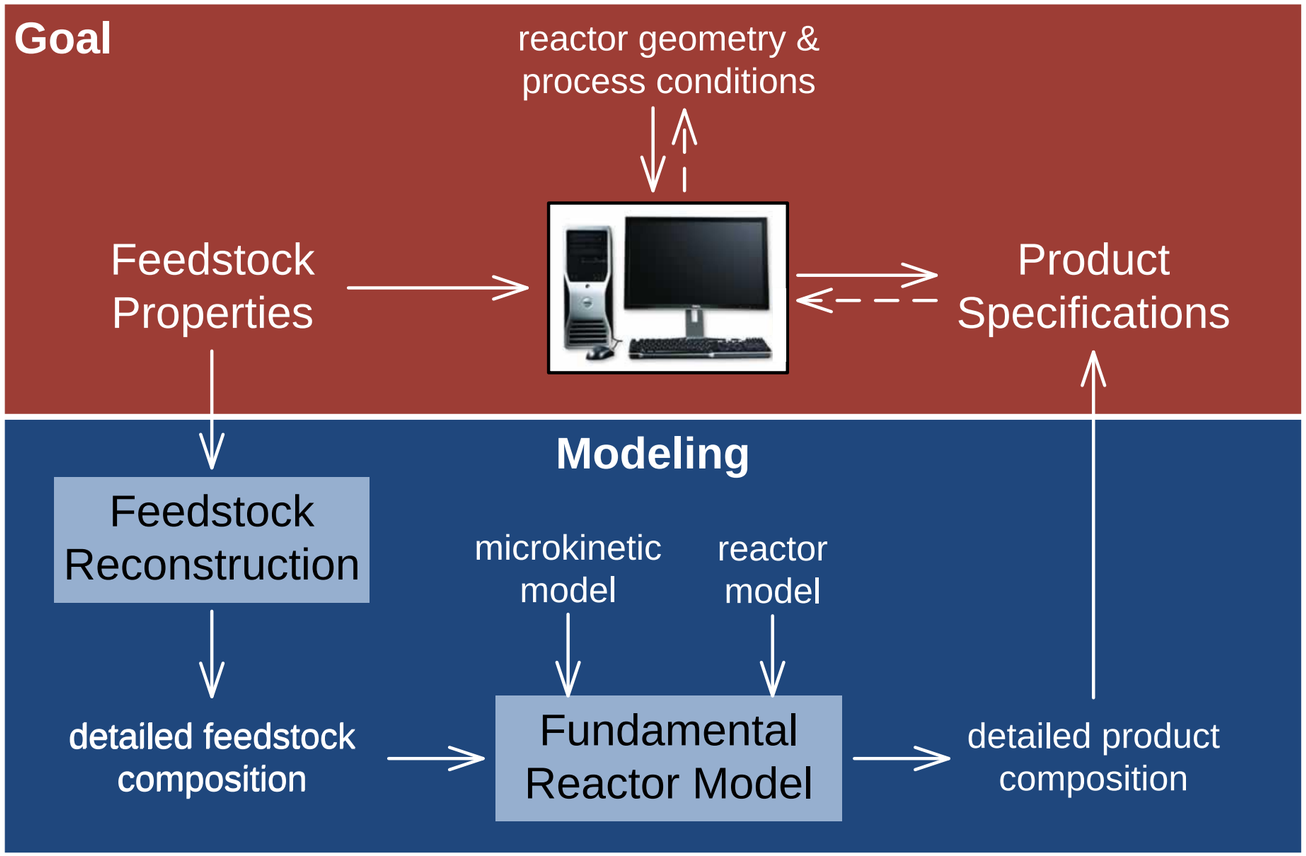


Symoens, S. H.; Aravindakshan, S. U.; Vermeire, F. H.; De Ras, K.; Djokic, M. R.; Marin, G. B.; Reyniers, M.-F.; Van Geem, K. M., QUANTIS: Data quality assessment tool by clustering analysis. *International Journal of Chemical Kinetics* **12019,** 51, (11), 872-885.

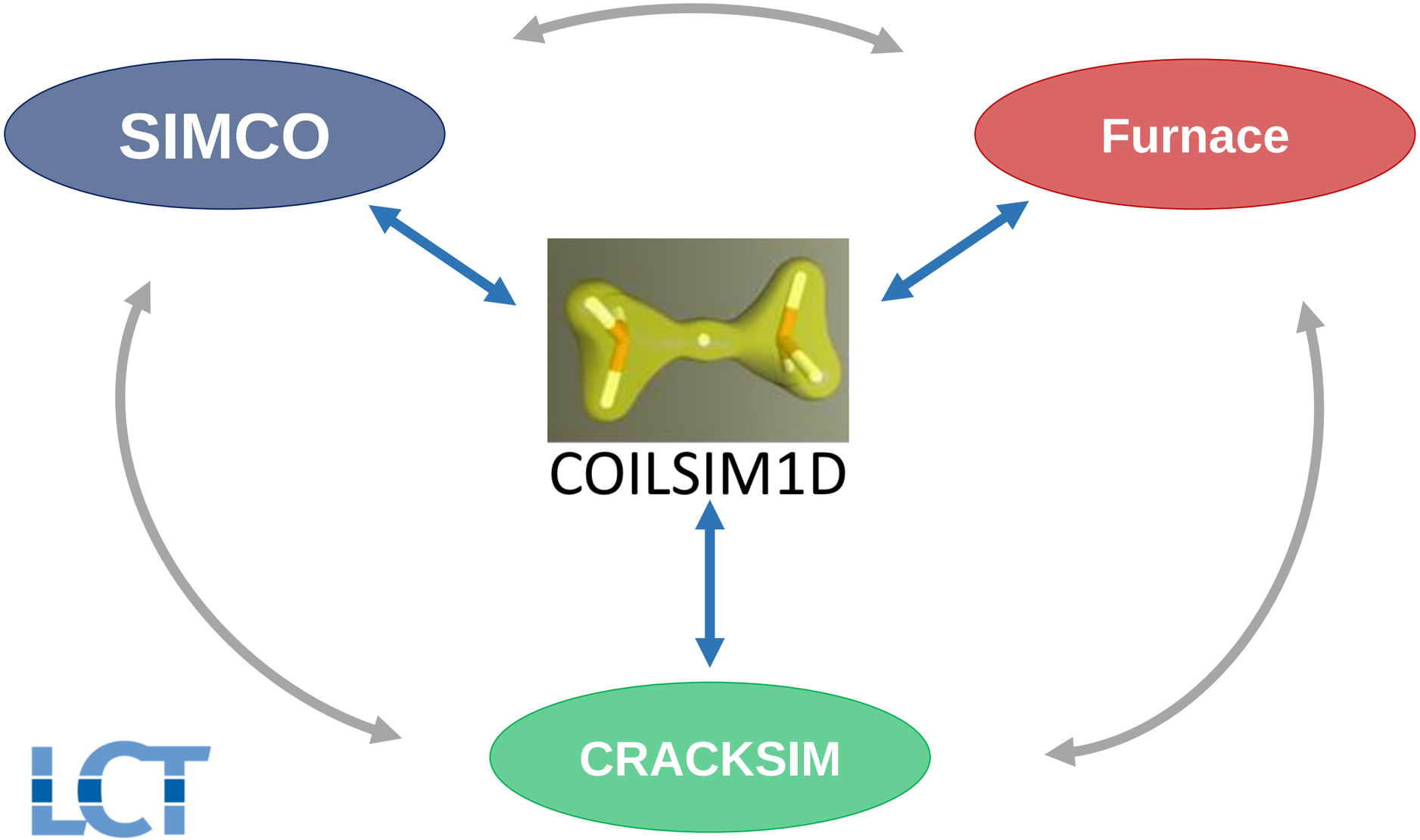
Good data was the start of COILSIM

Fundamental modeling strategy

from feed to product



Key elements of COILSIM



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SIMCO: Feedstock Reconstruction

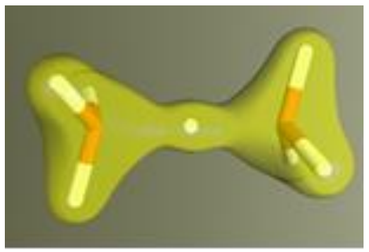
– A detailed model requires a detailed molecular composition

Bulk properties / Commercial indices

- Gaseous feeds
- Naphthas
- Gas condensates
- Kerosene
- HVGO
- VGO
- …

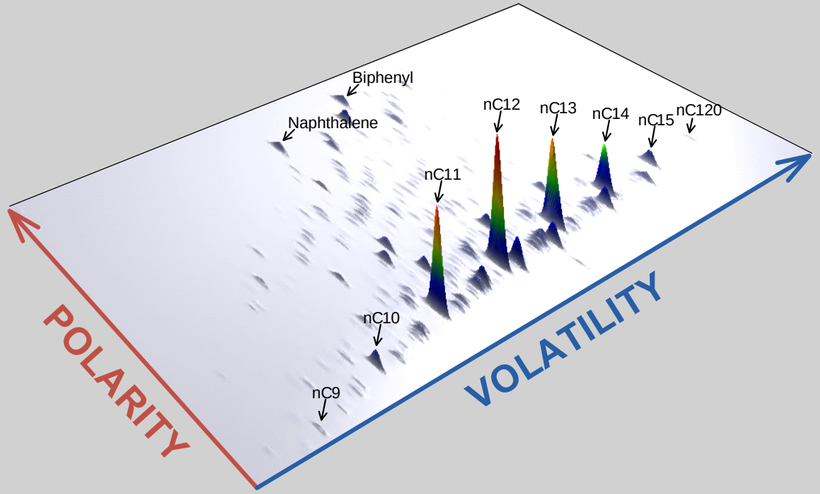
SIMCO

Molecular feed composition



COILSIM1D

Detailed product distribution



Validation by means of GCxGC

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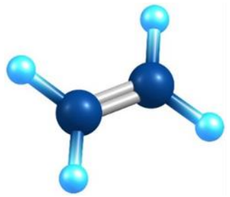
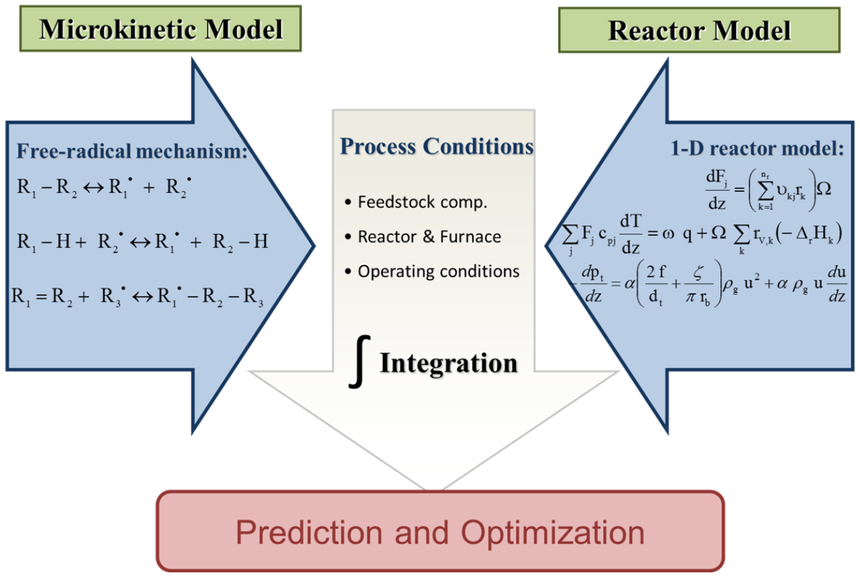
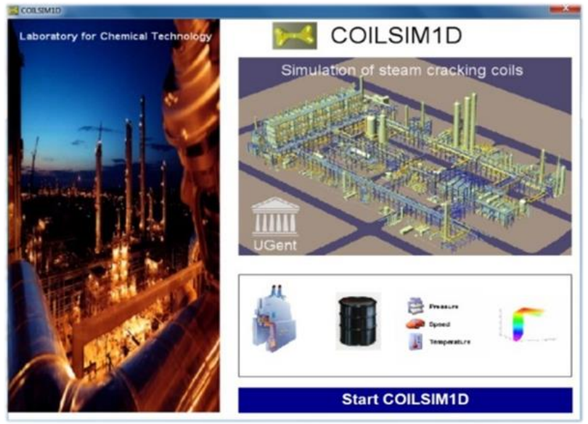
COILSIM1D



COILSIM1D





LCT Laboratory for Chemical Technology

- Broadest and most accurate kinetic model for steam cracking
  - 785+ molecules
  - 43 radicals
  - 300,000+ reactions
- Based on high level Ab initio data, and kinetics re-fitted with experimental data (pilot and industrial)
- The result of decades of expertise in independent research and modelling of thermal cracking reactions with exceptional validation facilities

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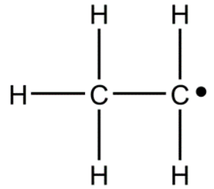
https://www.lct.ugent.be/
https://www.avgi.be/

Pyrolysis chemistry

Radical chemistry – radicals are molecules with an unpaired valence electron

for example: ethyl radical,  ,

Reactions can be classified in so-called **reaction families**:

1) **Scission**

C-C $C_1{-}C_2 \rightarrow {\bullet}C_1 + {\bullet}C_2$

C-H $C_1{-}H \rightarrow {\bullet}C_1 + {\bullet}H$

Net formation of radicals, very reactive species

2) **Hydrogen abstraction**

Intermolecular

by H• $C_1{-}H + {\bullet}H \rightarrow {\bullet}C_1 + H{-}H$

by C• $C_1{-}H + {\bullet}C_2 \rightarrow {\bullet}C_1 + C_2{-}H$

Intramolecular $\bullet C_1\text{-}(C)_n\text{-}C_2\text{-}H \rightarrow H\text{-}C_1\text{-}(C)_n\text{-}C_2\bullet$

3) **β-scission & reverse radical addition**

Intermolecular $\bullet C_1\text{-}C_2\text{-}C_3 \rightarrow C_1{=}C_2 + \bullet C_3$

$\bullet C_1\text{-}C_2\text{-}H \rightarrow C_1{=}C_2 + \bullet H$

Intramolecular $\bullet C_1\text{-}(C)_n\text{-}C_2{=}C_3 \rightarrow cy(C_1\text{-}(C)_n\text{-}C_2\bullet\text{-}C_3)$

$\bullet C_1\text{-}(C)_n\text{-}C_2{=}C_3 \rightarrow cy(C_1\text{-}(C)_n\text{-}C_2)\text{-}C_3\bullet$

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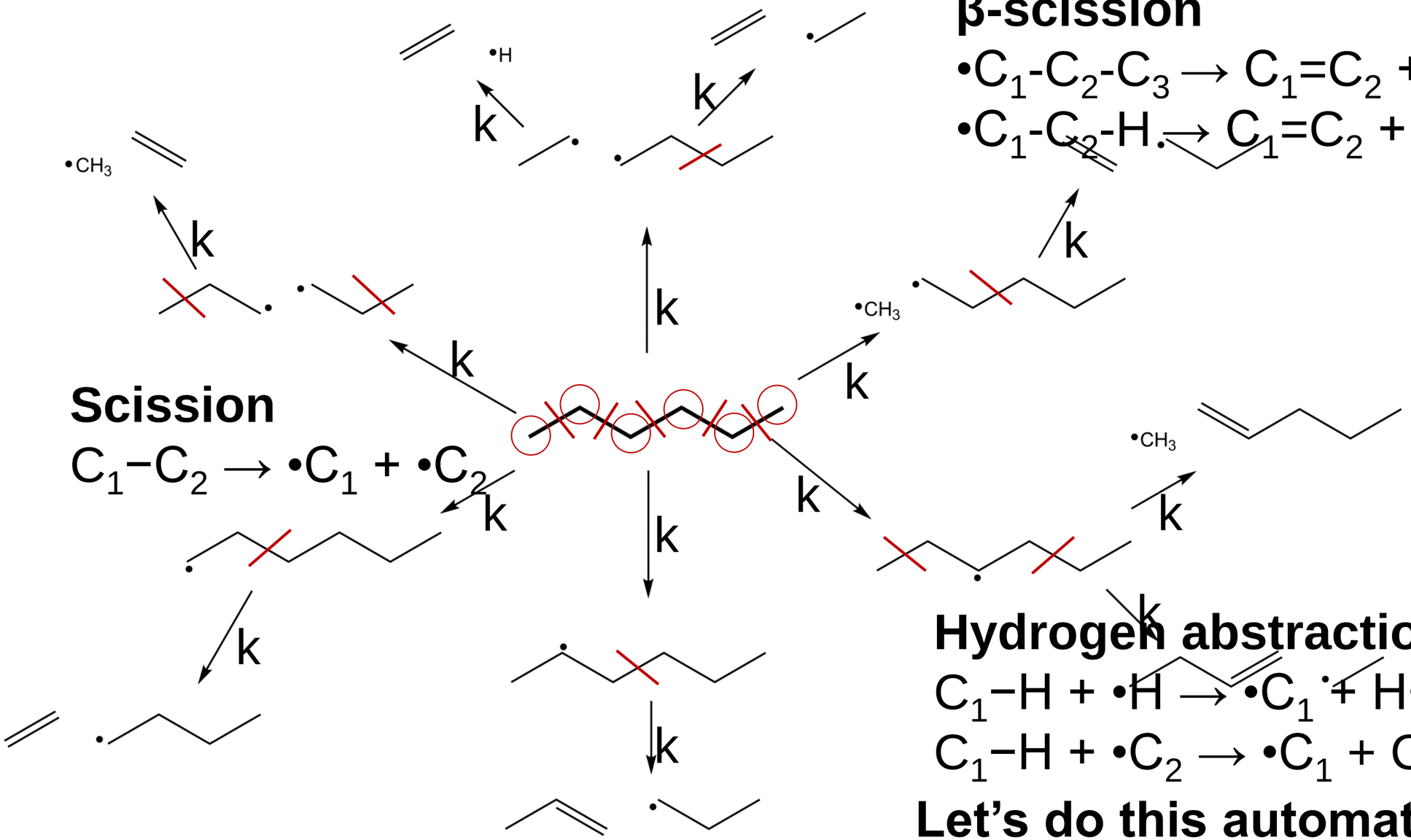
How does this occur?



β-scission

$\bullet C_1\text{-}C_2\text{-}C_3 \rightarrow C_1{=}C_2 + \bullet C_3$

$\bullet C_1\text{-}C_2\text{-}H \rightarrow C_1{=}C_2 + \bullet H$

Scission

$C_1{-}C_2 \rightarrow \bullet C_1 + \bullet C_2$

Hydrogen abstraction

$C_1{-}H + \bullet H \rightarrow \bullet C_1 + H{-}H$

$C_1{-}H + \bullet C_2 \rightarrow \bullet C_1 + C_2\text{-}H$

Let's do this automatically!

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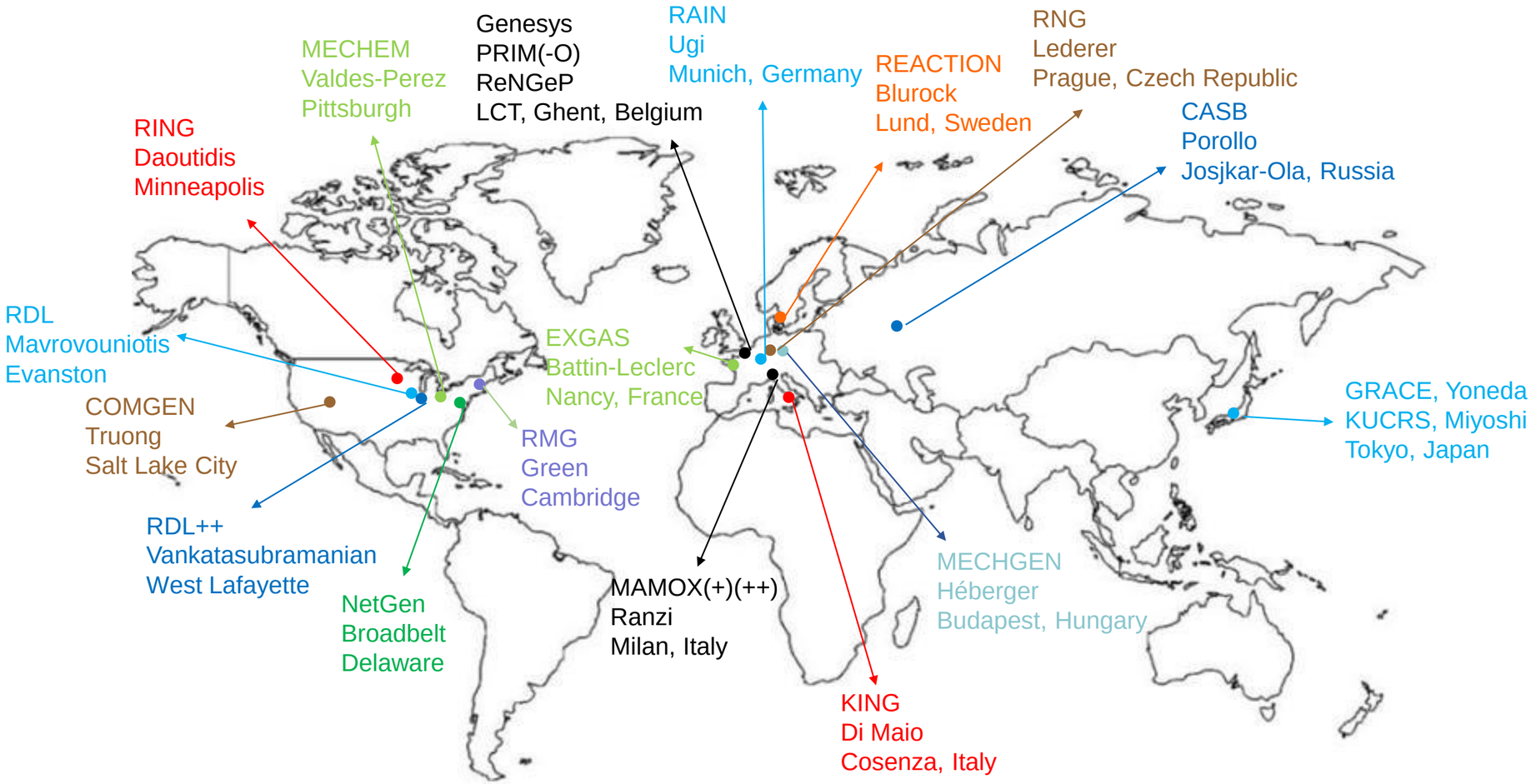
Network generators



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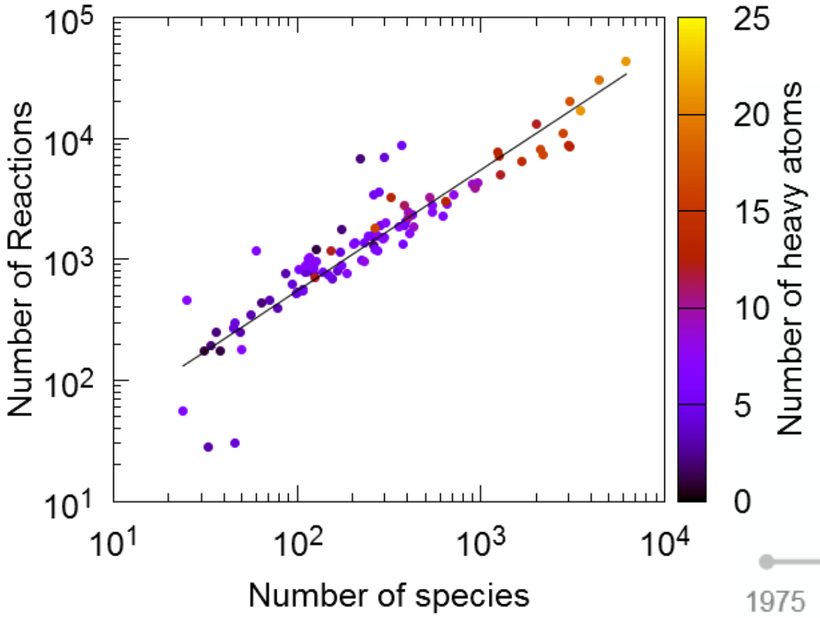
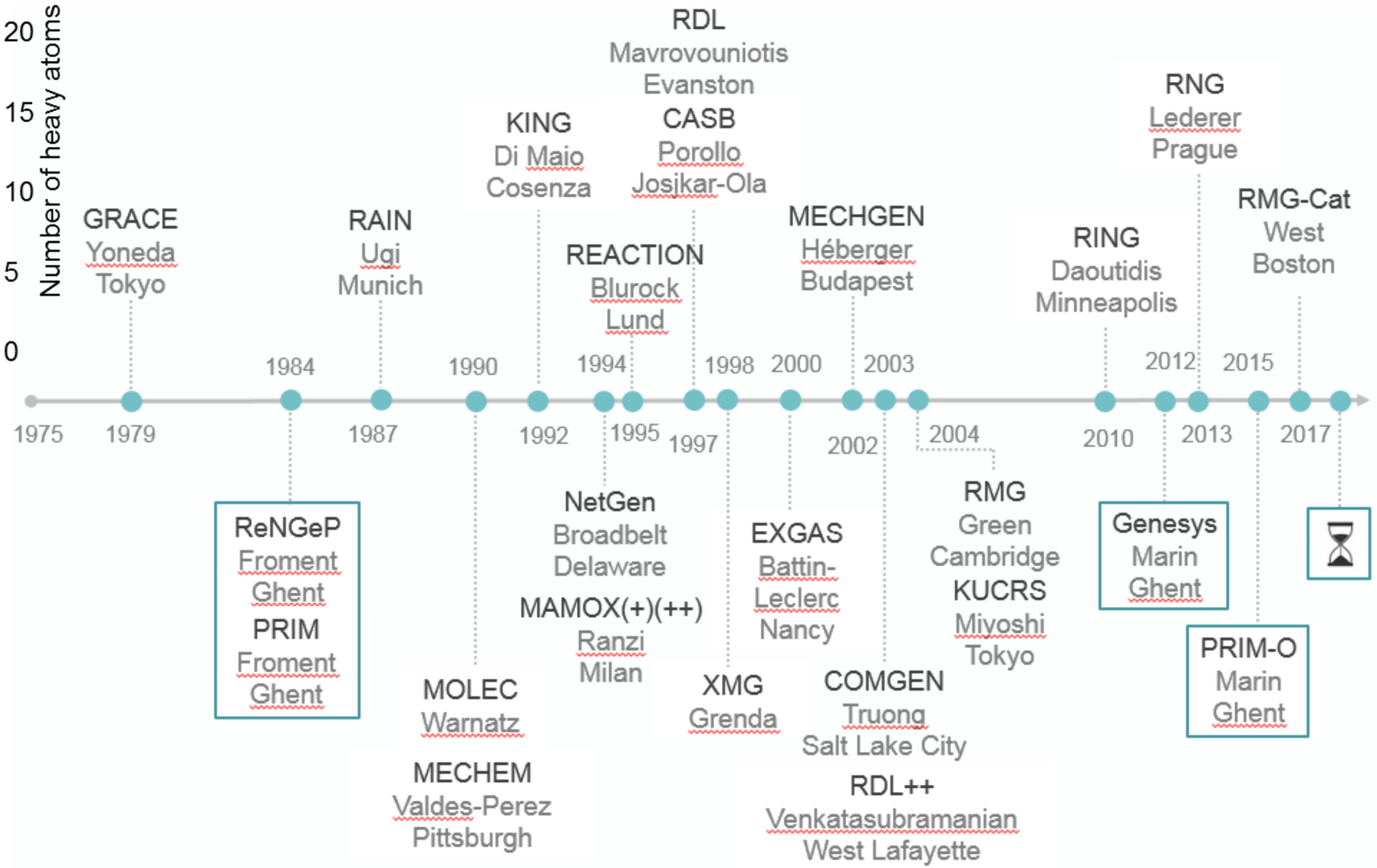
Network generation





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GENESYS : GENEration of reacting SYStems

RDKit
Open-Source Cheminformatics and Machine Learning

OpenBabel

CDK

- Computer sciences, chemistry and mathematics
- Open source projects
- Advanced species representation
- Advanced algorithms (e.g. structure based virtual screening)
- Widely applicable
  - Pharmacophore discovery
  - Protein structure elucidation
  - Quantitative structure-activity relationships

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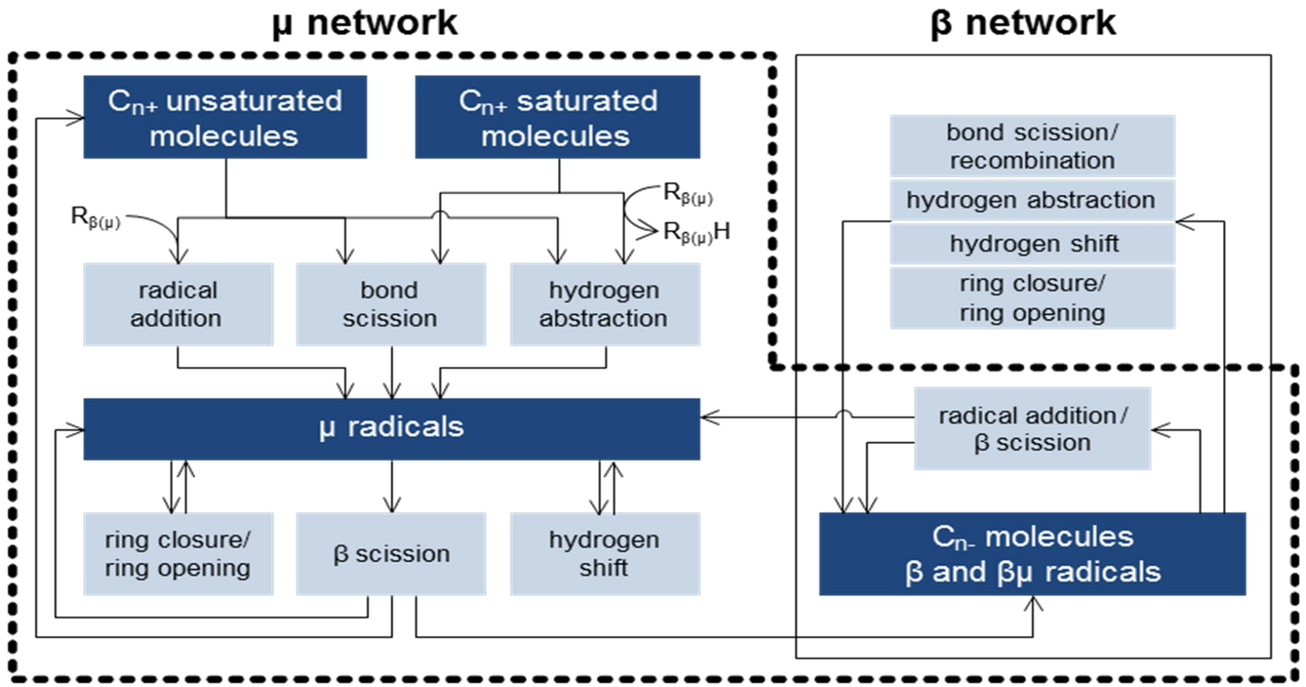
COILSIM1D ~ Microkinetic network



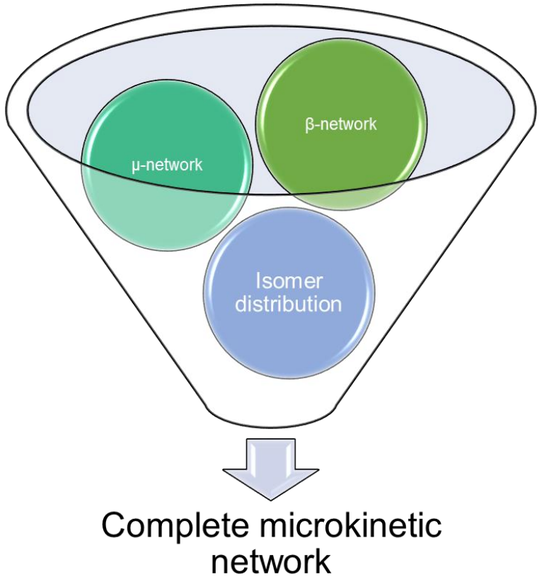
- μ network

  Application of PSSA on μ-radicals (C_{+6}) leads to a significant reduction of differential equations to solve

- β network

  Bi and monomolecular reactions of considered species

- Per feed/primary product molecule
- Per initiation mode
  - Bond scission
  - Hydrogen abstraction
  - Various radical additions
- Library of independent sub-networks



Van Geem, K. M., et al. (8508). "Challenges of modeling steam cracking of heavy feedstocks." Oil & Gas Science and Technology-Revue de l'IFP **63**(1): 79-94

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COILSIM1D ~ Microkinetic network

Thermal Cracking of Hydrocarbons

Free Radical mechanism :

- Bond-dissociation and Radical recombination

$$R_1 - R_2 \leftrightarrow R_1^{\bullet} + R_2^{\bullet}$$

- Hydrogen abstraction (intra and inter molecular)

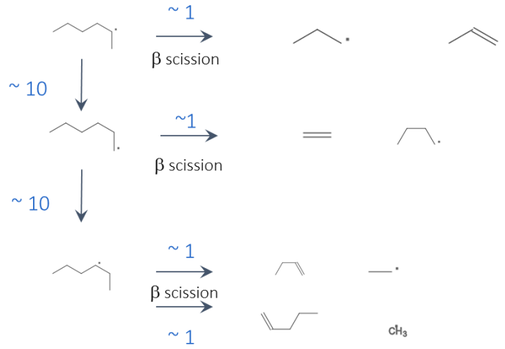
$$R_1 - H + R_2^{\bullet} \leftrightarrow R_1^{\bullet} + R_2 - H$$

- Radical addition and β-scission (intra and inter molecular)

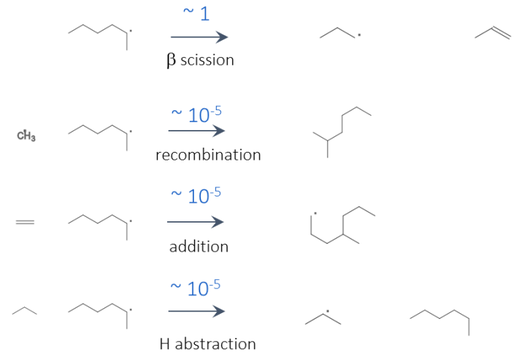
$$R_1 = R_2 + R_3^{\bullet} \leftrightarrow R_1^{\bullet} - R_2 - R_3$$

Initiation & termination

Propagation



Relative reaction rates



Orders of magnitude difference between bi- and monomolecular reactions

μ-radical Hypothesis:

"*Monomolecular reactions dominate for long chain radicals*"

Distinction between 2 sub-networks

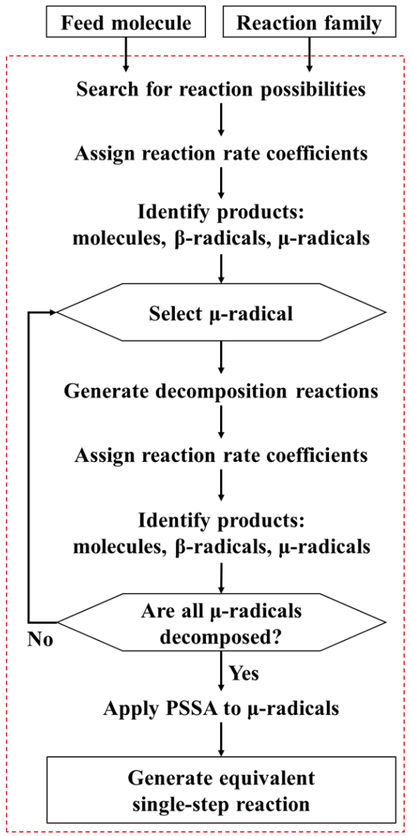
Rice, F. (1931). "The thermal decomposition of organic compounds from the standpoint of free radicals. I. Saturated hydrocarbons." Journal of the American Chemical Society **53**(5): 1959-1972.

Ranzi, E., et al. (1983). "Initial product distributions from pyrolysis of normal and branched paraffins." Ind. Eng. Chem. Fundam.;(United States) **22**(1).

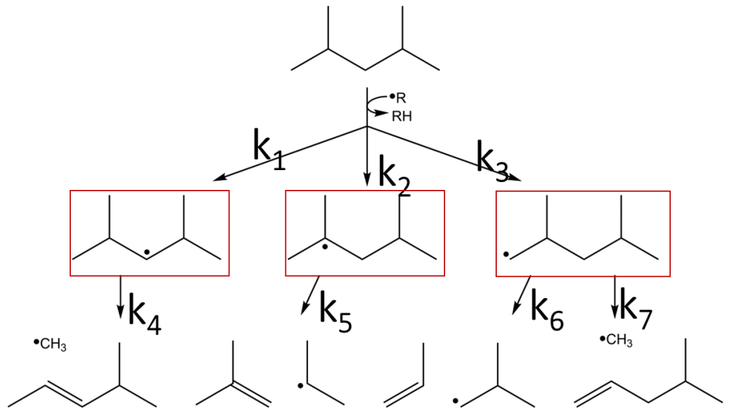
Clymans, P. and G. Froment (1984). "Computer-generation of reaction paths and rate equations in the thermal cracking of normal and branched paraffins." Computers & Chemical Engineering **8**(2): 137-142..

COILSIM1D ~ Microkinetic network

μ network



Example : H-abstraction of 2,4 dimethyl pentane



Application of Pseudo Steady State Approximation

$$\frac{dC_{\mu_1}}{dt} = k_1 C_M - k_4 C_{\mu_1} = 0$$

$$\frac{dC_{\mu_2}}{dt} = k_2 C_M - k_5 C_{\mu_2} = 0$$

$$\frac{dC_{\mu_3}}{dt} = k_3 C_M - (k_6+k_7) C_{\mu_3} = 0$$

Solving towards C_{μ_i}

$$C_{\mu_1} = \frac{k_1}{k_4} C_M$$

$$C_{\mu_2} = \frac{k_2}{k_5} C_M$$

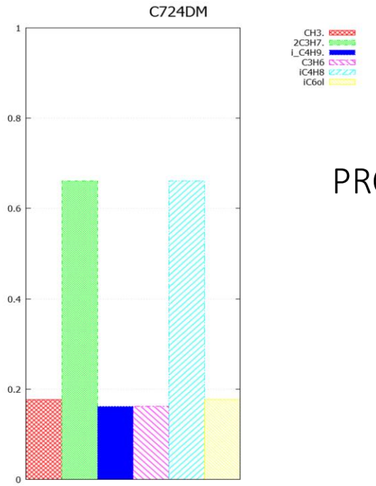
$$C_{\mu_3} = \frac{k_3}{k_6 + k_7} C_M$$

$$R_{fO} = k_5 C_{\mu_2} = k_5 \frac{k_2}{k_5} C_M \qquad R_{fR} = k_6 C_{\mu_1} = k_6 \frac{k_3}{k_6 + k_7} C_M$$

So-called PRC'S

$$feed \rightarrow \sum_{j=1}^{n_{ol}} \frac{k^{pseudo}(O_j)}{\sum_i^r k_i} + \sum_{j=1}^{n_{rad}} \frac{k^{pseudo}(\beta_j)}{\sum_i^r k_i}$$

Equivalent single step reaction



PRC'S at 800°C

De Bruycker, R., et al. (85120). "Steam cracking of bio-derived normal and branched alkanes: Influence of branching on product distribution and formation of aromatics." Journal of Analytical and Applied Pyrolysis 122(Supplement C): 468-478.

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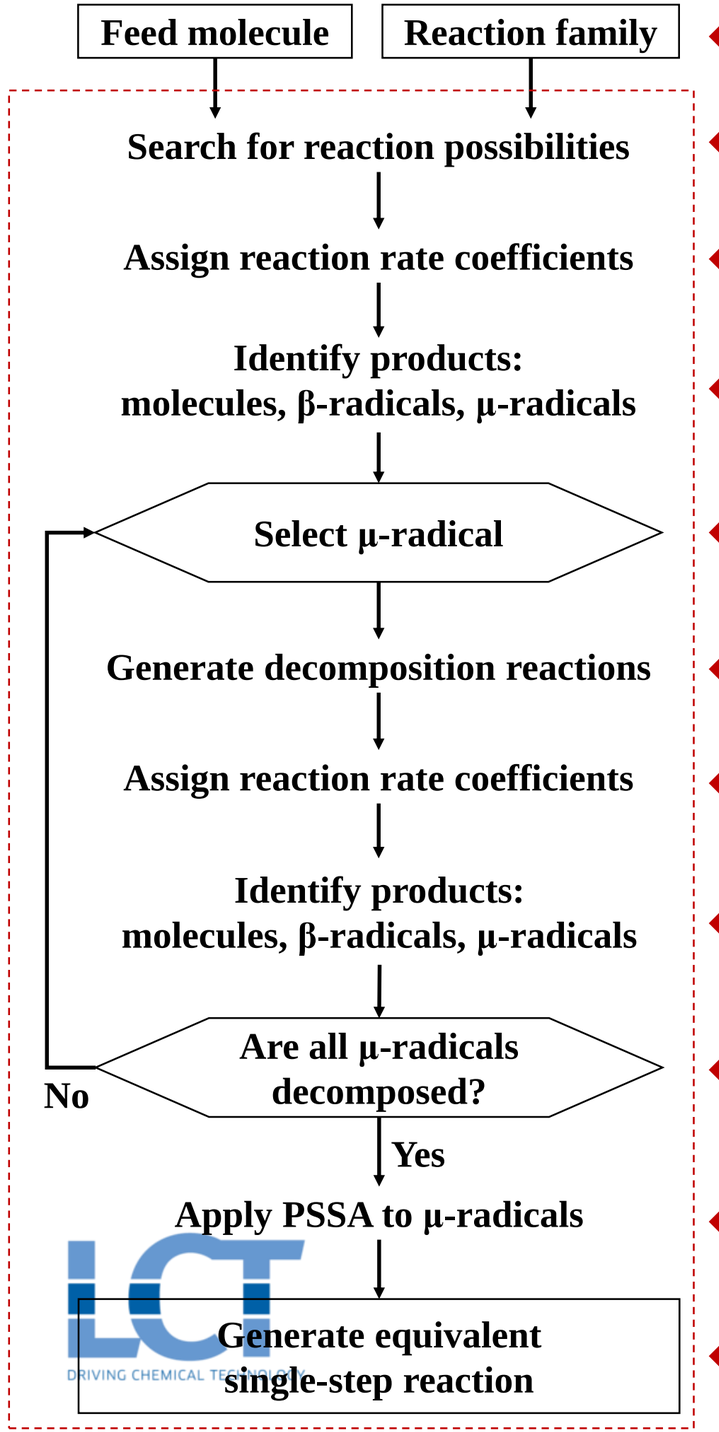
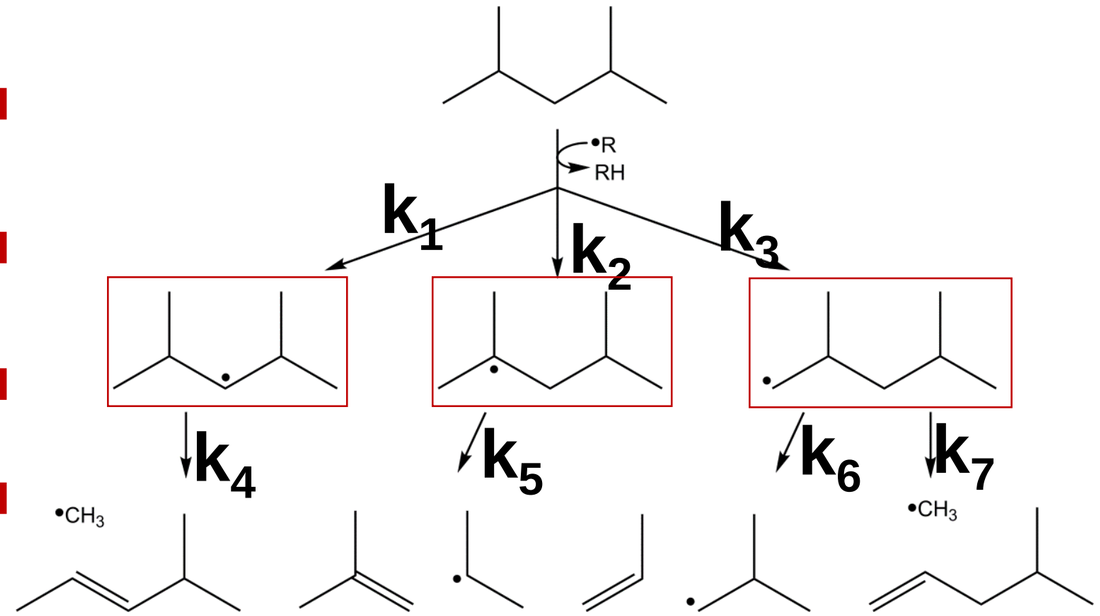
PRIM-O algorithm





$$\mathrm{CC(C)CC(C)C} + \bullet\,\mathrm{R} \xrightarrow{k_1+k_2+k_3} \mathrm{RH} + \frac{k_1}{k_1+k_2+k_3}\,\mathrm{CC=CC(C)C} + \frac{k_2}{k_1+k_2+k_3}\,(\mathrm{IC_4H_8} + \mathrm{CC}\bullet\mathrm{C}) + \frac{k_3}{k_1+k_2+k_3}\,\frac{k_6}{k_6+k_7}\,(\bullet\,\mathrm{IC_4H_9} + \mathrm{C_3H_6}) + \frac{k_3}{k_1+k_2+k_3}\,\frac{k_7}{k_6+k_7}\,\mathrm{C=CCC(C)C} + \left(\frac{k_1}{k_1+k_2+k_3} + \frac{k_3}{k_1+k_2+k_3}\,\frac{k_7}{k_6+k_7}\right) CH_3$$

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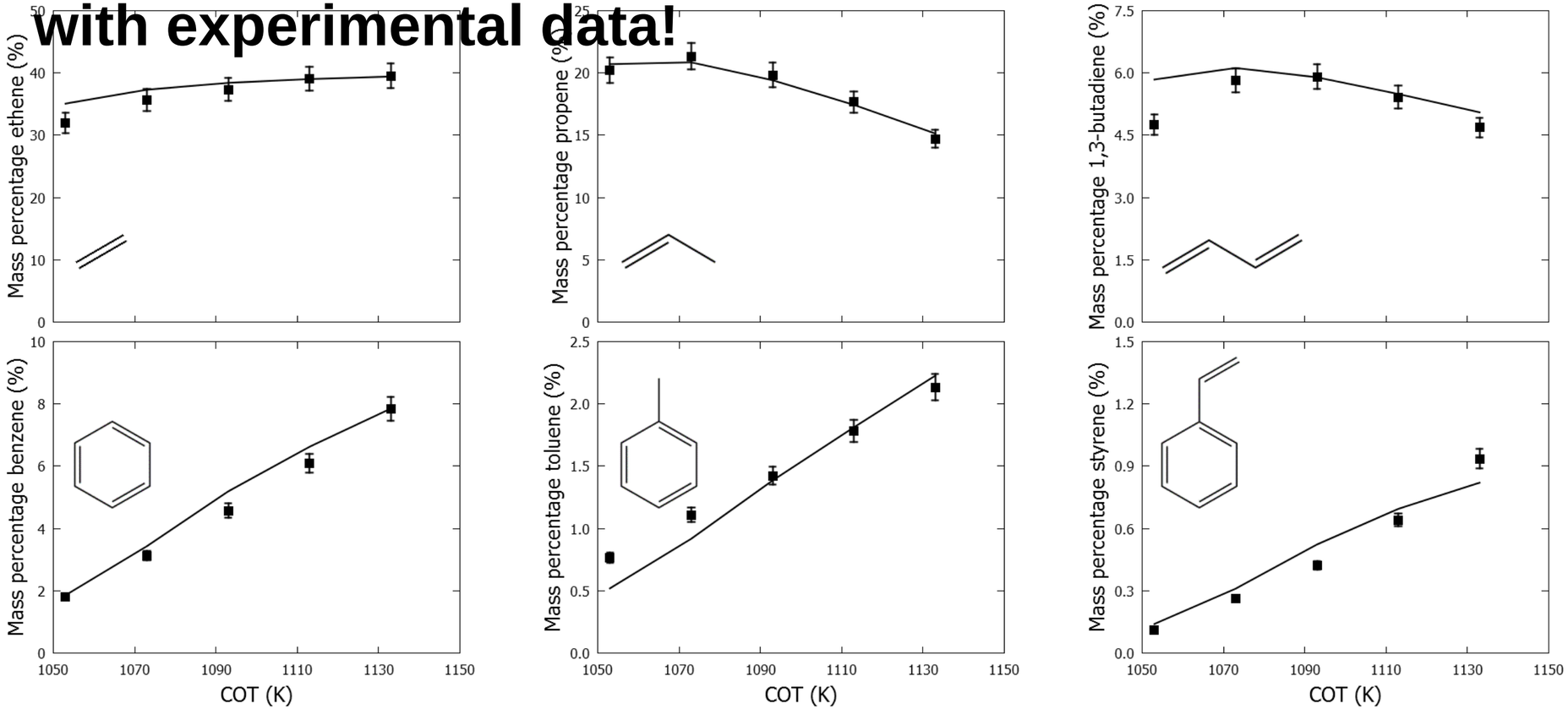
How accurate is our kinetic model?

Validation by comparing kinetic model predictions with experimental data!



Experimental yields during steam cracking of bio-derived hydrocarbons

Feedstock composition: $MW_{average}$ = 230g/mol 51wt% normal alkanes – 49wt% branched alkanes

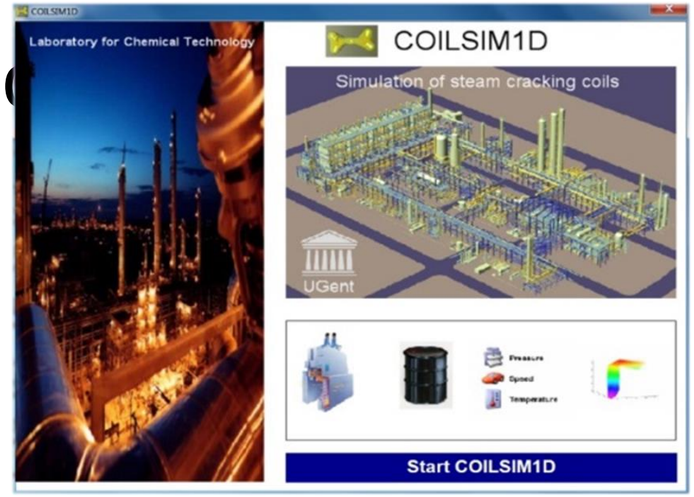
$F_{HC,0}$ = 0.04 g/s, $F_{H2O,0}$ = 0.02 g/s, P = 0.17 MPa

Model calculated yields, calculated using CHEMKIN using the plug flow reactor module

COILSIM1D ~ key features

Possibilities with COILSIM1D

- Boost profitability with highly accurate simulati
  - Yield maximization
  - Process optimization



- High flexibility
  - Model validated for broad range of feeds
  - Main reactor geometries supported
  - User-defined reactor geometry (a.k.a. ‘open version’)
  - User-defined operating conditions

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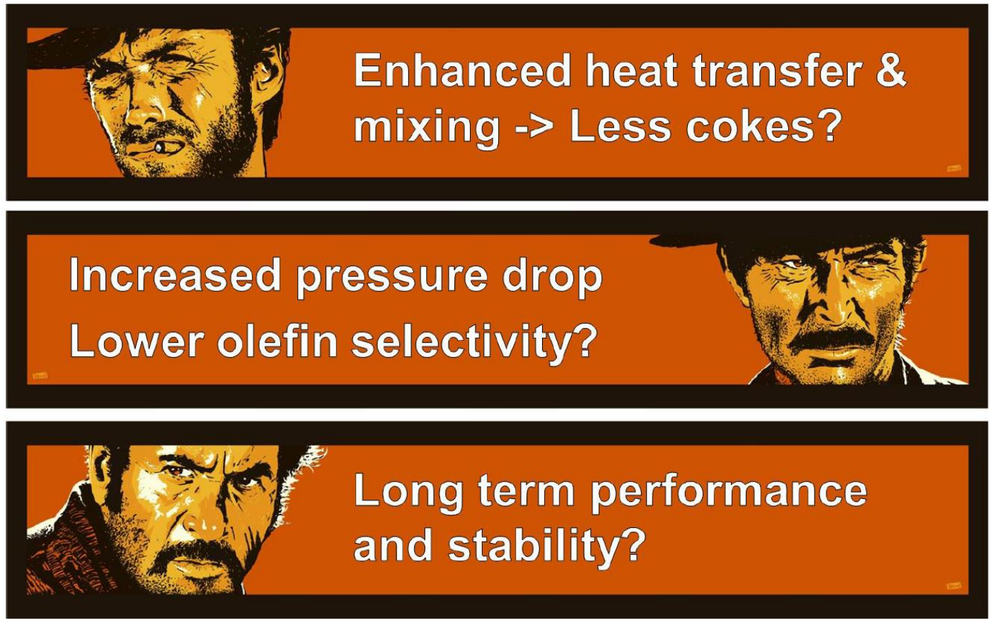
3D reactor technologies: coking



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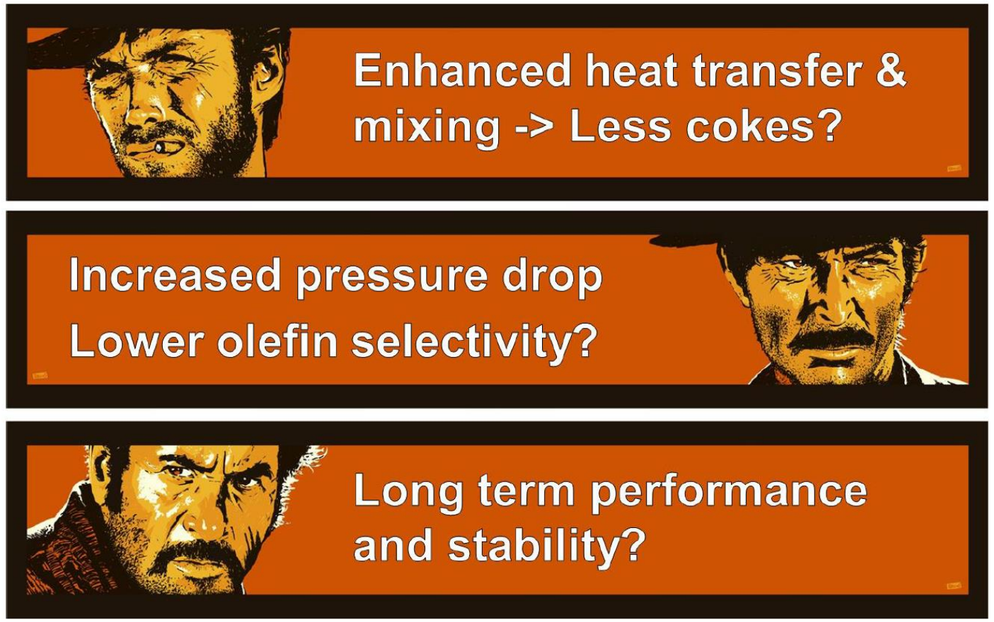
3D reactor technologies - coking



Reduction of hot regions

- less overcracking
- higher propylene selectivity

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Coke formation in steam cracking

Endothermic process at temperatures of 800–900 °C

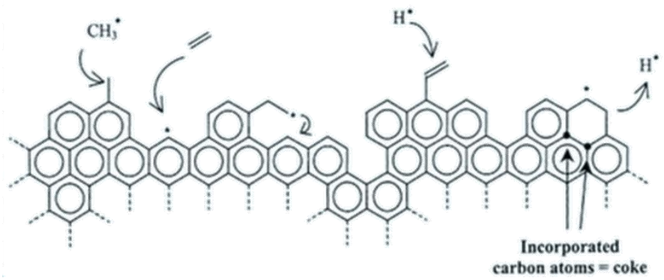
Deposition of a carbon layer on the reactor surface

⟹ Reduced thermal efficiency

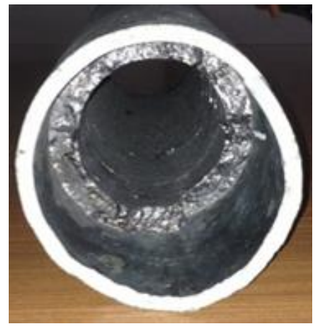
⟹ High pressure causes loss of product selectivity

⟹ Coil carburization and thermal stress

Coke reduction method: 3D reactor technology



$$r_C = \sum_i c_i \cdot A_i \cdot \exp\left(\frac{-E_{a,i}}{R T_{int}}\right)$$



Coil cracking due to differences in thermal expansion rate

Hot spots due to inhomogeneous coke formation

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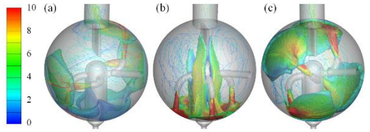
Nova Chemicals, 12002; Linde Group; Muños et al., 12013; Albright et al., 1988; Muños et al., 12014

Improving jet stirred reactors



Ideally mixed lab scale reactor

⟹ Flexible, fast and low-cost experiments for intrinsic kinetics

⟹ Quasi-homogeneous gas phase composition

⟹ Jet stirred reactor (JSR)

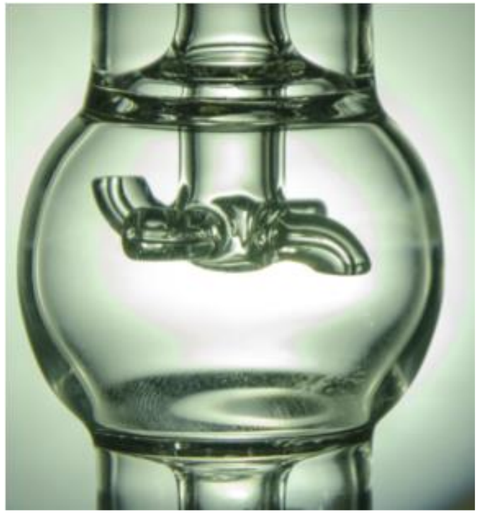
High velocity jets induce mixing via turbulence generation

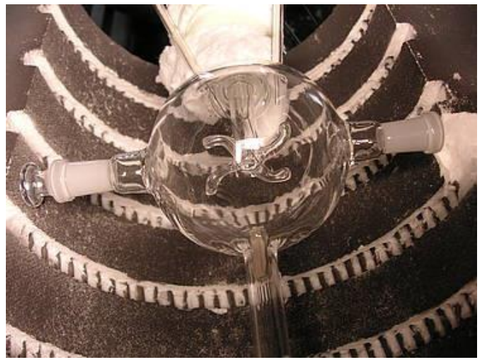
Gas-phase kinetics study

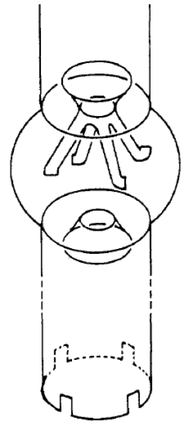
- ✓ Oxidation of fuels
- ✓ Pyrolysis of hydrocarbons
- ✓ Nitrous oxide formation
- ✓ Ignition phenomena

Gas-solid kinetics study

- ✓ Chemical vapor deposition
- ✓ Coke formation in steam cracking







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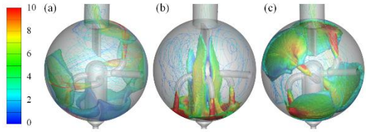
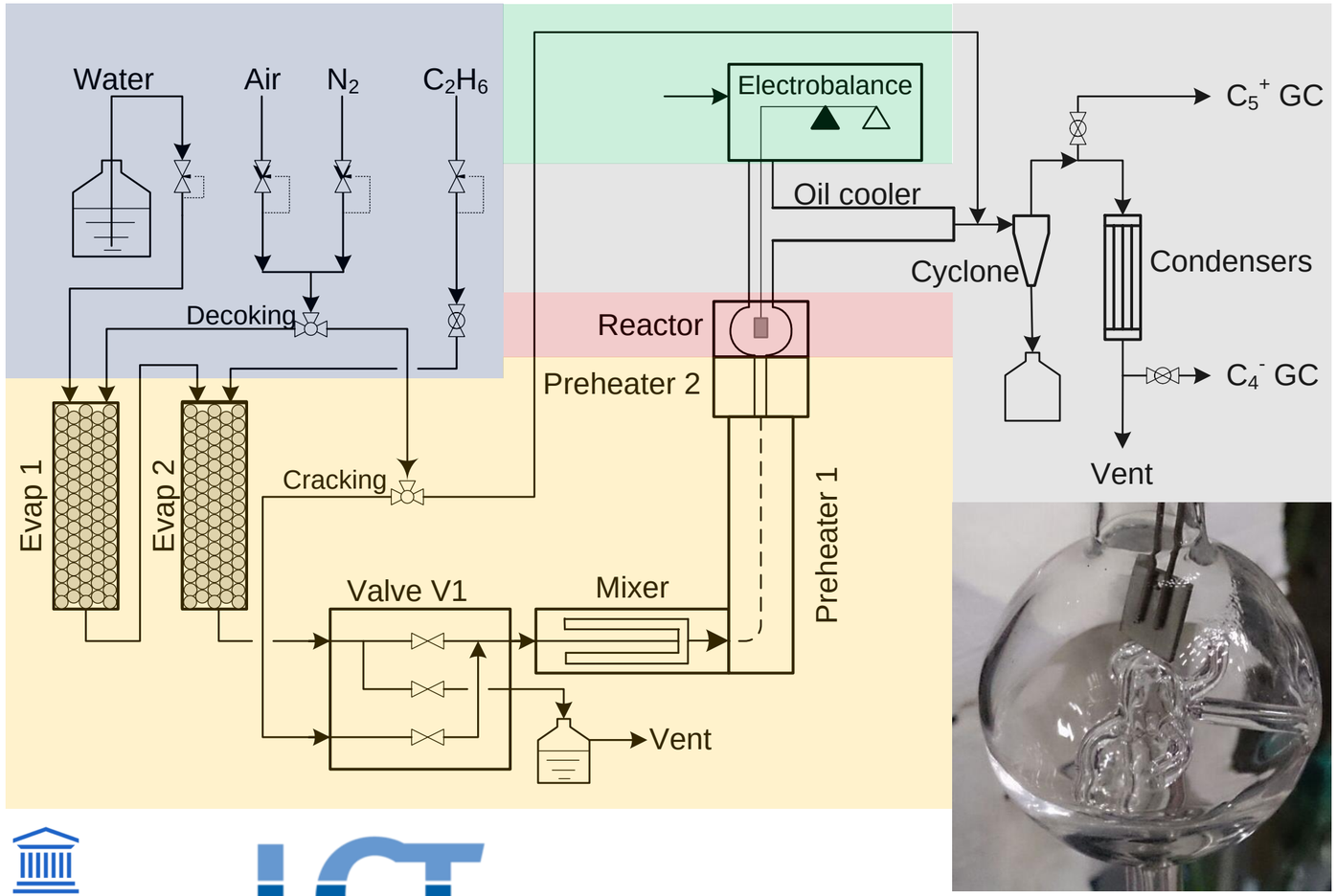
Reyniers, P. A. et al. Int. J. Chem. Kinet. 120120, 48, 556.

Improving jet stirred reactors



Jet stirred reactor at the Laboratory for Chemical Technology

Feed section | Preheating section | Reactor section | Electrobalance | Analysis section



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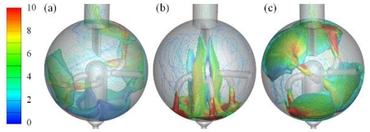
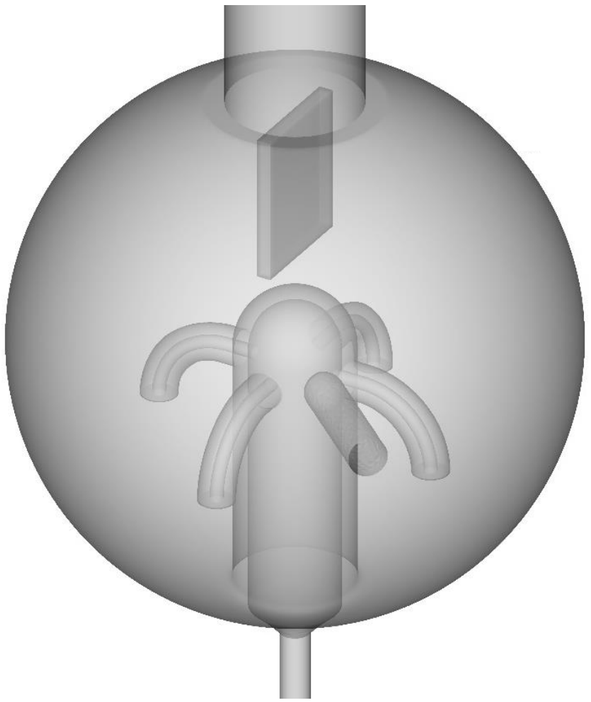


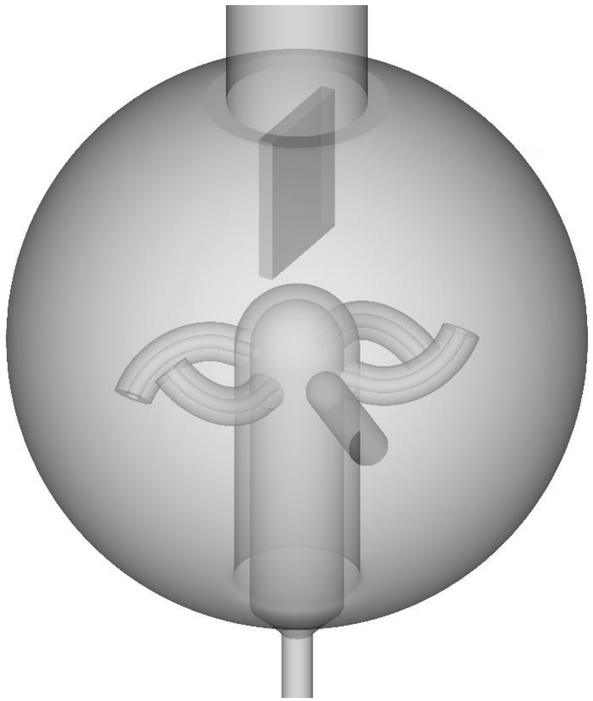
Three proposed geometries to maximize the gas phase homogeneity via residence time distribution simulations and reactive simulations of ethane cracking

90° case

down case



45° case



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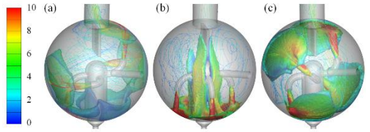
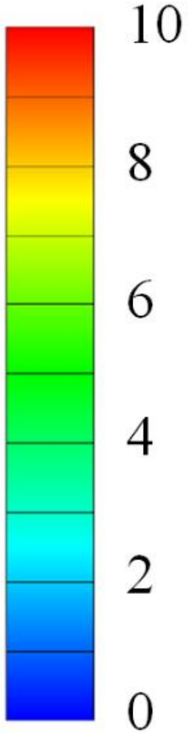
Reyniers, P. A. et al. Int. J. Chem. Kinet. 120120, 48, 556.

Improving jet stirred reactors

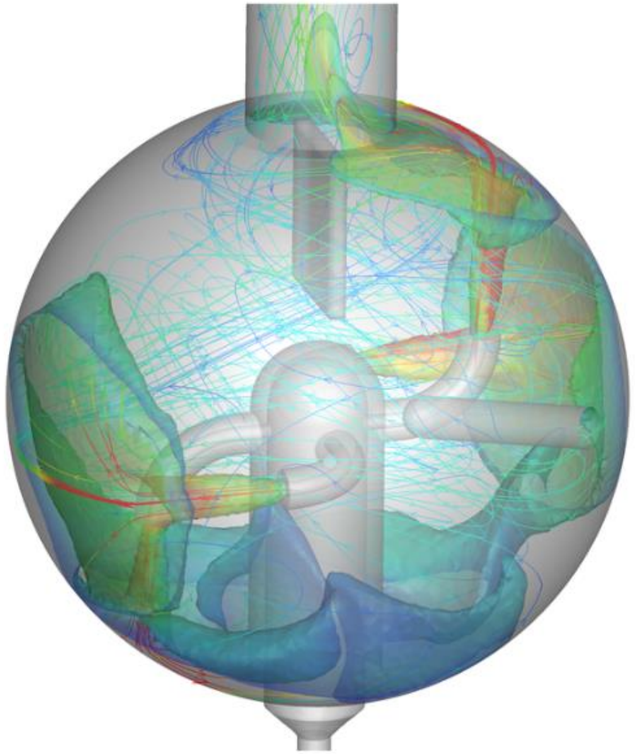


Distinctive differences in the flow pattern between geometries, with the 45° case exhibiting the highest degree of homogeneity

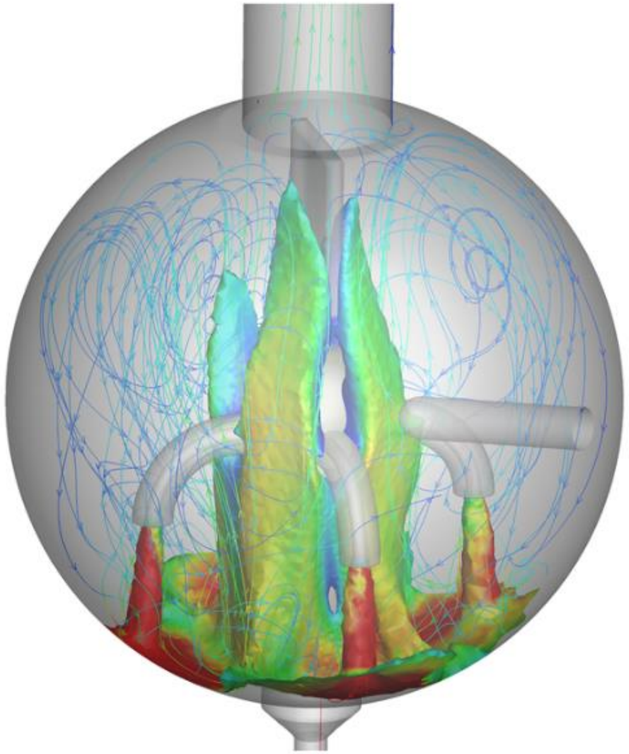
Velocity magnitude [m/s]



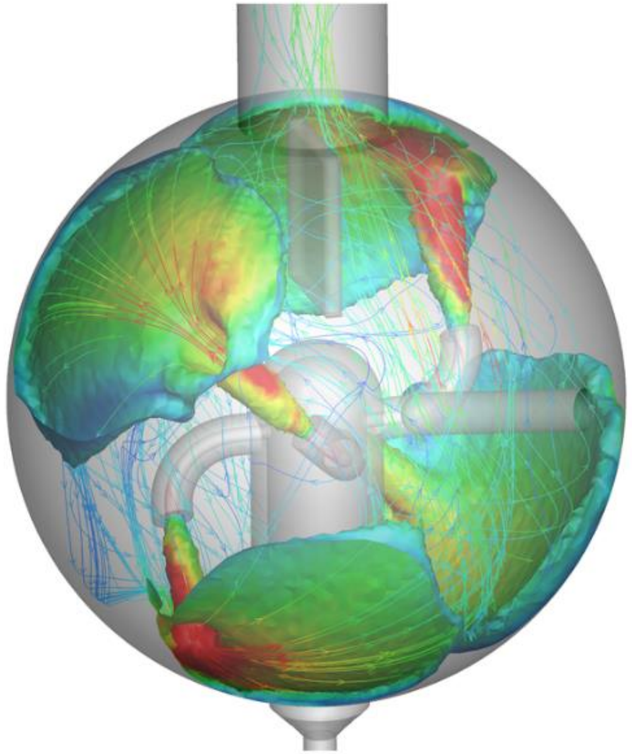
90° case



down case



45° case



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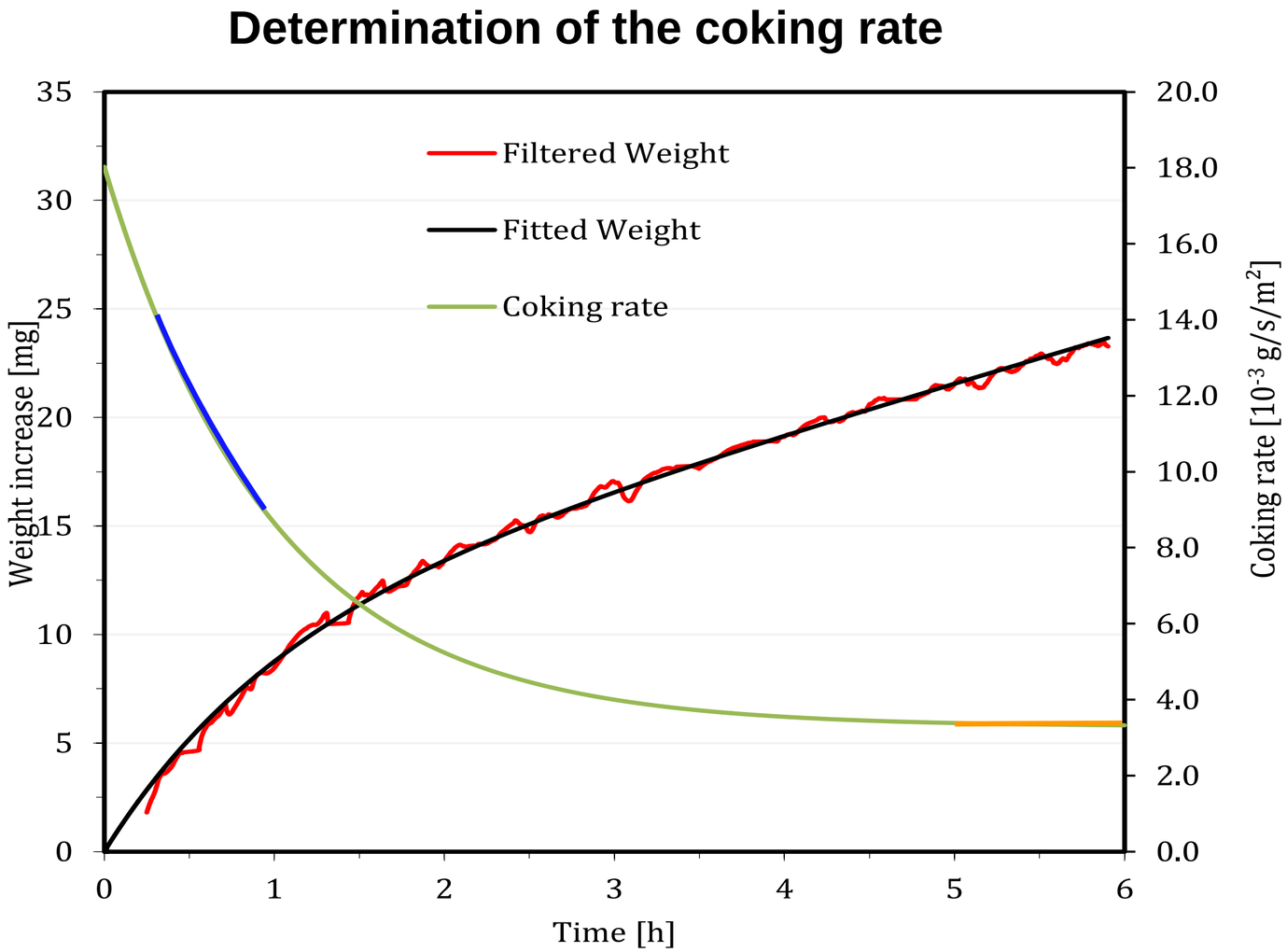
Reyniers, P. A. et al. Int. J. Chem. Kinet. 120120, 48, 556.

MSB data post processing



- ✓ **Initial (catalytic) coking rate** = Average coking rate value from 15 min to 1 hour of cracking

- ✓ **Asymptotic (pyrolytic) coking rate** = Average coking rate value during the last hour of cracking

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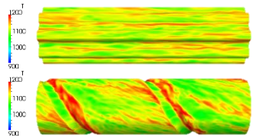
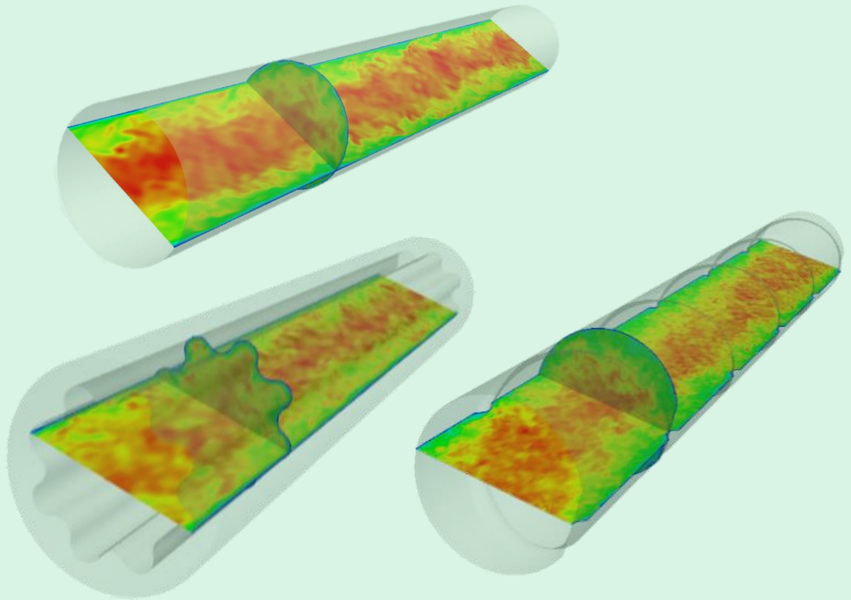
Towards LES with detailed kinetics



1D simulations are not sufficient to capture all phenomena

1D Simulation	BARE	FINNED	RIBBED
$\Delta P/\Delta P_{Bare}$	1.00	1.22	2.17
U/U_{Bare}	1.00	1.21	1.50
$T_{gas/cokes}$ [K]	1079.4	1066.4	1054.5
Rel. r_{coke}	-	-4.8%	-43.1%
Rel. yield C_2H_4	-	-0.27%	-1.47%
Rel. yield C_3H_6	-	+0.03%	+0.13%

~ 10^1 CPU seconds



~ 10^6 CPU seconds

⟹ 3D CFD simulations are **computationally expensive** but **necessary** to obtain correct results

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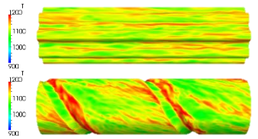
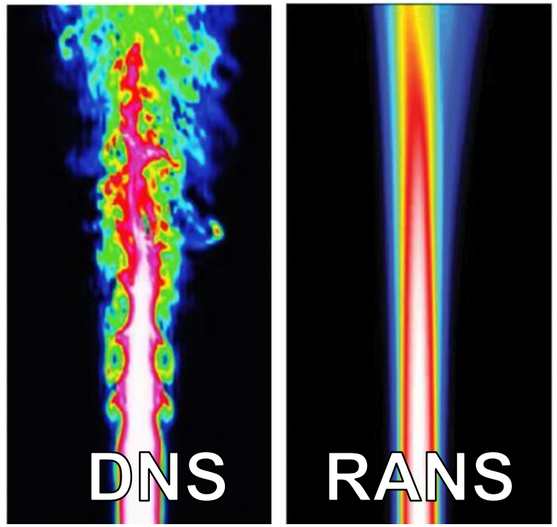
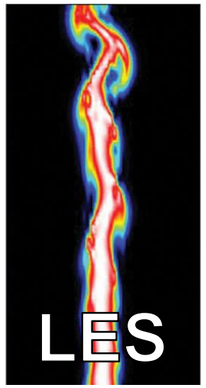
MODELING and measuring Turbulence



Resolve all turbulence		Model all turbulence
Most accurate and robust		Less expensive
Lots of physical insight		Average = intuitive
Extremely expensive		Models are fitted to specific flows
Uncertainty from other sources		Limited physical insight, qualitative

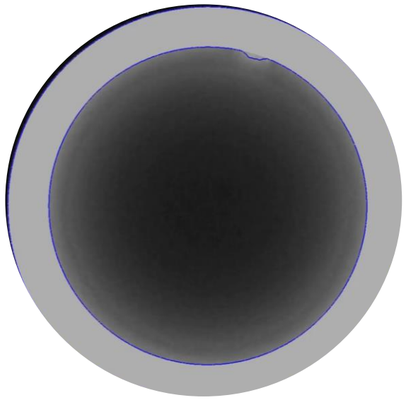




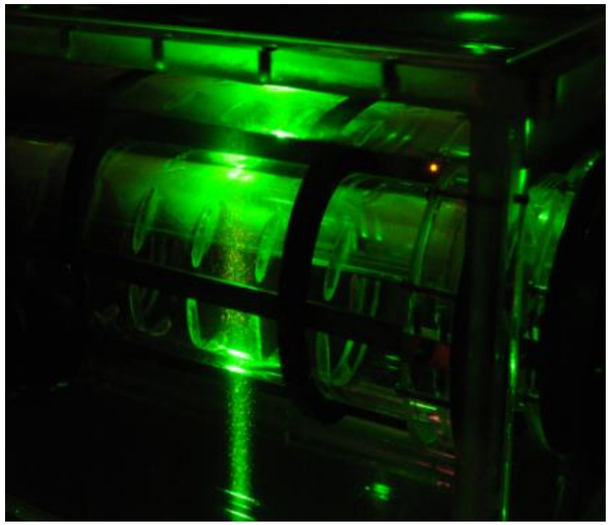
The in-between: large eddy simulation

- Resolve the large flow-determining eddies
- Model the smaller, more uniform eddies

X-ray microscopy



Particle Image Velocimetry



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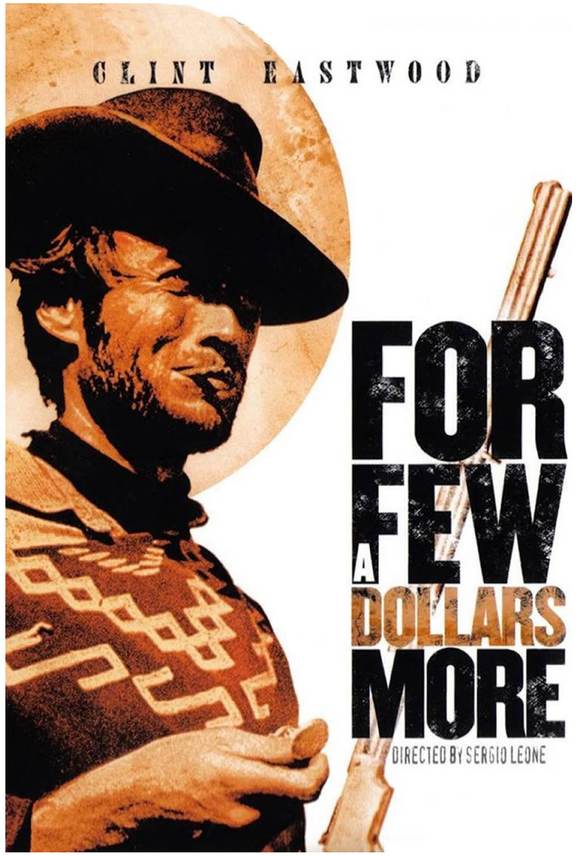
L. Gicquel, P. Givi; AccuWeather

3D reactor technologies – 12017 & 12018



FACULTY OF ENGINEERING AND ARCHITECTURE

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

124B
479642
IMPROOF: INTEGRATED MODEL GUIDED PROCESS OPTIMIZATION OF STEAM CRACKING FURNACES

K.M. Van Geem, F. Battin-Leclerc, G. Bellos, G. Heynderickx, W. Buysschaert, B. Cuenot, M.R. Djokic, T. Faravelli, G. Theis, D. Jakobi, P. Lenain, A.E. Muñoz, J. Olver, J.N. Dedeyne, S. Vangaever, P. Honnerová, Z. Veselý, P. Oud

2017 Spring National Meeting, San Antonio, Texas, March, 28, 2017

Advances in coil material

- increased run length
- increased coil lifetime

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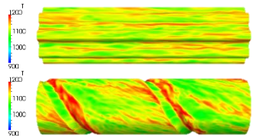
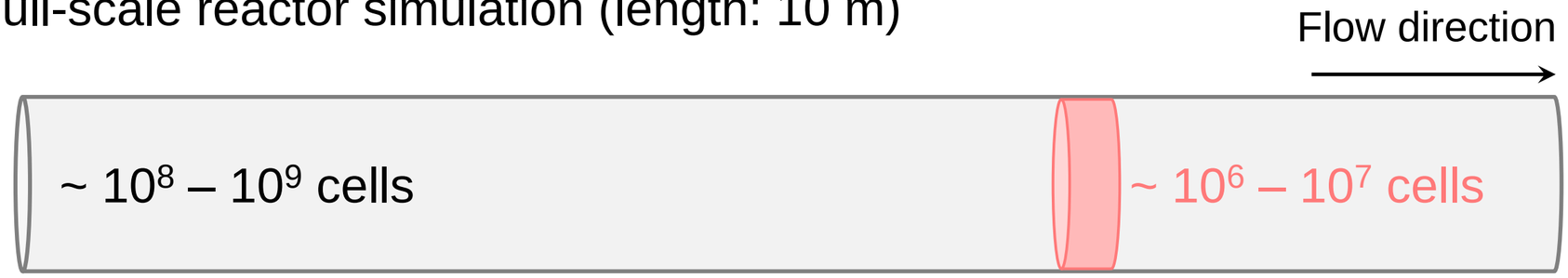
Towards LES with detailed kinetics



Full-scale reactor simulation (length: 10 m)



~10^5 – 10^6 iterations required to reach steady-state solution

Trick: **streamwise periodicity**

Computational domain can be reduced by using **streamwise periodic** boundary conditions

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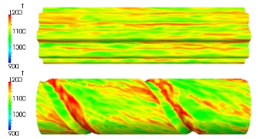
Patankar, S. V. et al. J. Heat Transfer 1977, 99, 180.

Towards LES with detailed kinetics



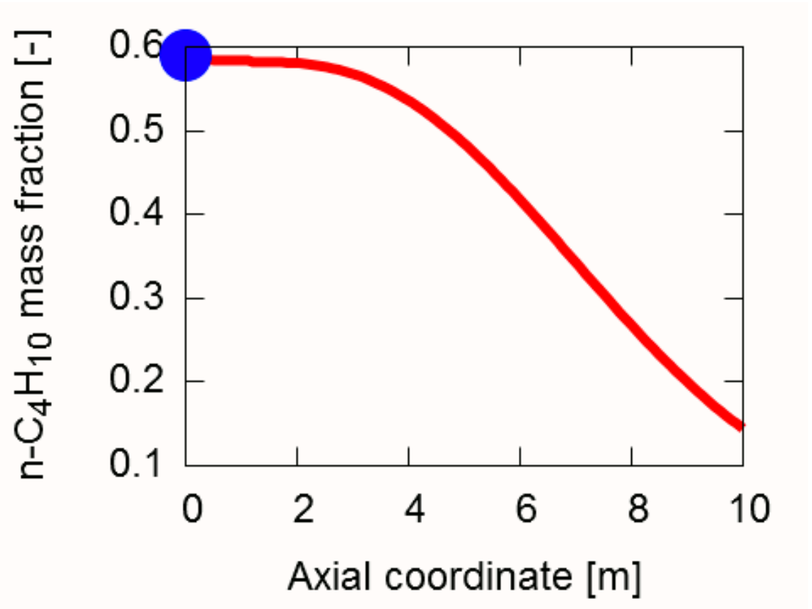
Assume velocity as **fully-developed** over the short computational volume

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 1200+

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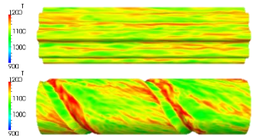
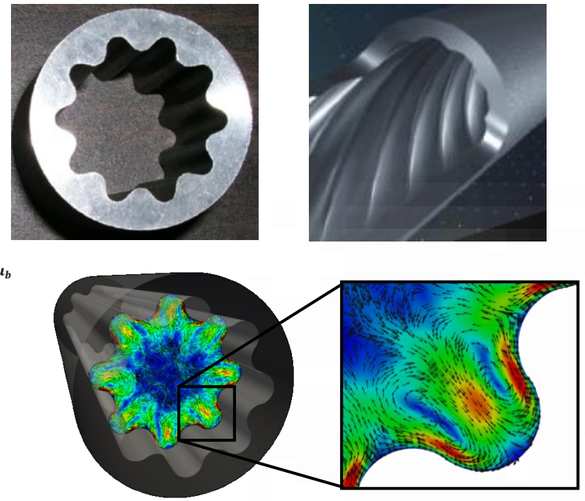
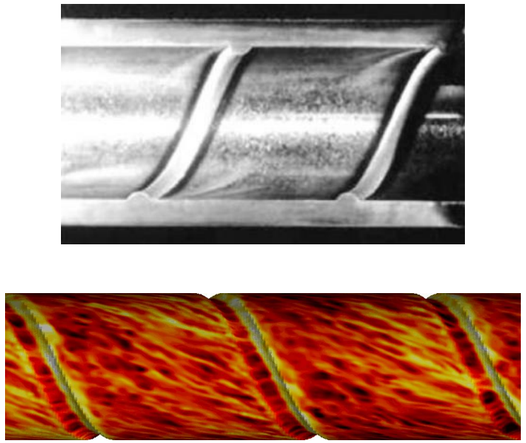
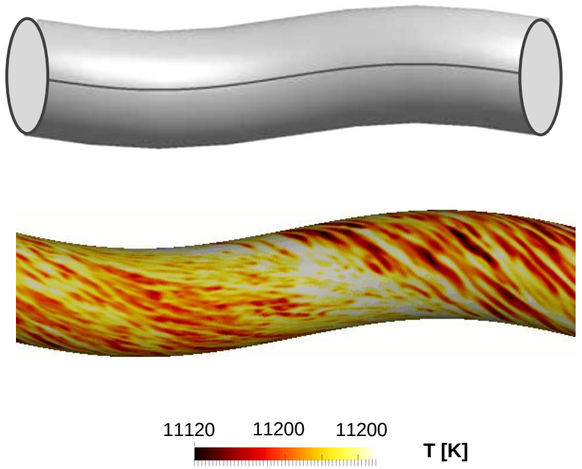
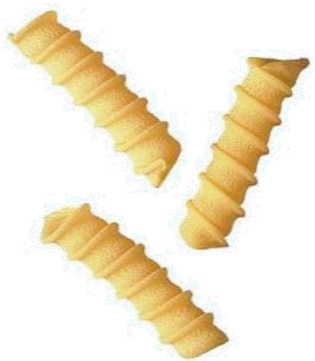
Van Cauwenberge, D. J. et al. AIChE J. 12017, 63, 1715.

Enhanced reactor designs



KBR / S+C **Straight / rifled fins**	Kubota **(Slit- / X-) MERT®**	Lummus/Sinopec **IHT®**	Technip **Swirl Flow Tube®**
1988, 12002, 12011	1996, 12003, 12009	12009	12011
			
			

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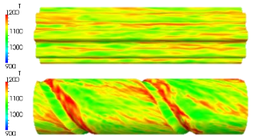
Van Cauwenberge, D. J. et al. Chem. Eng. J. 12015, 282, 66.

Towards LES with detailed kinetics

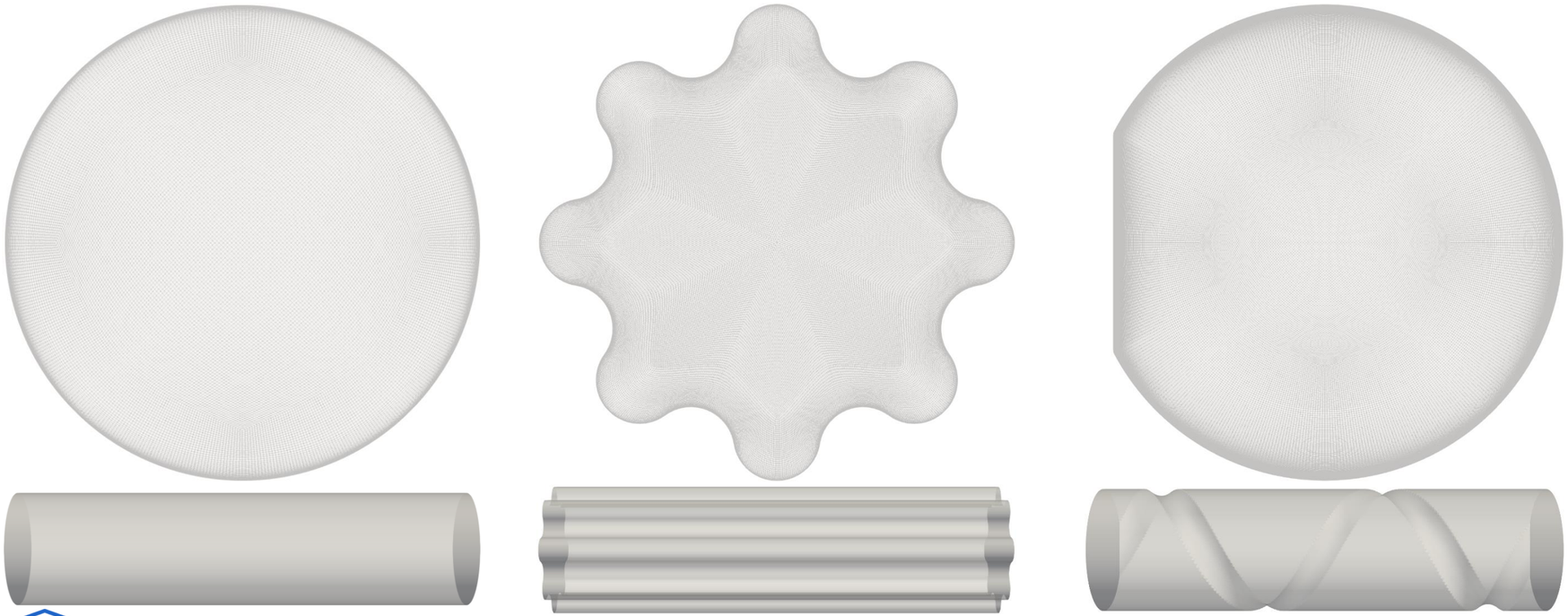


Simulation of a bare, finned and ribbed reactor

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)



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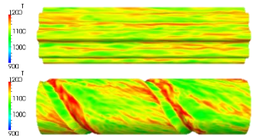
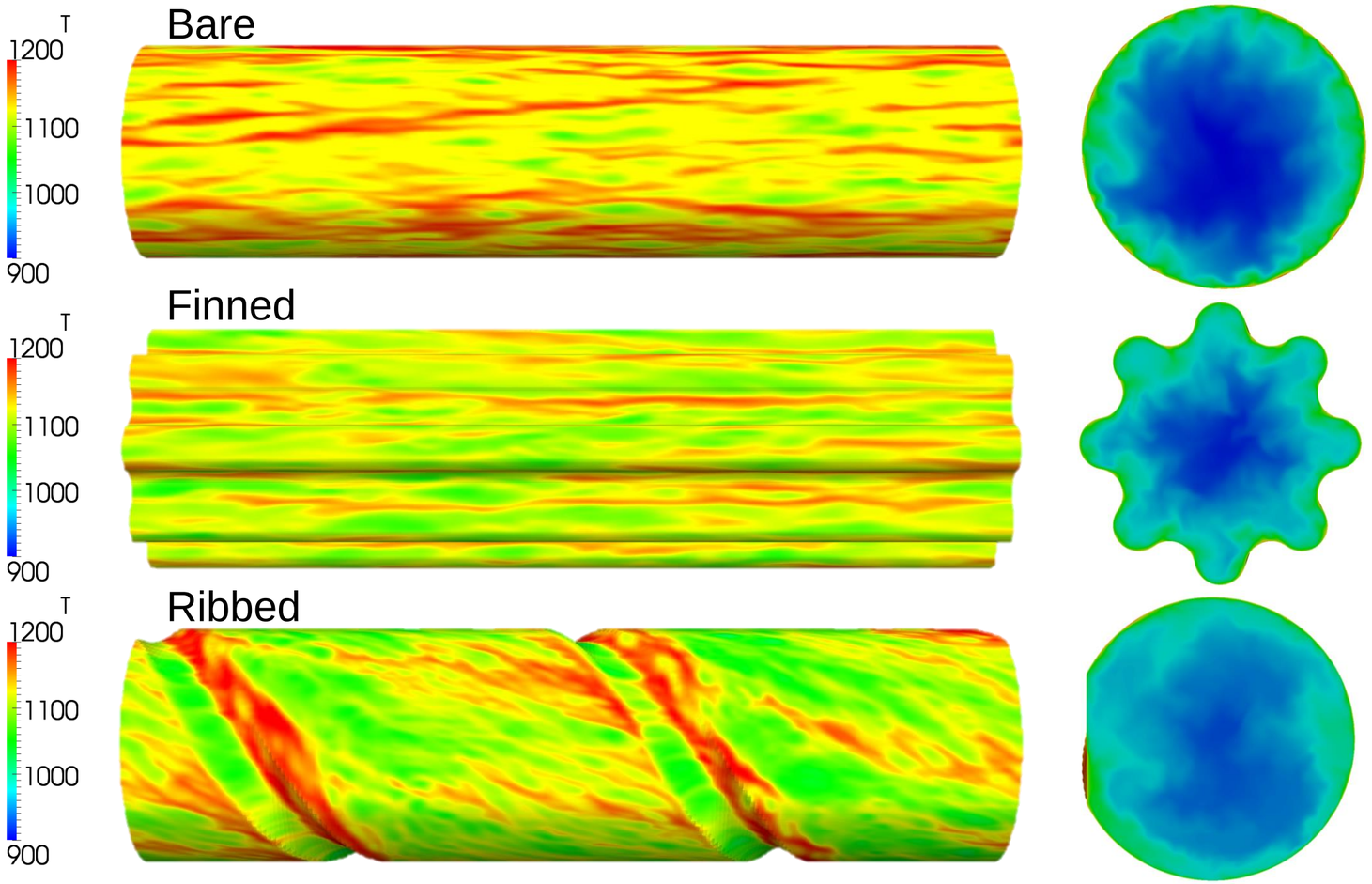
Reyniers, P. A. et al. 24th International Symposium on Chemical Reaction Engineering, Minneapolis, MN, USA, 120120.

Towards LES with detailed kinetics



Importance of 3D simulations – instantaneous temperature [K]



Lower average wall temperature

High temperature at trailing edge of the rib

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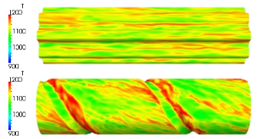
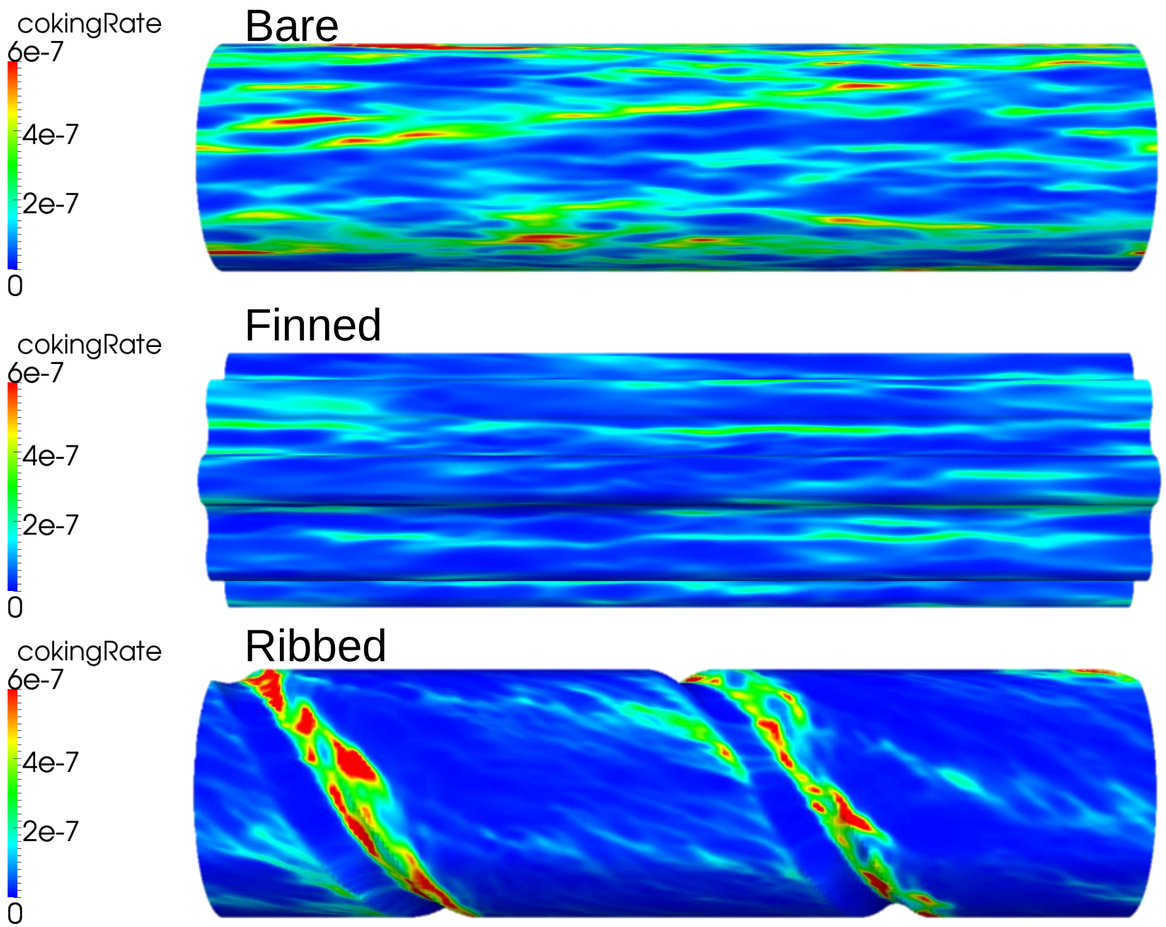
Reyniers, P. A. et al. 24th International Symposium on Chemical Reaction Engineering, Minneapolis, MN, USA, 120120.

Towards LES with detailed kinetics



Importance of 3D simulations – instantaneous rate of coke formation [kg m^{-2} s^{-1}]



Lower rate of coke formation due to lower average wall temperature

Coke formation highest at trailing edge

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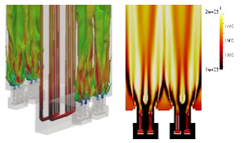
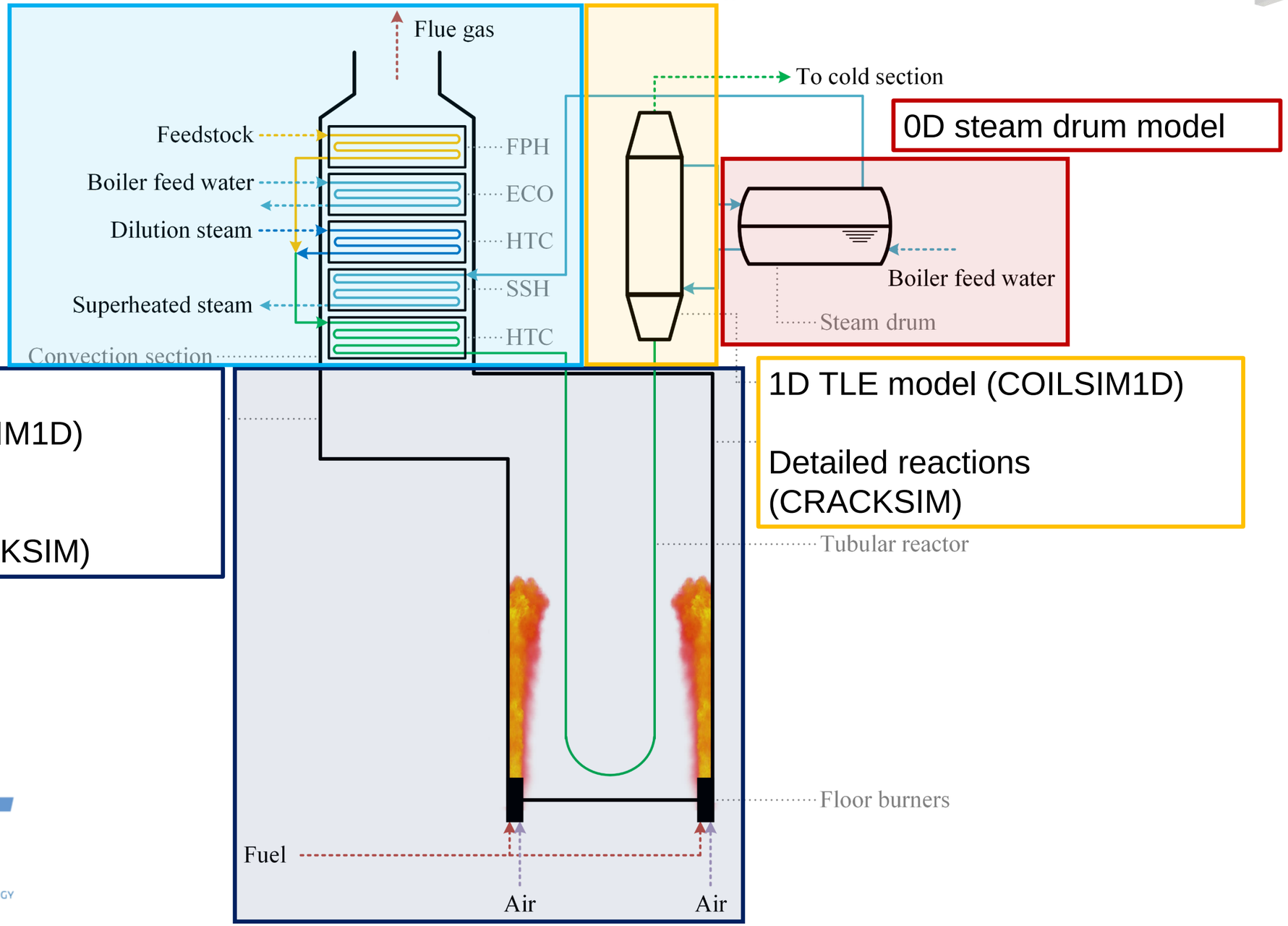
Reyniers, P. A. et al. 24th International Symposium on Chemical Reaction Engineering, Minneapolis, MN, USA, 120120.

Steam cracking furnace modeling



1D convection section model (COILSIM1D 4.0)

No reactions



0D steam drum model

3D furnace model (CFD)
1D reactor model (COILSIM1D)

Iteratively coupled
Detailed reactions (CRACKSIM)

1D TLE model (COILSIM1D)

Detailed reactions (CRACKSIM)

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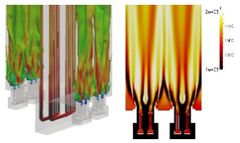
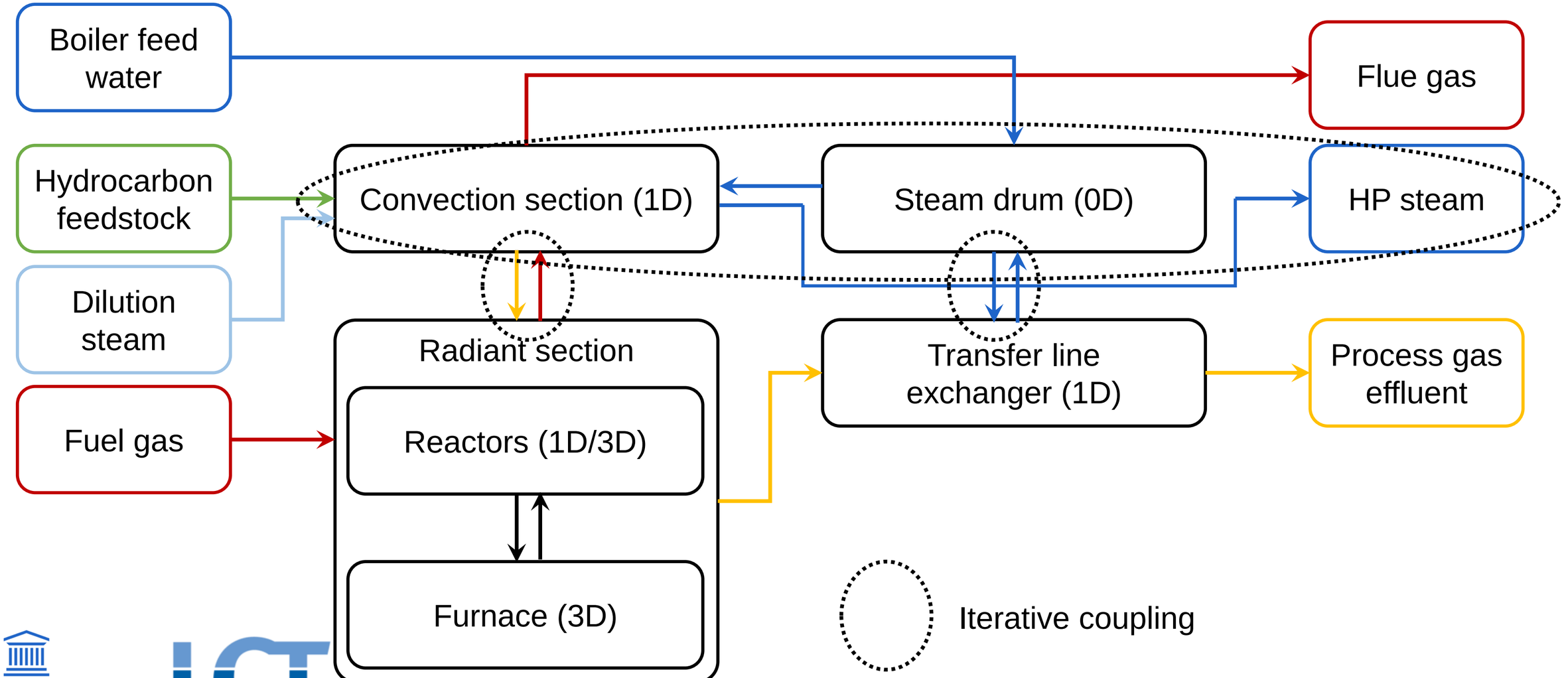
Coupling between individual parts



Assess influence of furnace improvements on overall heat balance



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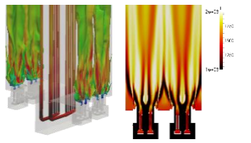
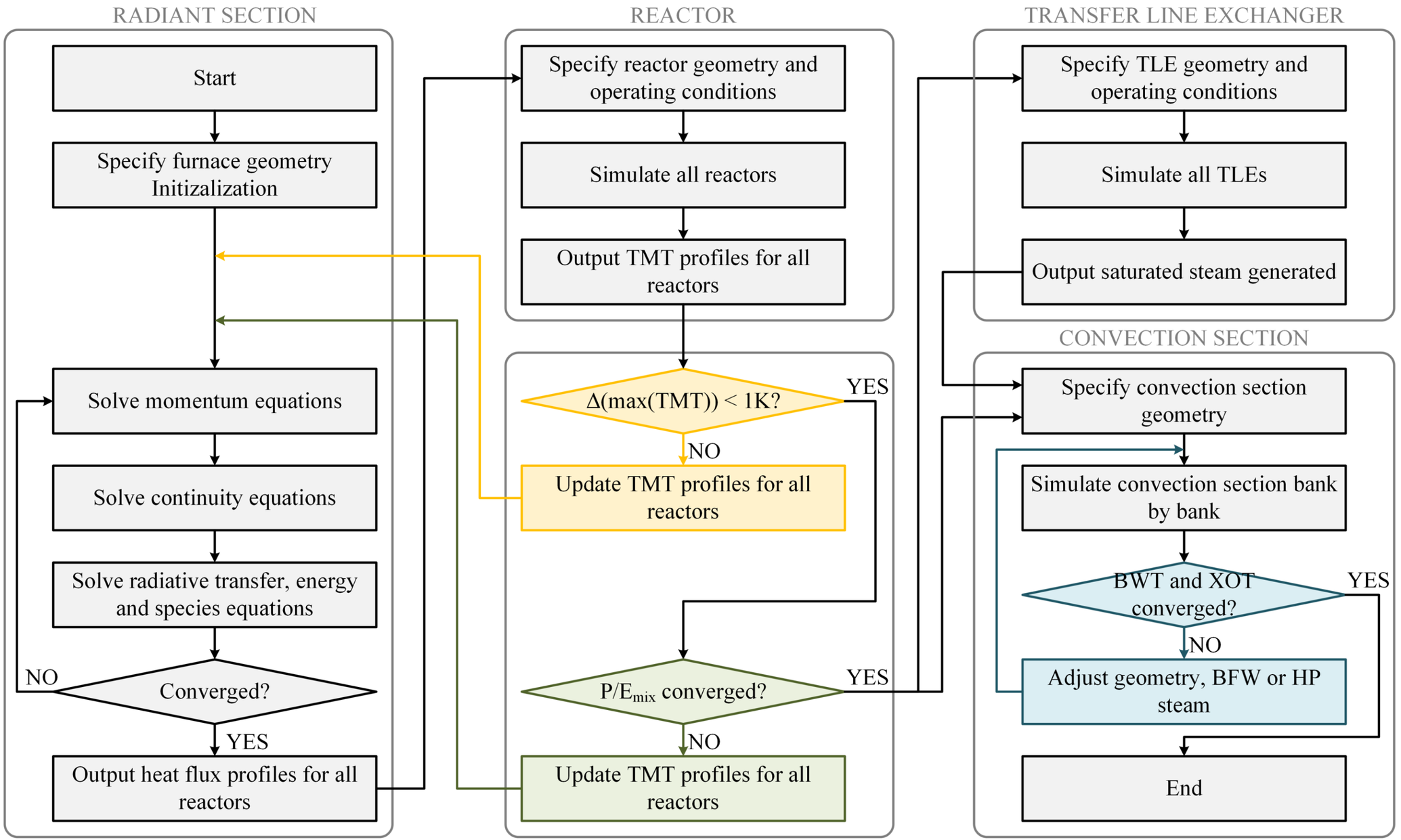
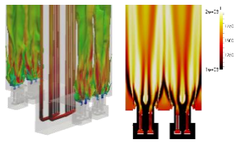
Coupling between individual parts

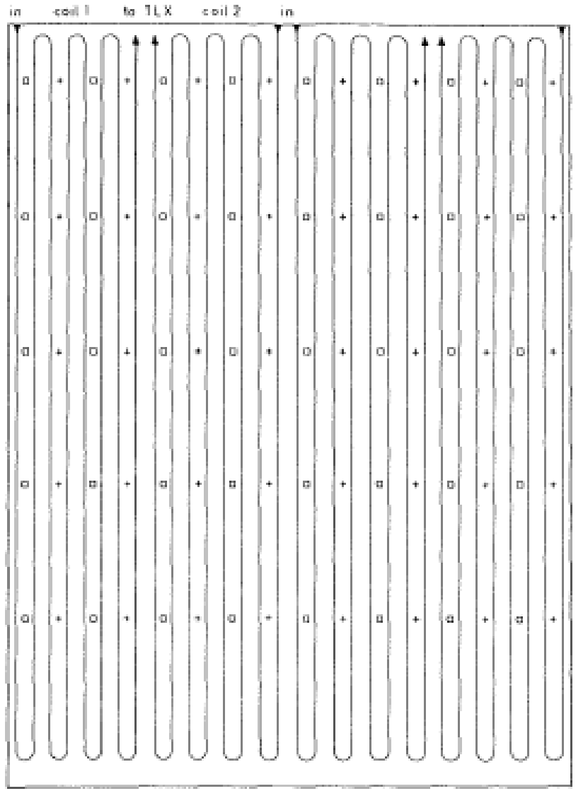




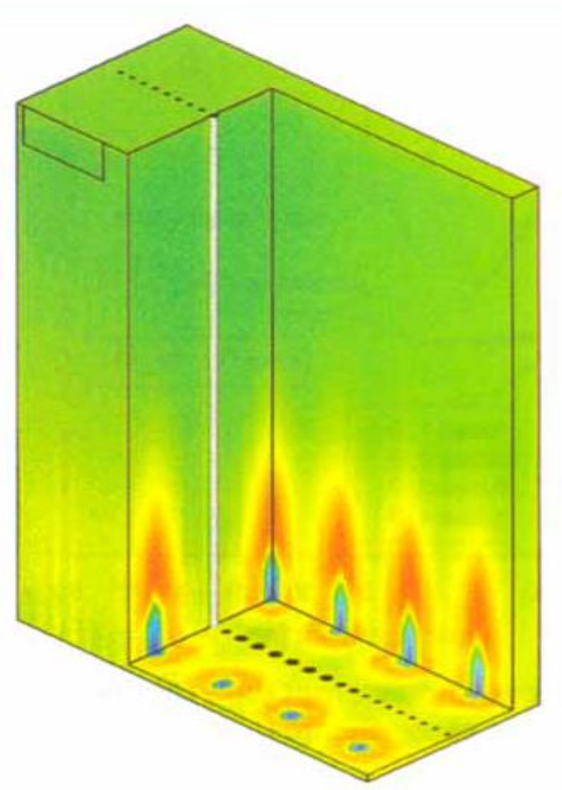
furnace modeling – the past



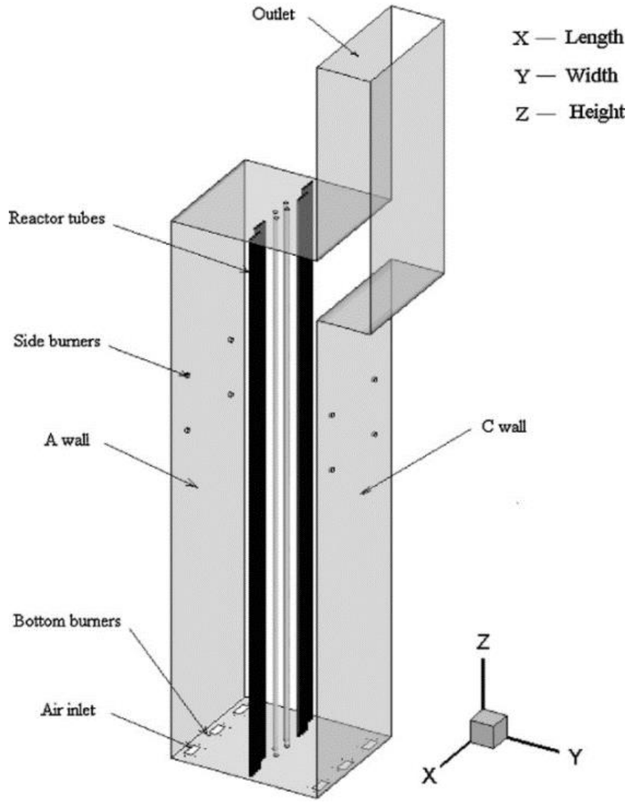
1D simulations of the furnace side, accounting for flue gas flow pattern, turbulent mixing and combustion in a crude way



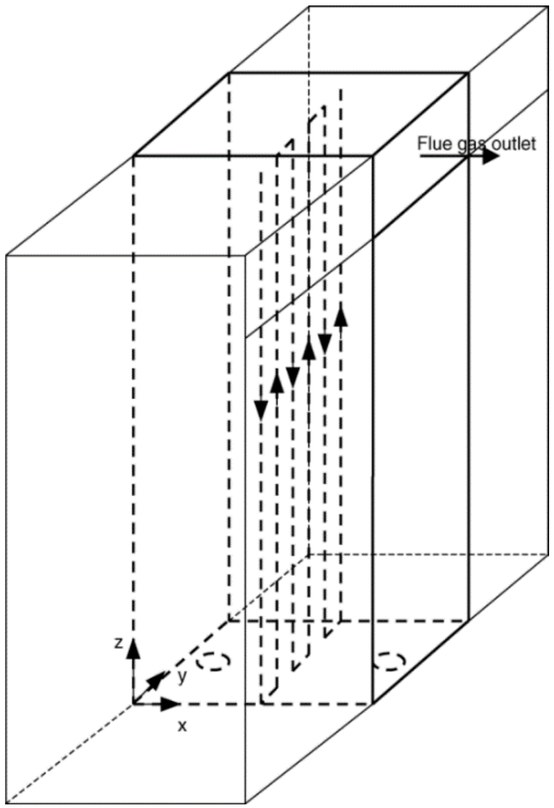
Plehiers et al. (1990)



Heynderickx et al. (12001)



Stefanidis et al. (12006)



Hu et al. (12012)

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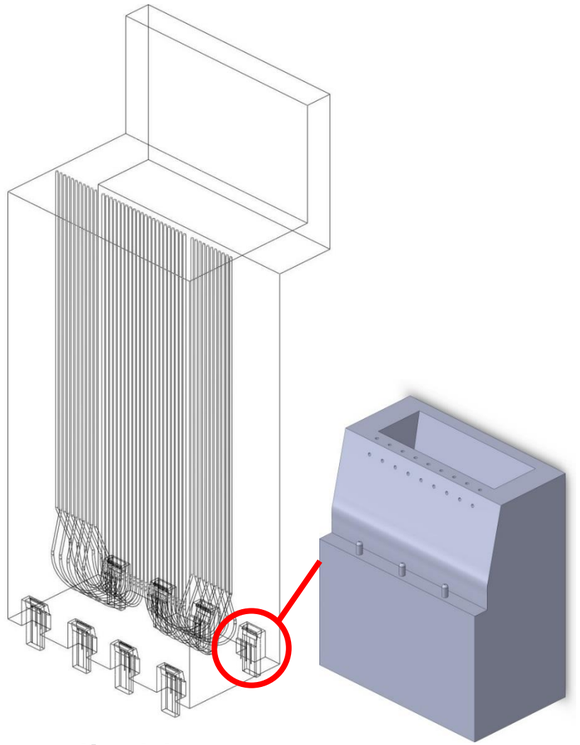
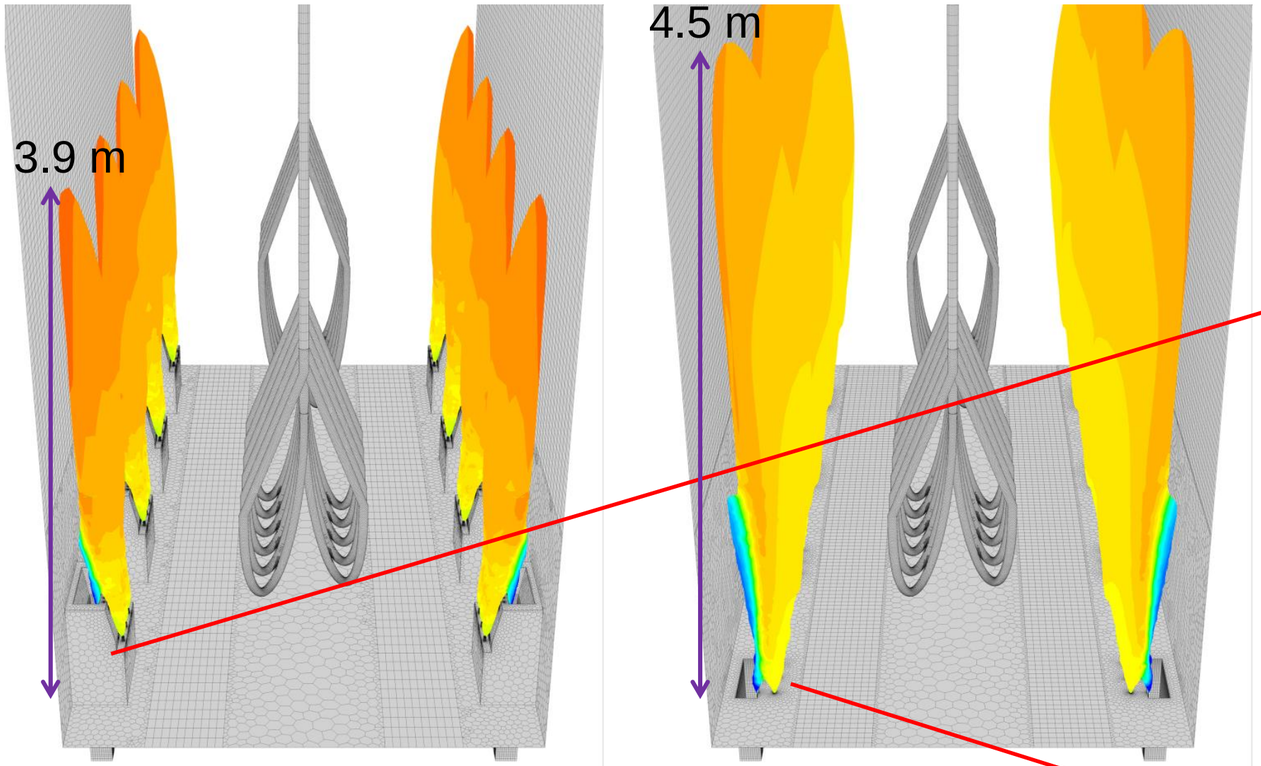
Plehiers, P. M. et al. Ind. Eng. Chem. Res. 1990, 29, 636-641. | Heynderickx, G. J. et al. AIChE J. 12001, 47, 388-400. | Stefanidis, G. D. et al. Comput. Chem. Eng. 12006, 30, 635-649. | Hu, G. et al. Comput. Chem. Eng. 12012, 38, 24-34.

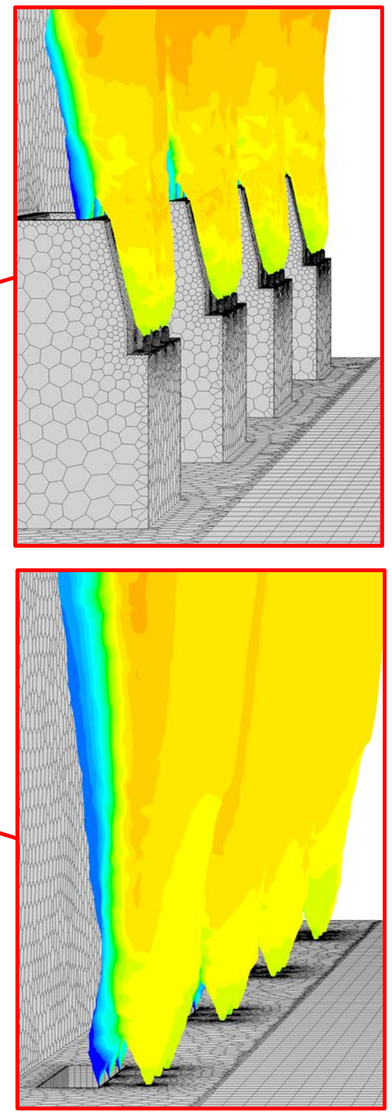
furnace modeling – the present



Detailed burner geometry



detailed simplified



- Detailed case
  - Shorter flame
  - Closer to the refractory

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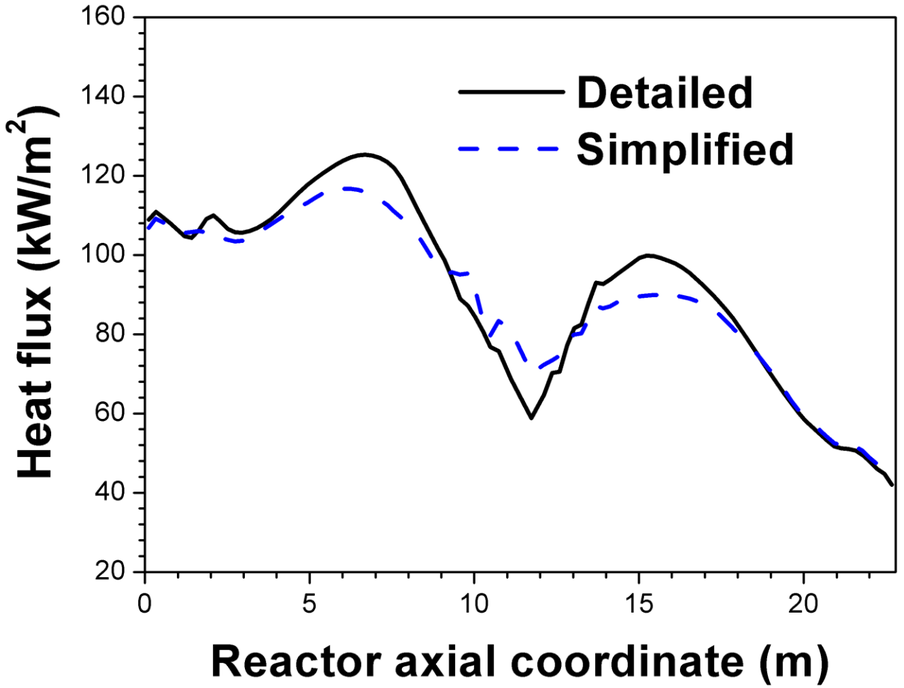
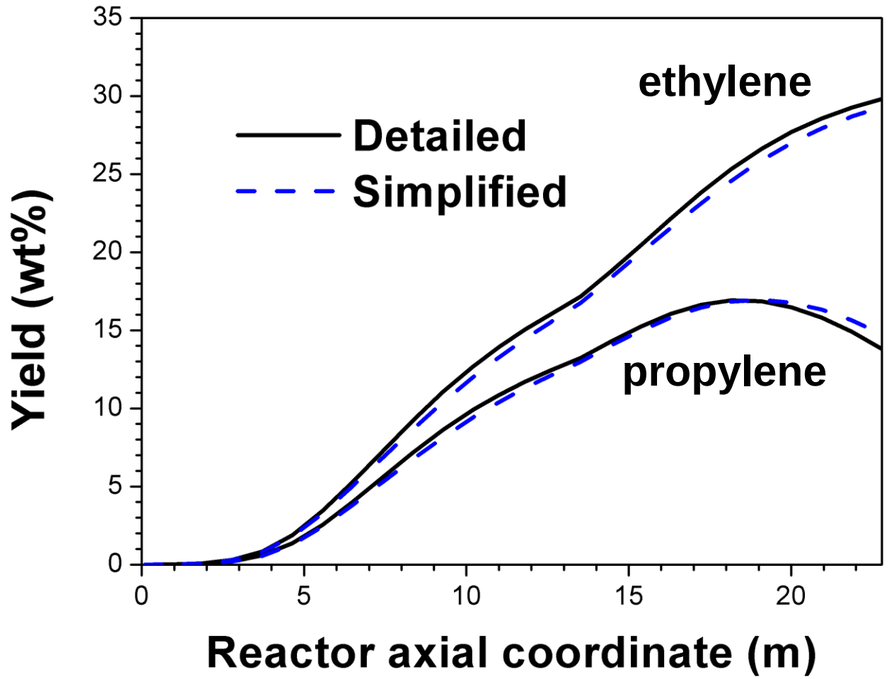
Zhang, Y. et al. AIChE J. 12015, 61, 936.

Heat flux and product yield



- **Detailed burner:**
  - +0.50% ethylene
  - -0.94% propylene



Heat flux profile is sensitive to the burner geometry

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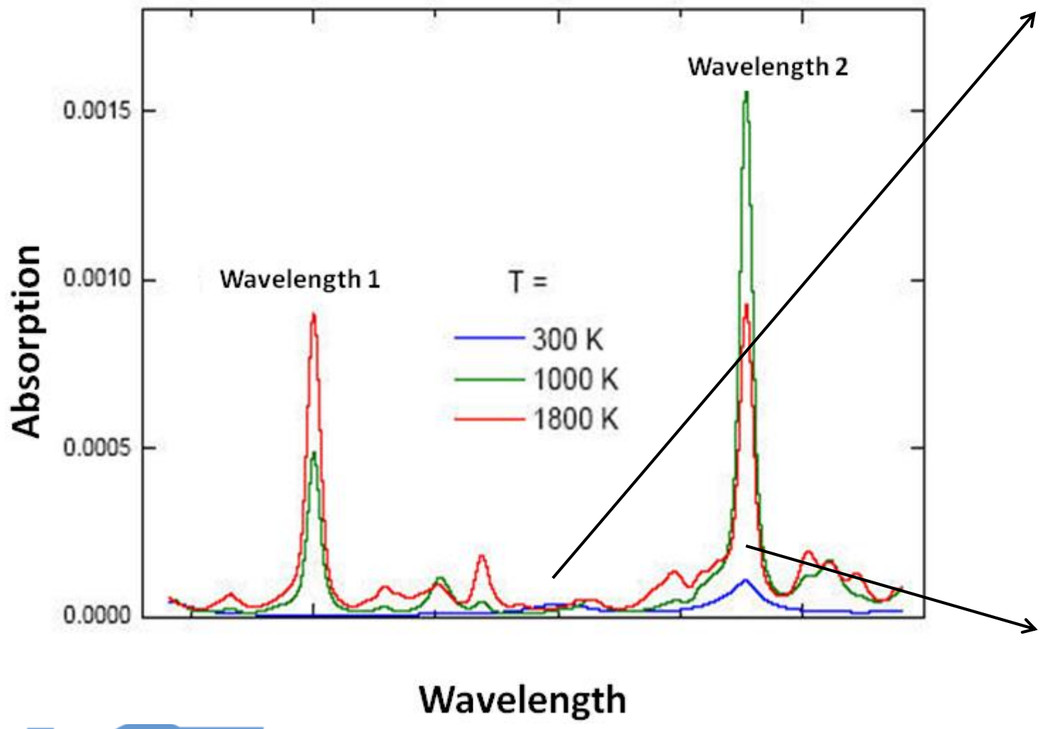
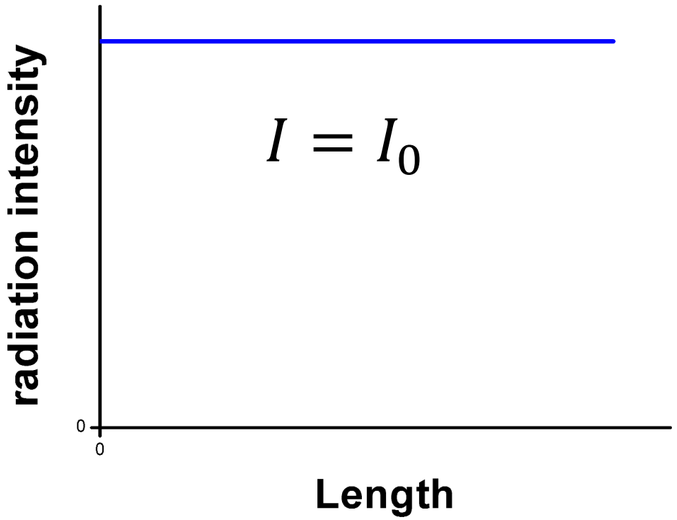
Flue gas radiative properties

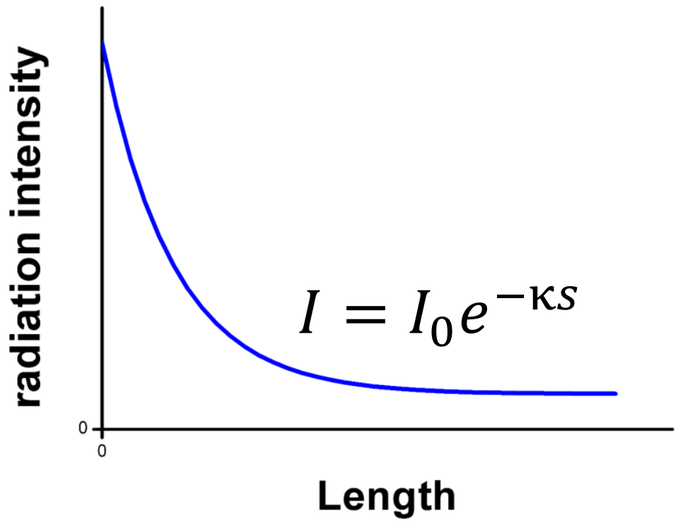
Non-gray characteristic



1) Spectral window



2) Absorption band



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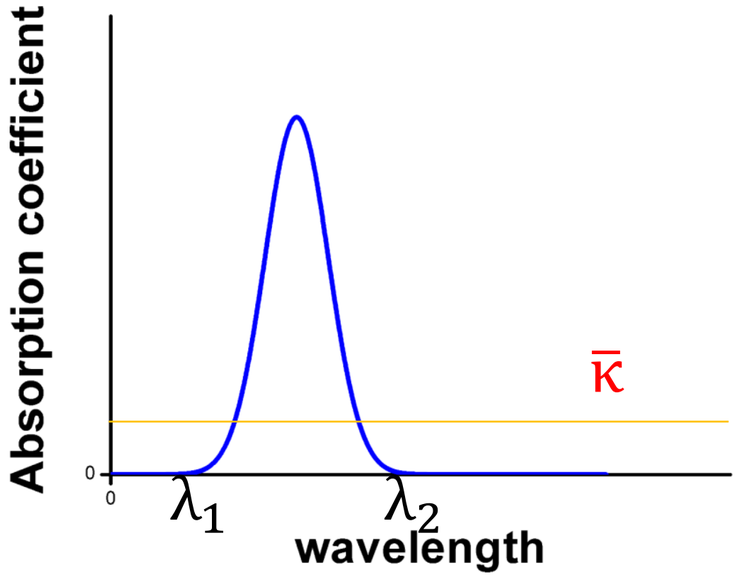
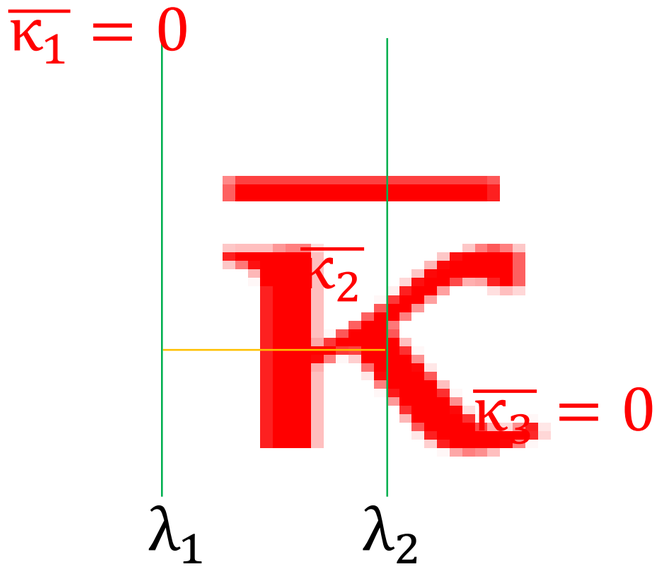
Gray gas/non-gray gas model



Gray gas model



Non-gray gas model

- **Average absorption coefficient over entire spectrum**

- **Absorption bands (K_2)**
- **Spectral windows (K_1 and K_3)**

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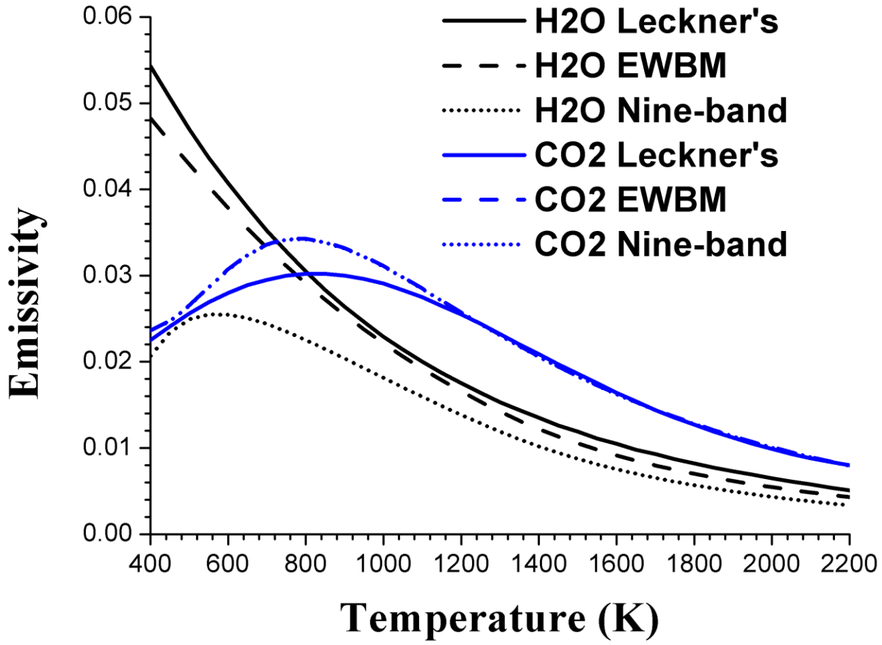
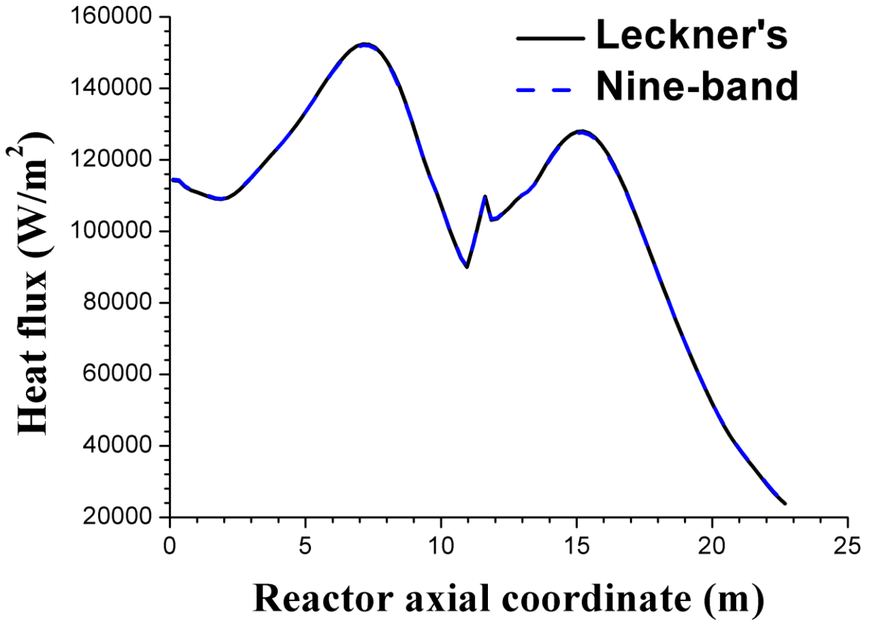
Validation of our non-gray gas model



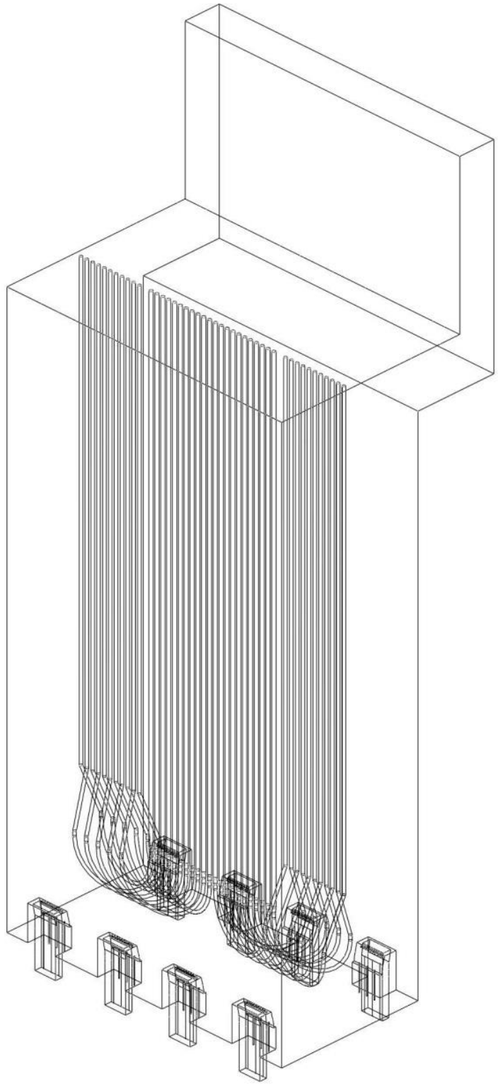
- **Small test furnace**
  - same burner
  - same reactor coil
  - same fuel/feedstock

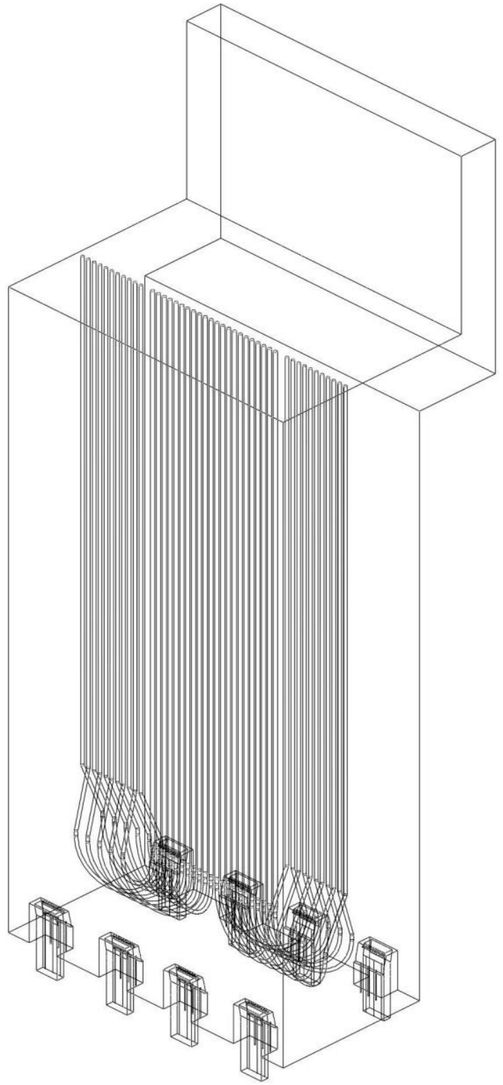
- **Nine-band model**
  - derived from exponential wide band model (EWBM)
- **Leckner's correlation**
  - emissivity correlation
  - 5% maximum error



Reliable non-gray model

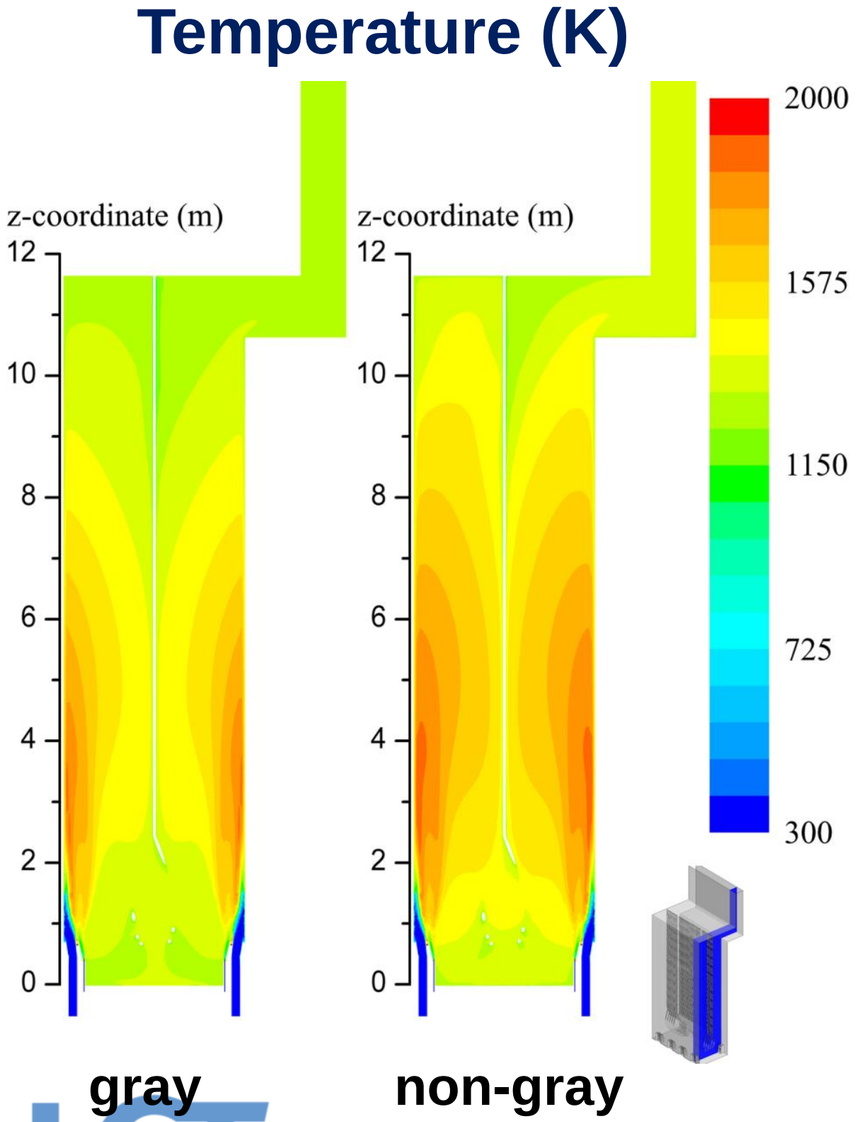
Gray vs. Non-gray

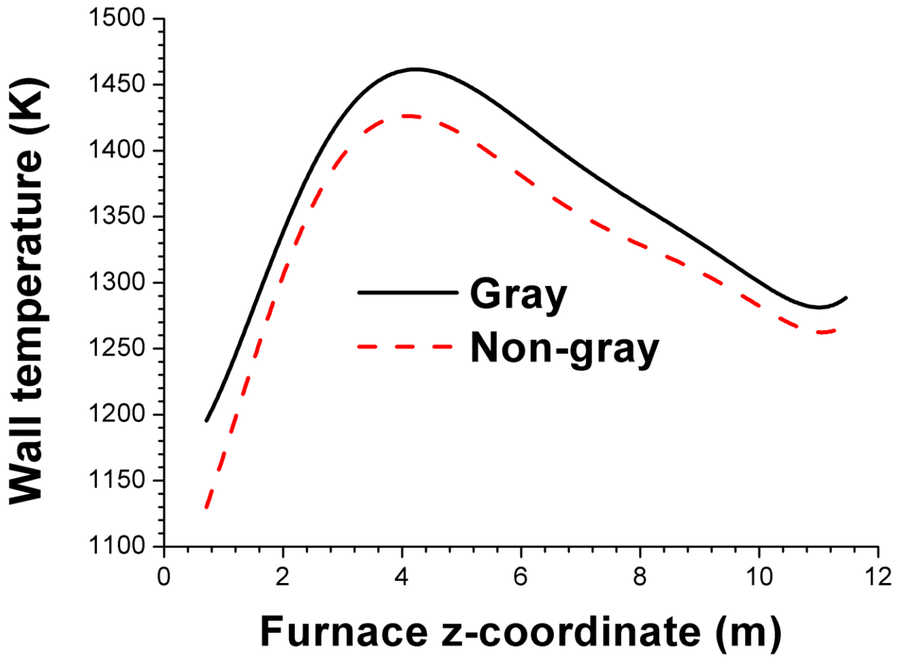




Gray gas model (WSGGM gray) **Non-gray model (Nine-band)**

Temperature contour





- **Non-gray gas model**
  - 70 K higher flue gas outlet temperature
  - 40 K lower refractory wall temperature

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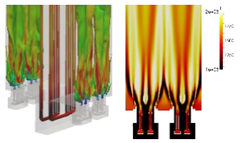
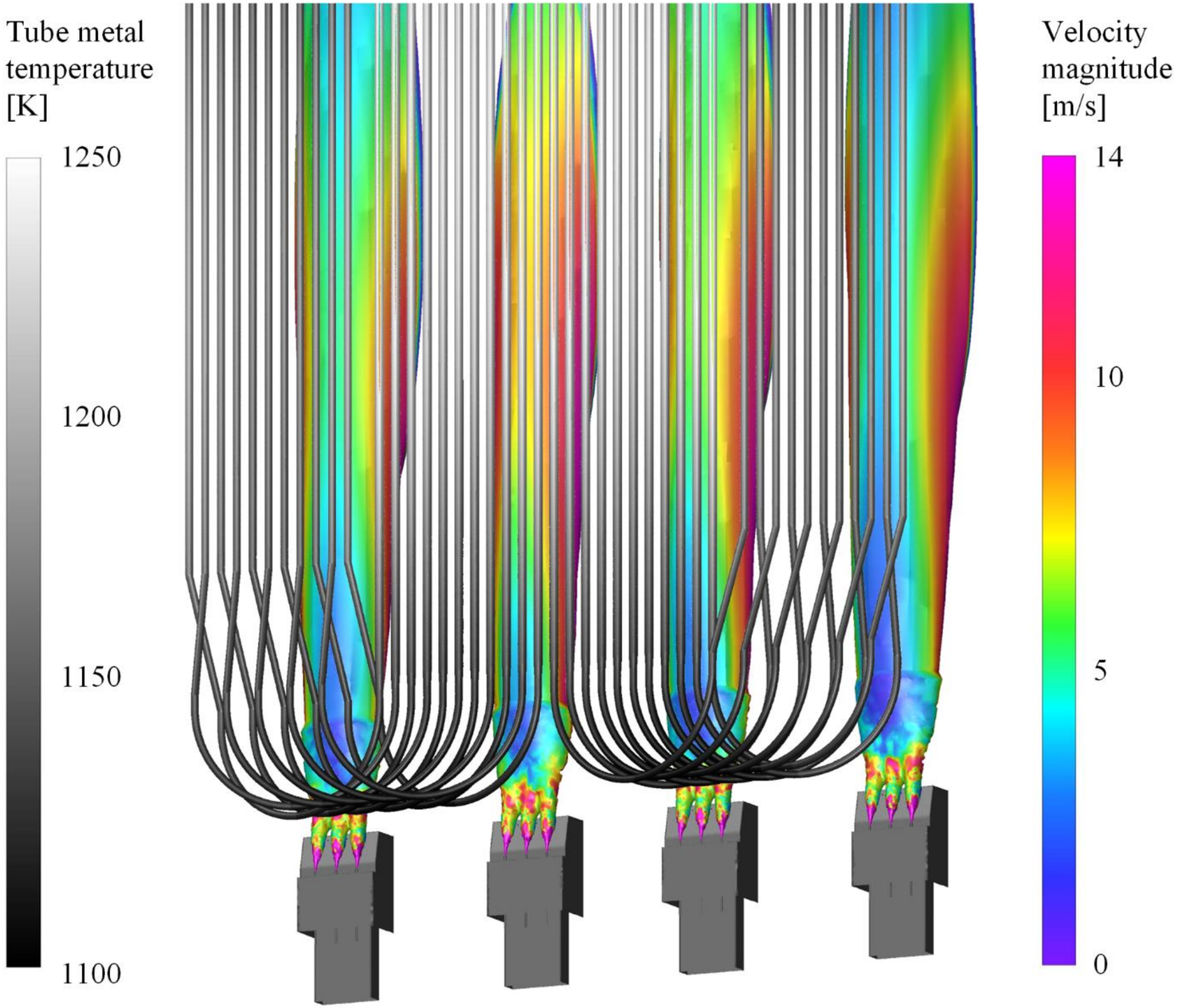
furnace modeling – the present





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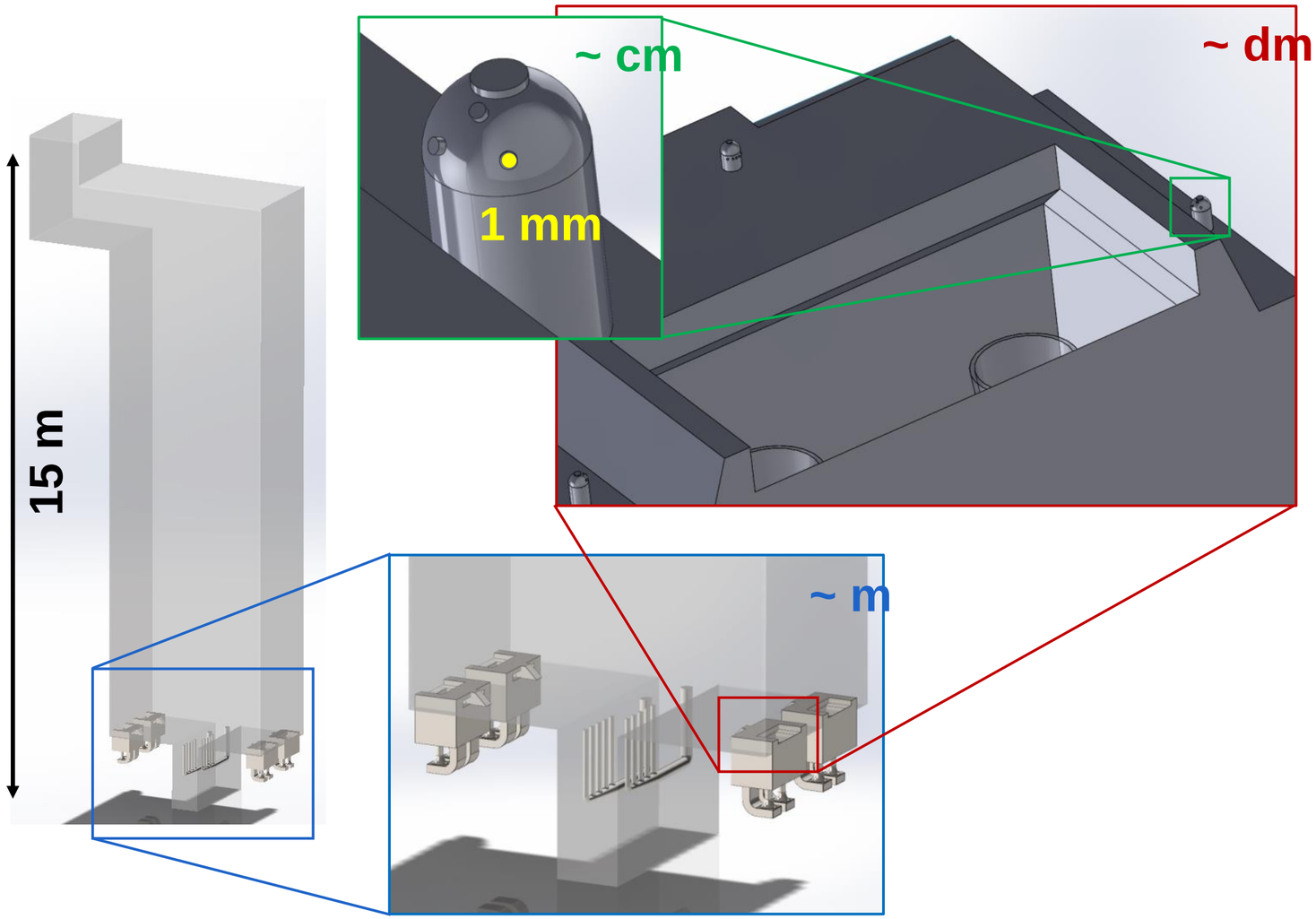
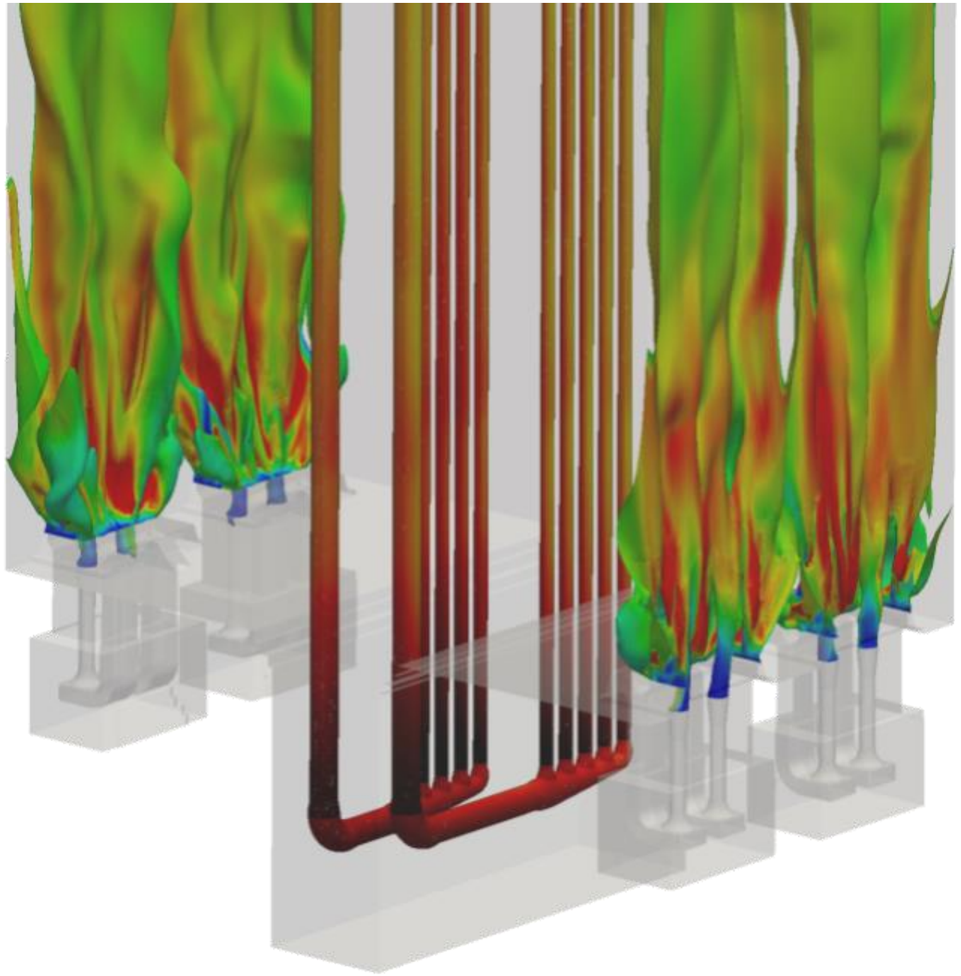
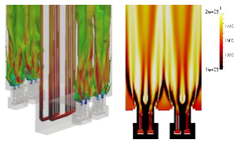
furnace modeling – the present







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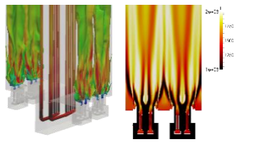
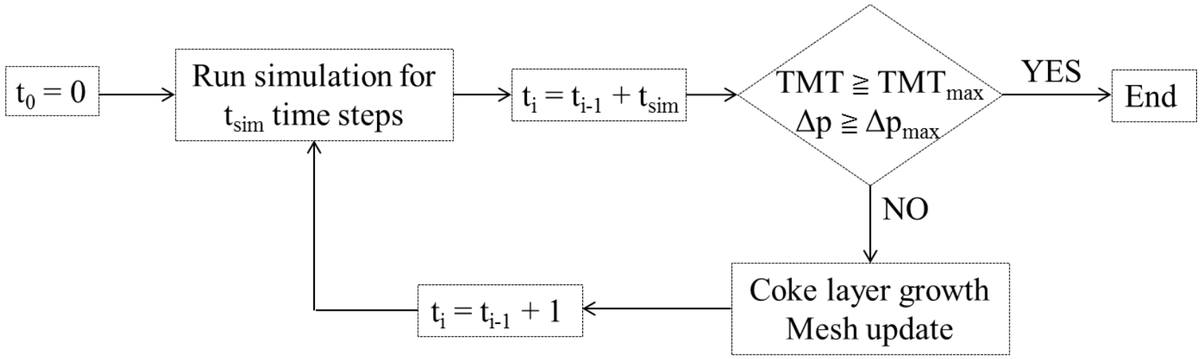
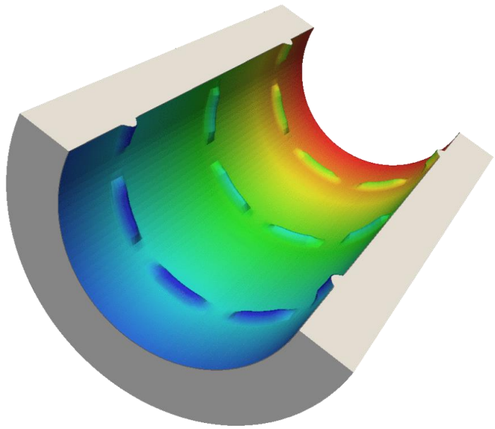
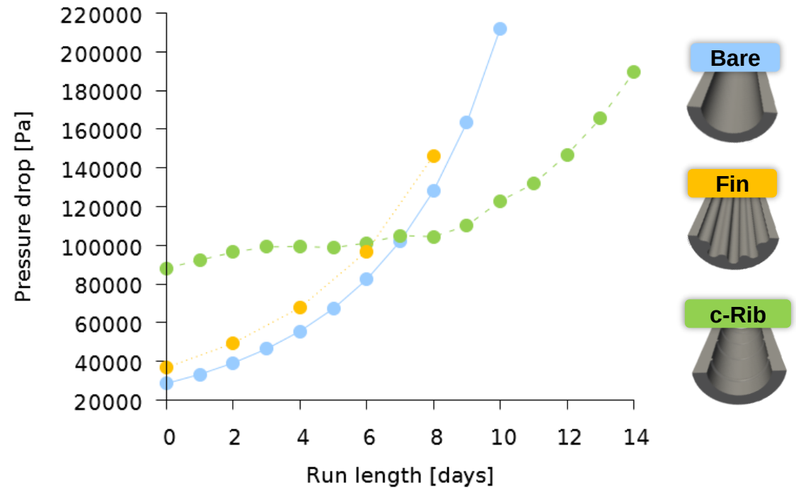
Dynamic run length simulation

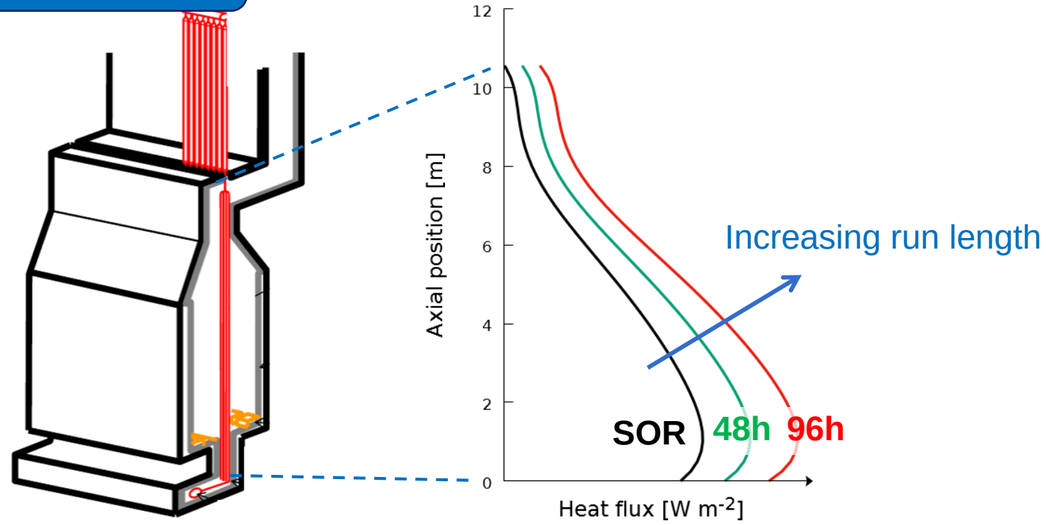




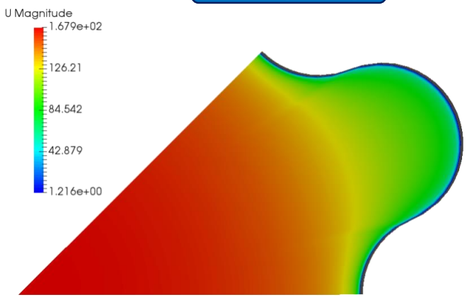




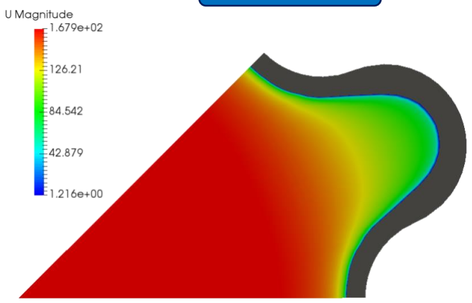
Propane Millisecond
29 species, 151 reactions

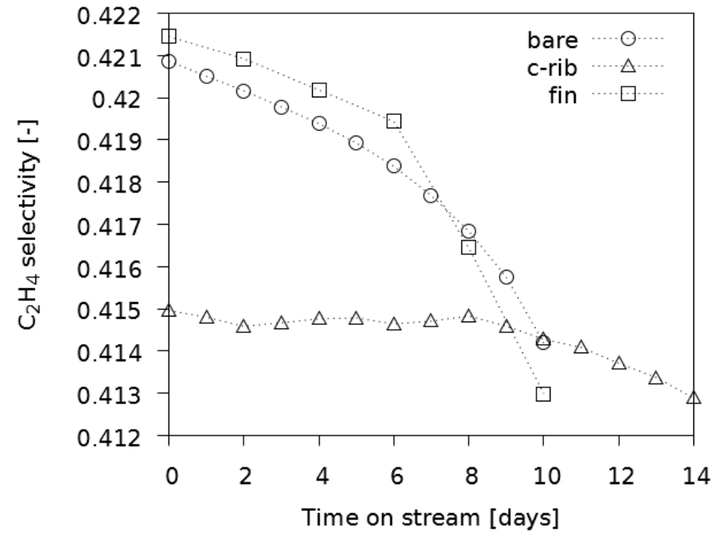


SOR (0 hrs)



48 hrs





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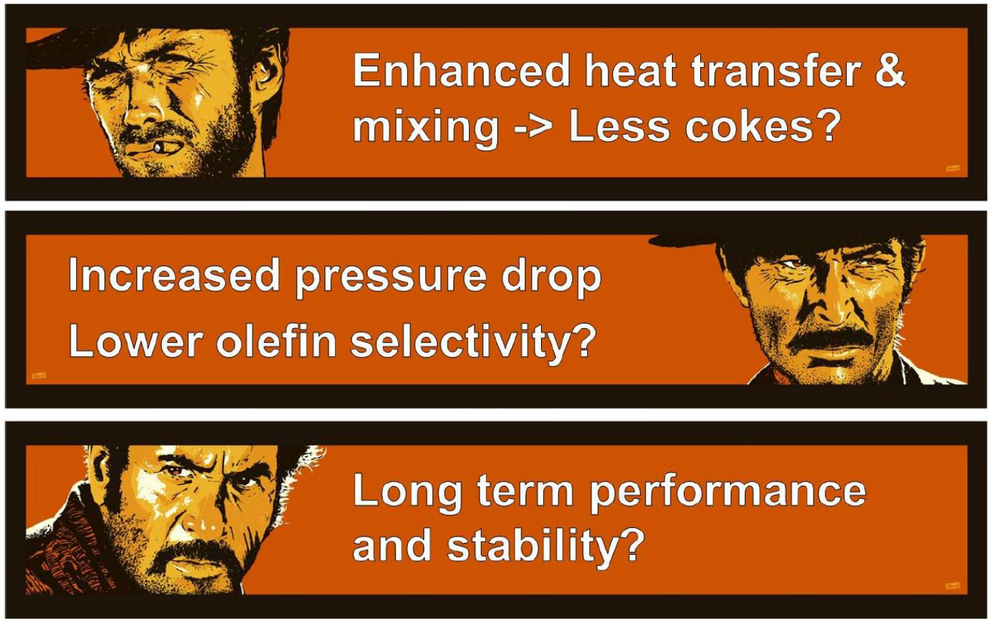
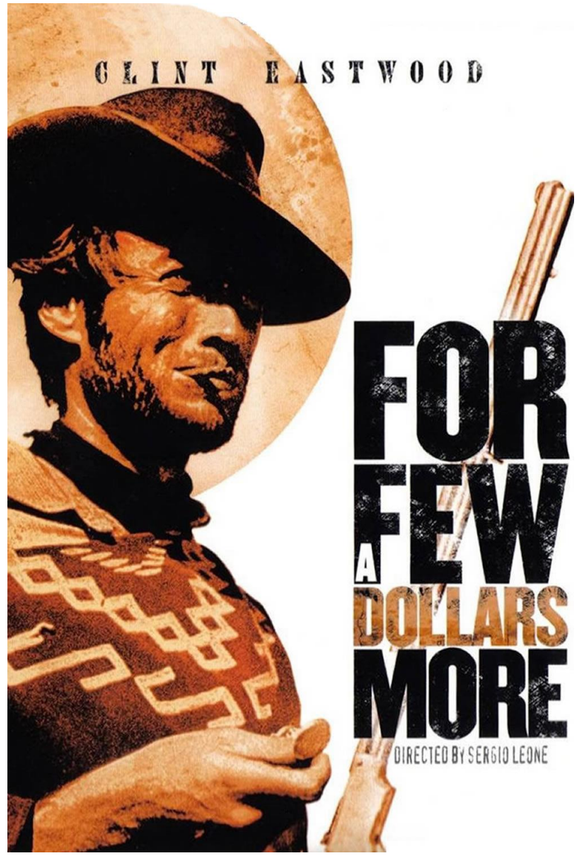
Vandewalle, L. A. et al. Chem. Eng. J. 12017, 329, 77-87.

3D reactor technologies - 12019





Improved coil design for a hole-in-one

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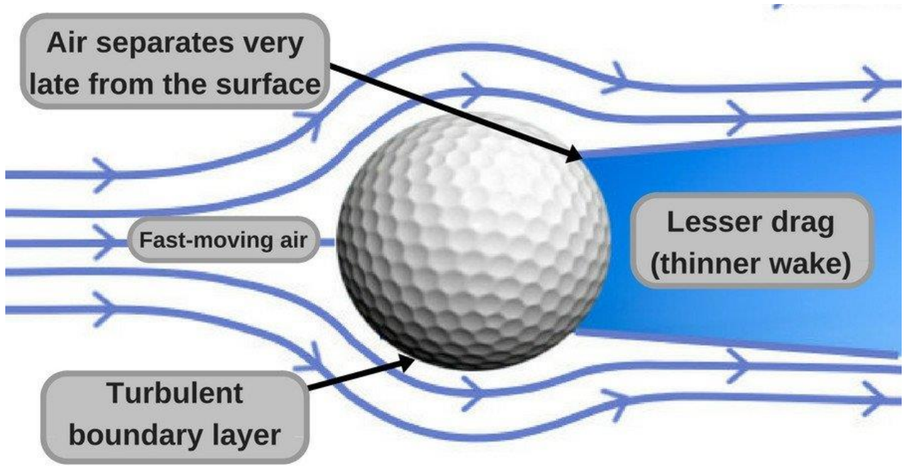
Golf and turbulent flow



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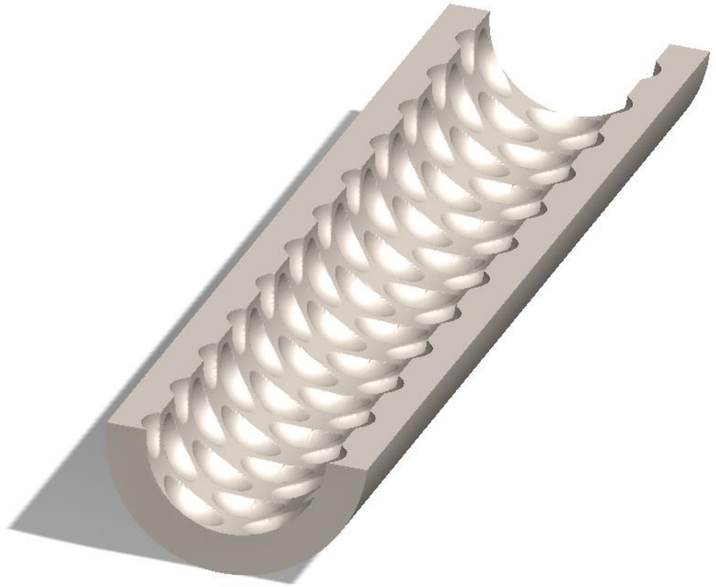
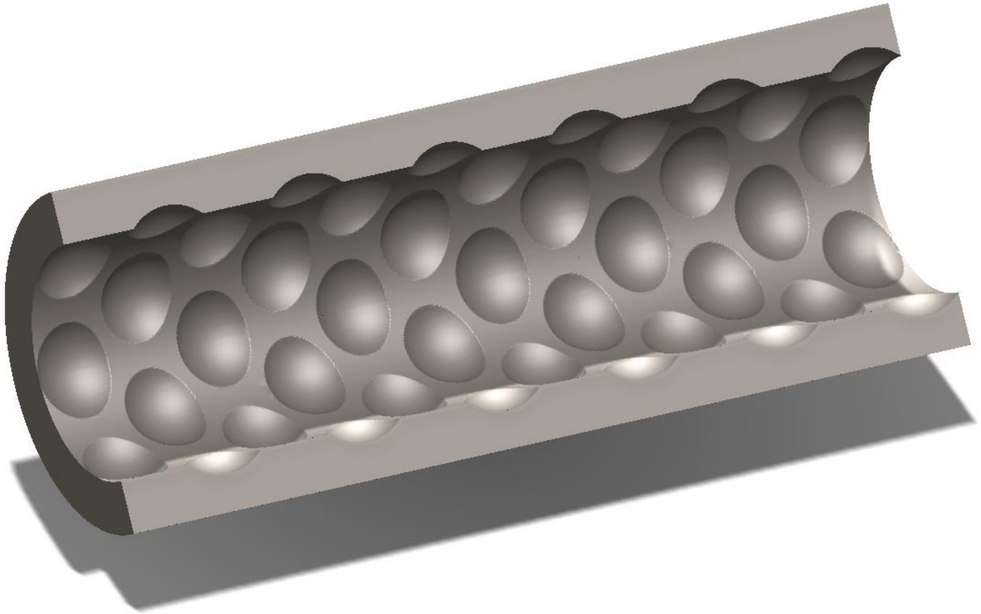
Golf meets a steam cracking coil





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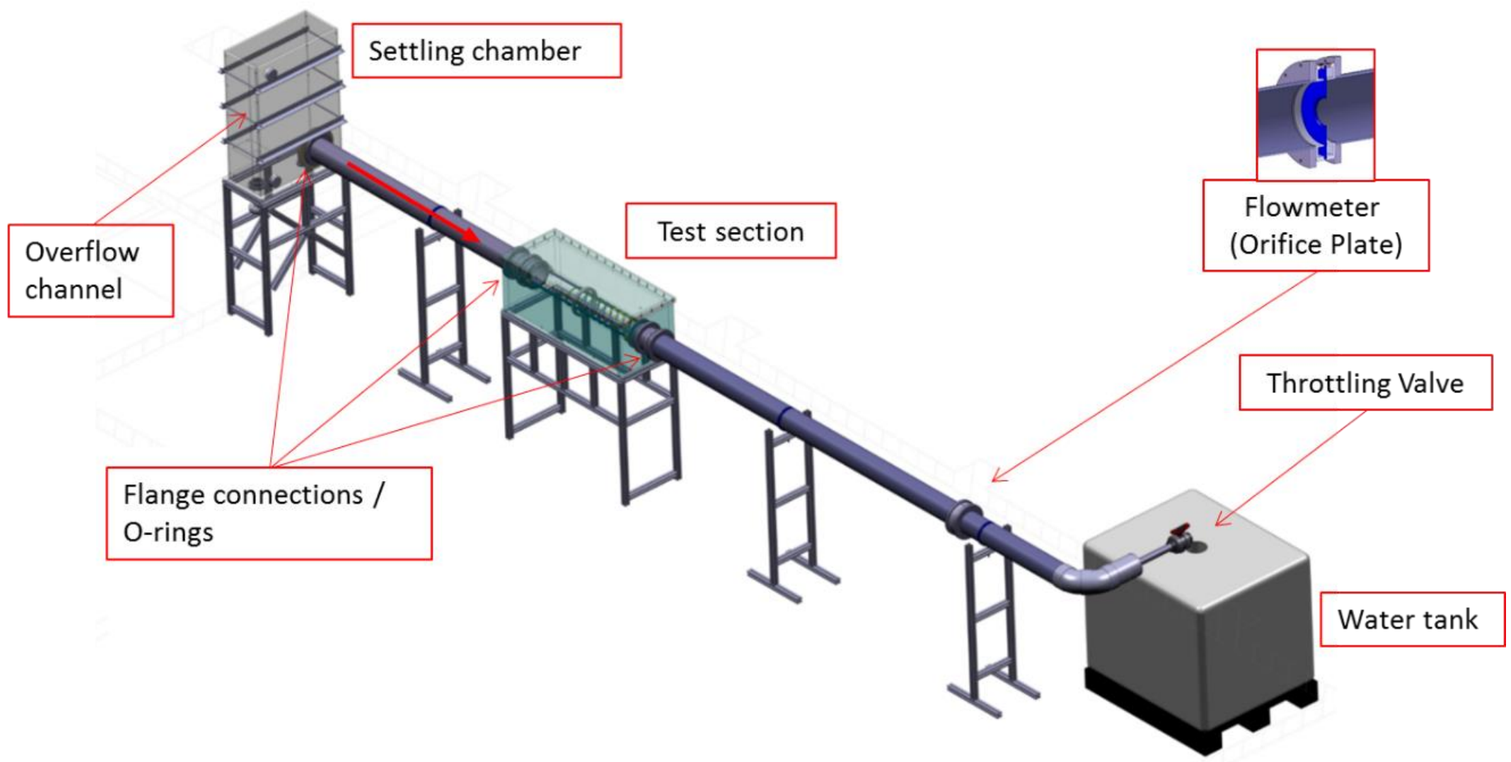
Experimental investigation – PIV setup



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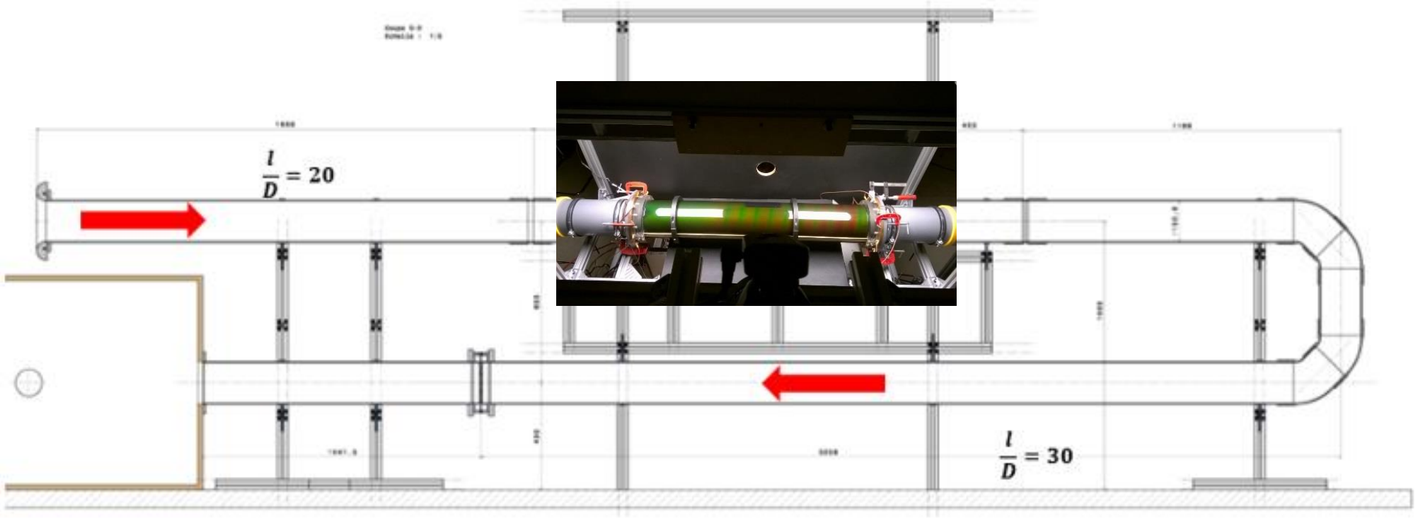
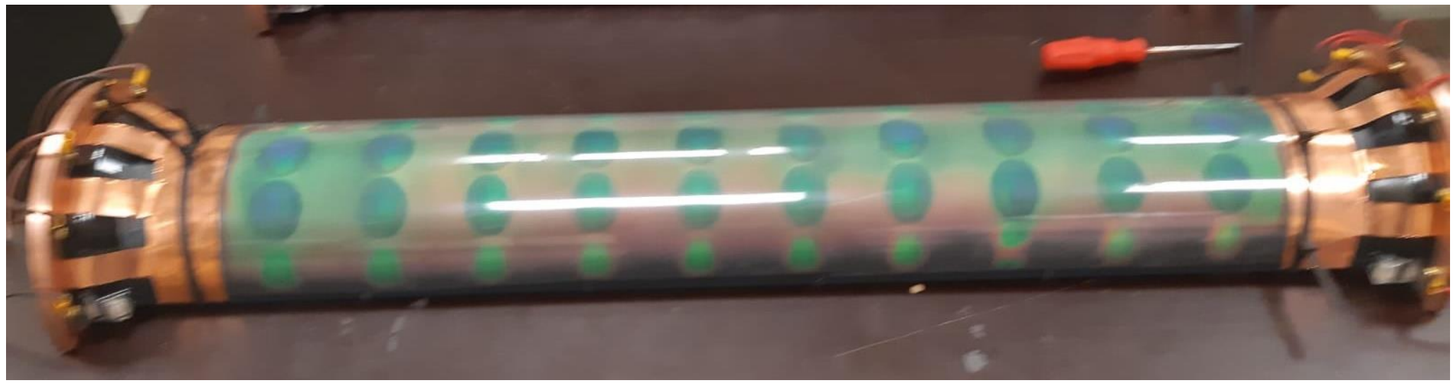
The von Karman Institute for Fluid Dynamics

Experimental investigation – Heat transfer setup





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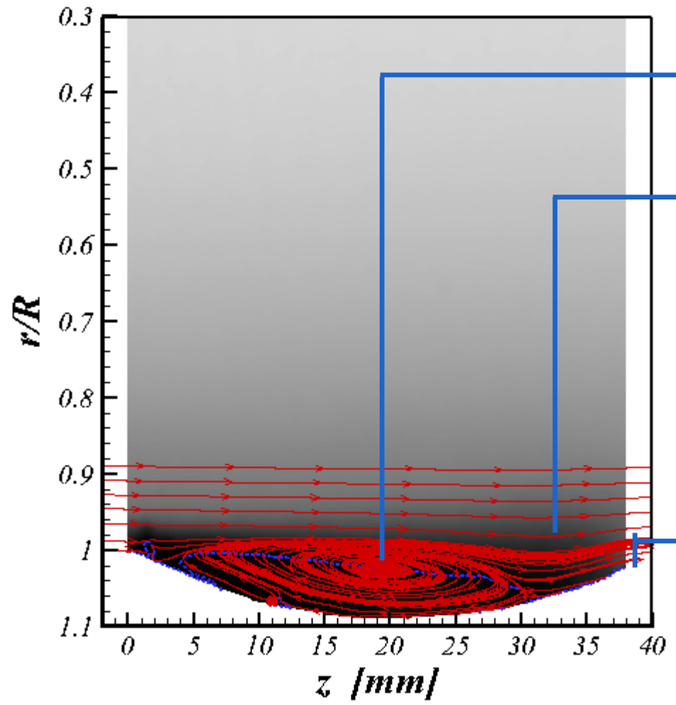
Flow in a dimpled coil



- Large swirling recirculation zone
- Perpendicular streamlines away from the wall
  - ➔ effect focused in near-wall region
  - ➔ low pressure drop
- Focused stream lines
  - ➔ high near-wall velocities
  - ➔ small thermal boundary layer
  - ➔ good heat transfer

Flow in dimpled coil exhibits desired properties

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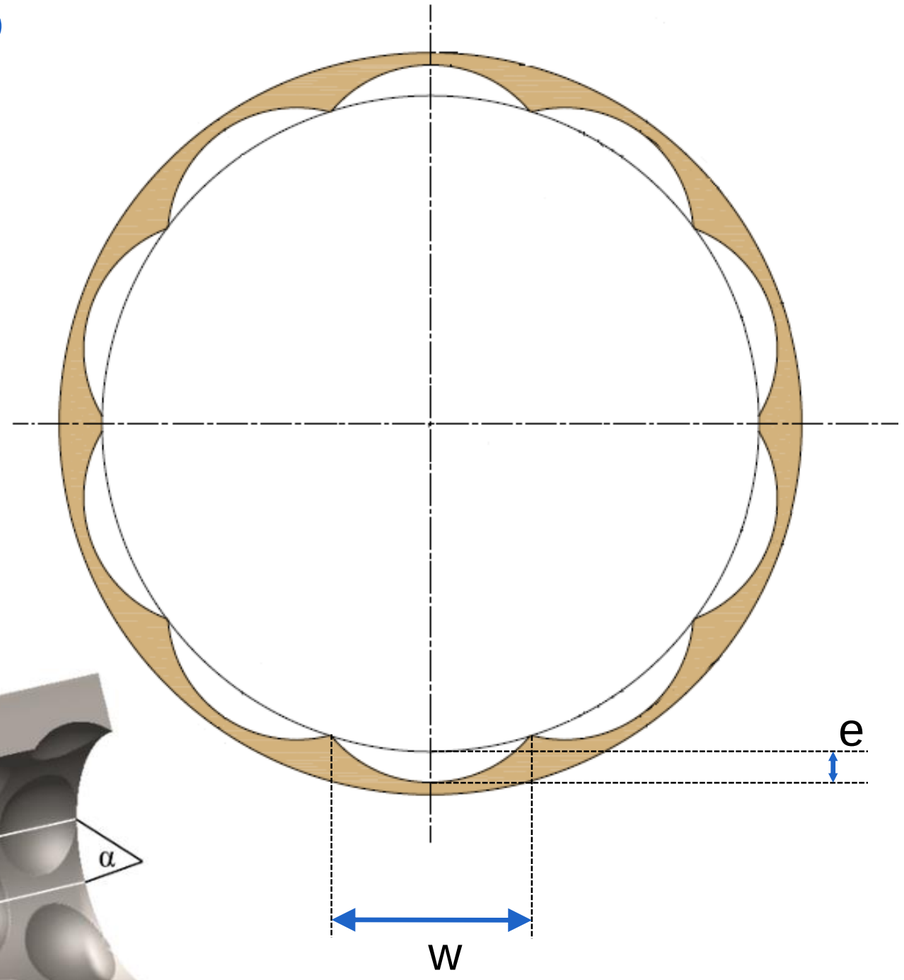
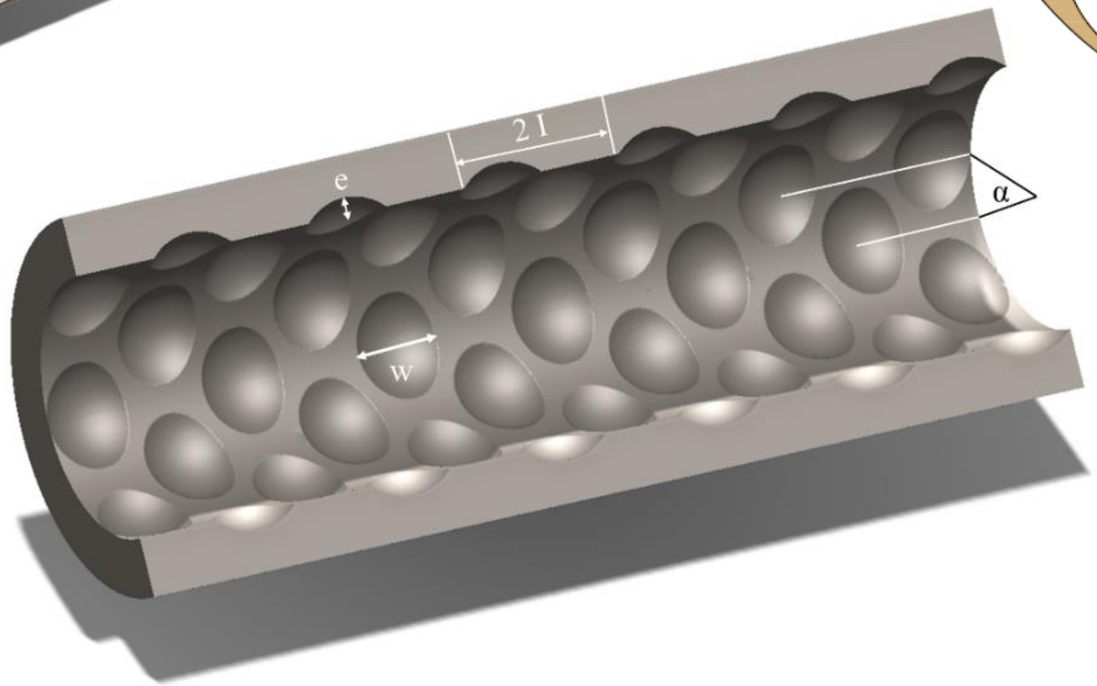
Effect of geometric parameters?





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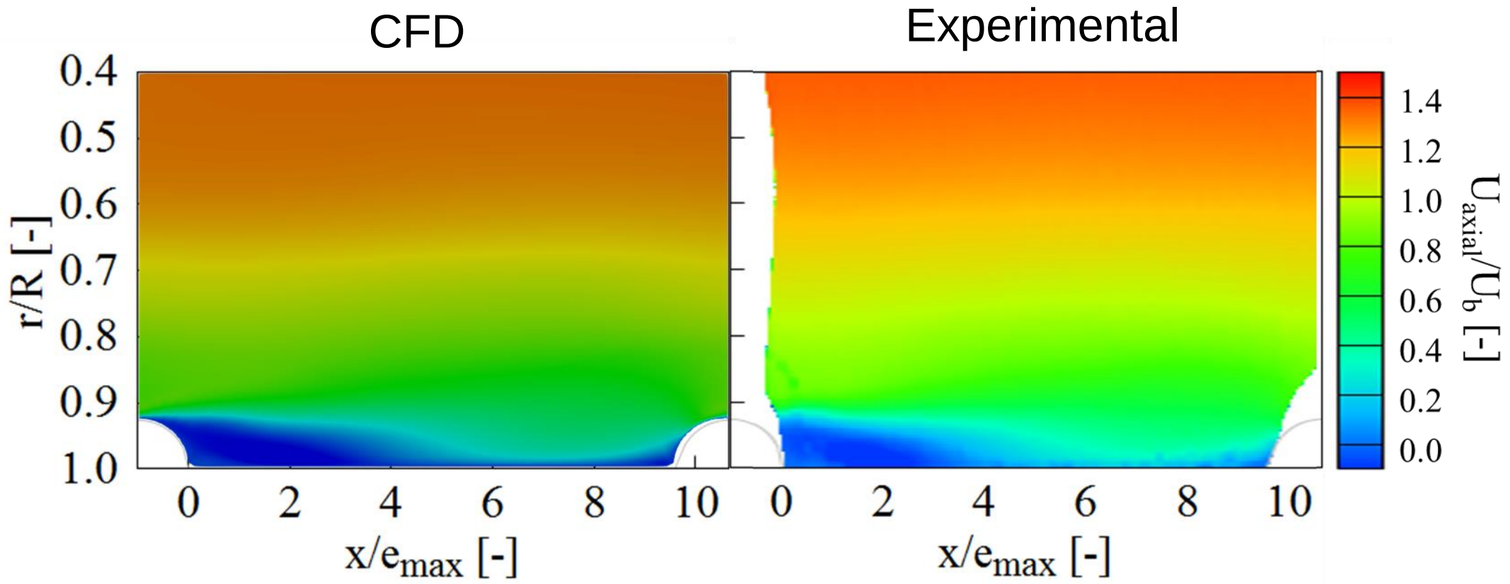
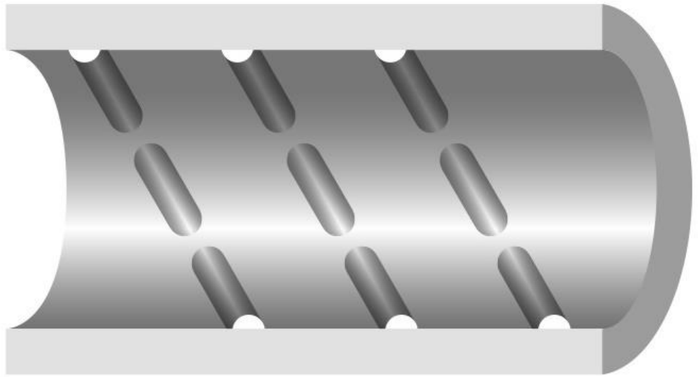
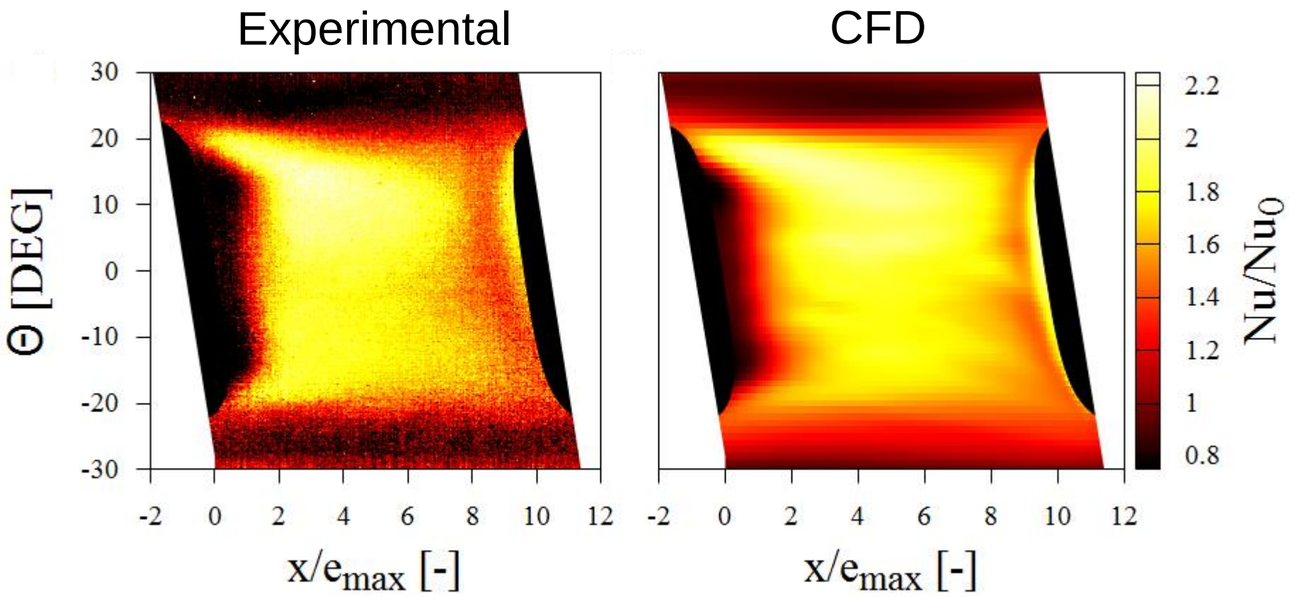
CFD validation







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The von Karman Institute for Fluid Dynamics

Impact of dimple depth

(a) Titleist Pro V1 (b) TaylorMade TP/Red LDP (c) Top Flite D2 Distance (d) Wilson Staff DX2 Distance

(e) Callaway Big Bertha (f) Nike PD 2 (g) MaxFli (h) Srixon AD333

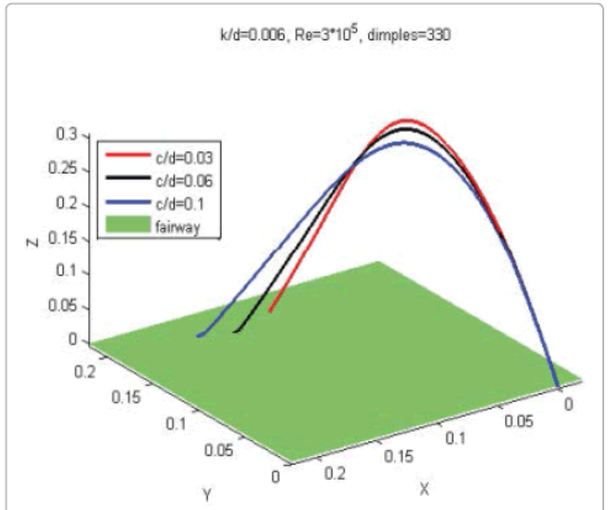

Figure 11: Three dimensional depictions of flight trajectories for varied dimple size.

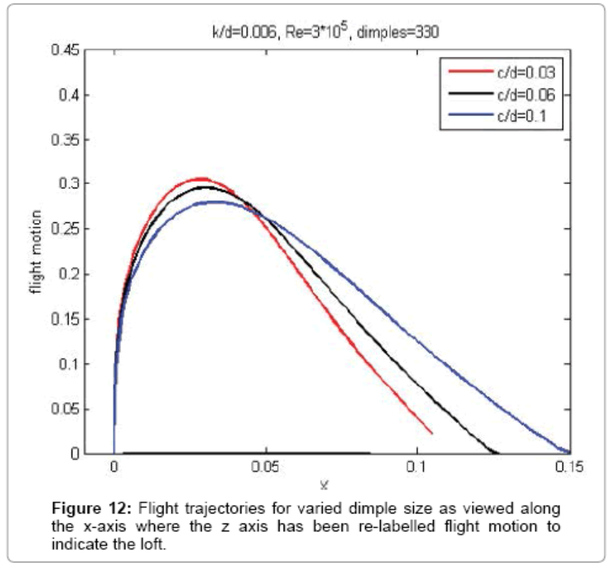

Figure 12: Flight trajectories for varied dimple size as viewed along the x-axis where the z axis has been re-labelled flight motion to indicate the loft.

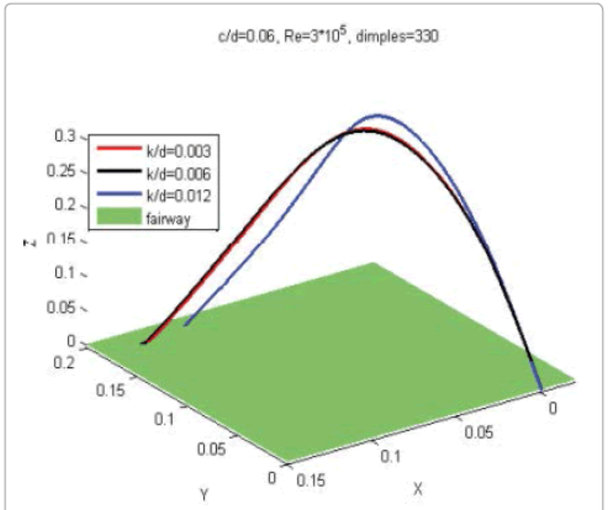

Figure 13: A simulation of the effect of dimple depth on the flight trajectory.

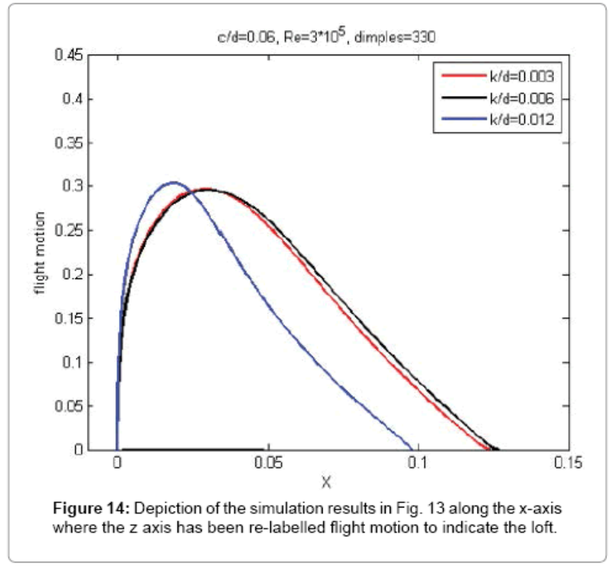

Figure 14: Depiction of the simulation results in Fig. 13 along the x-axis where the z axis has been re-labelled flight motion to indicate the loft.

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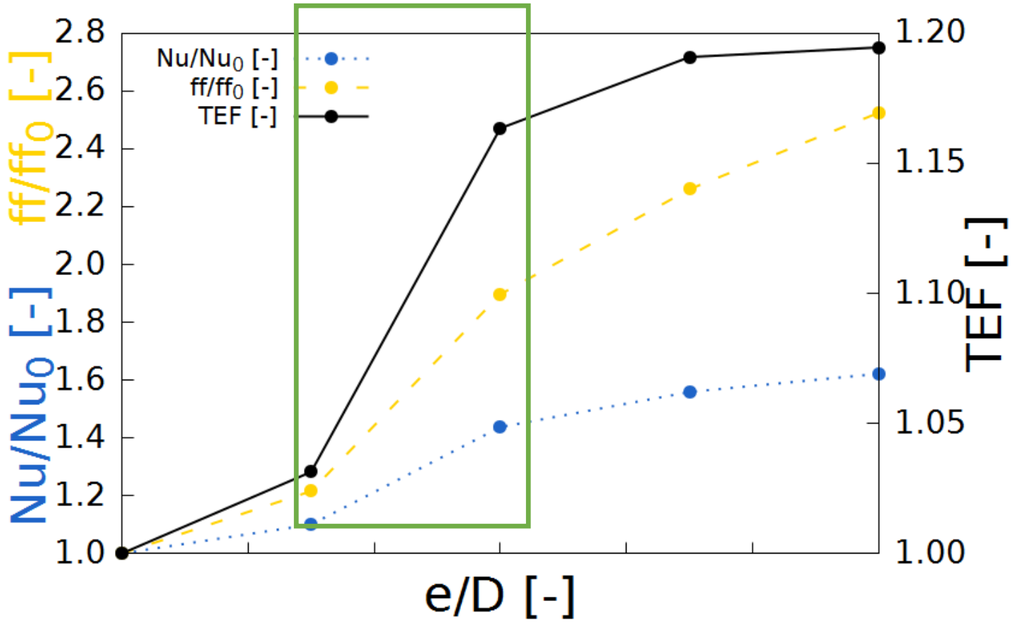
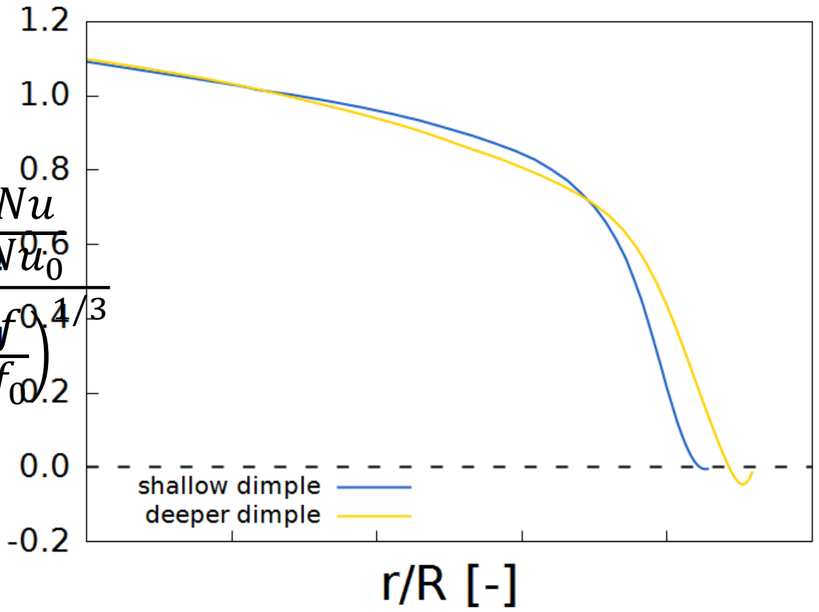
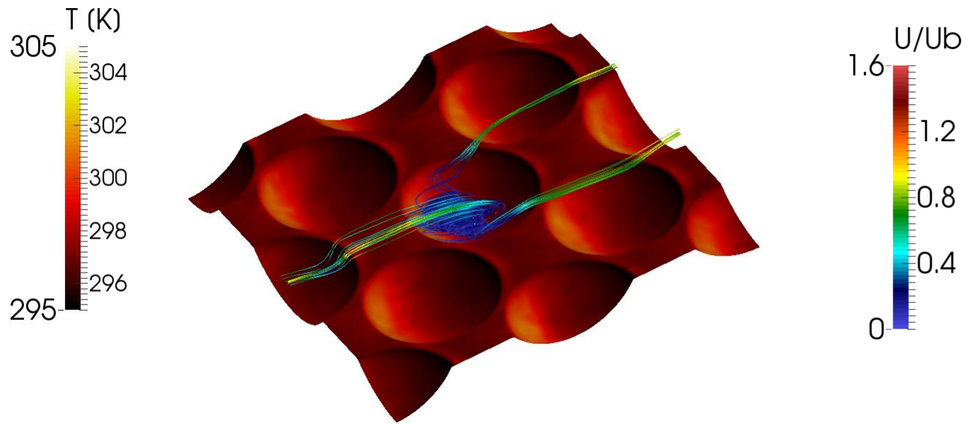
Wainaina M, Kimathi M, Malonza D, "Simulation of Dimple Characteristics on the Trajectories of a Dimpled Sphere (Golf Ball) in Motion," *J Appl Computat Math, 12018, Vol 7*, p. 386.

Impact of dimple depth (e)



$$TEF = \frac{\frac{Nu}{Nu_0}}{\left(\frac{ff}{ff_0}\right)^{1/3}}$$





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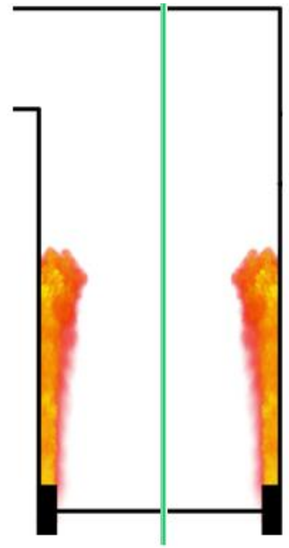
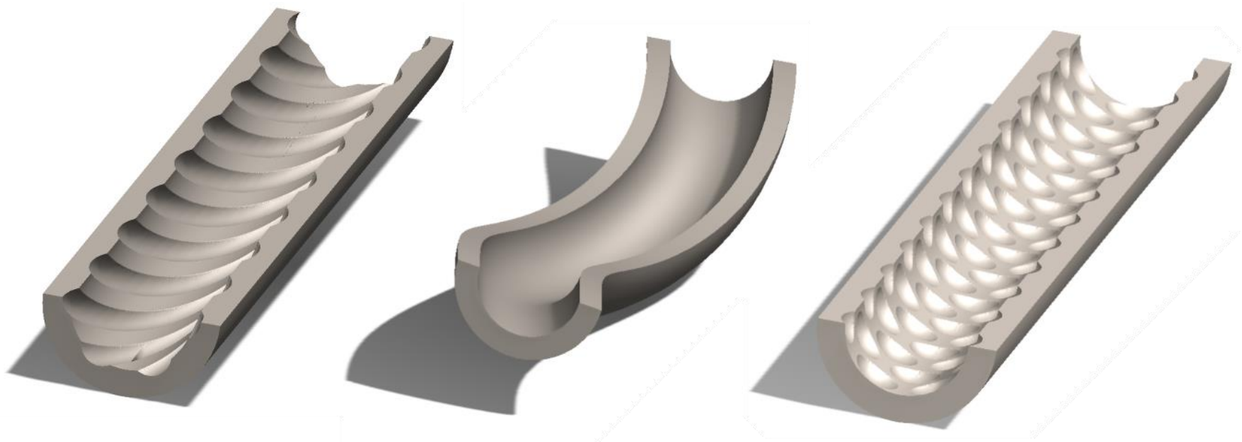
J. N. Dedeyne, D. J. Van Cauwenberge, P. A. Reyniers, K. M. Van Geem, and G. B. Marin, "Large eddy simulation of tubular reactors with spherical dimples," *Chemical Engineering Journal,* p. 122463, 12019.

Comparison with other reactor technologies

Process conditions	
Reactor length	11 m
Feedstock	118.54 kg/h propane
Steam dilution	0.326 kg/kg
Coil Inlet Temperature	903 K
Coil Outlet Pressure	170 kPa
Conversion	80.6 %





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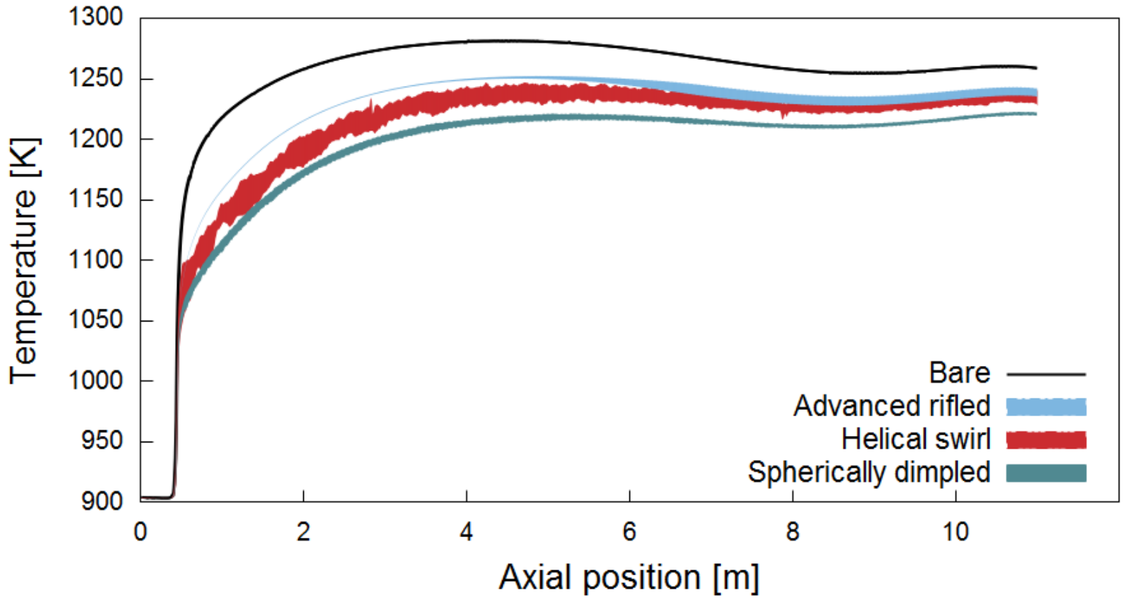
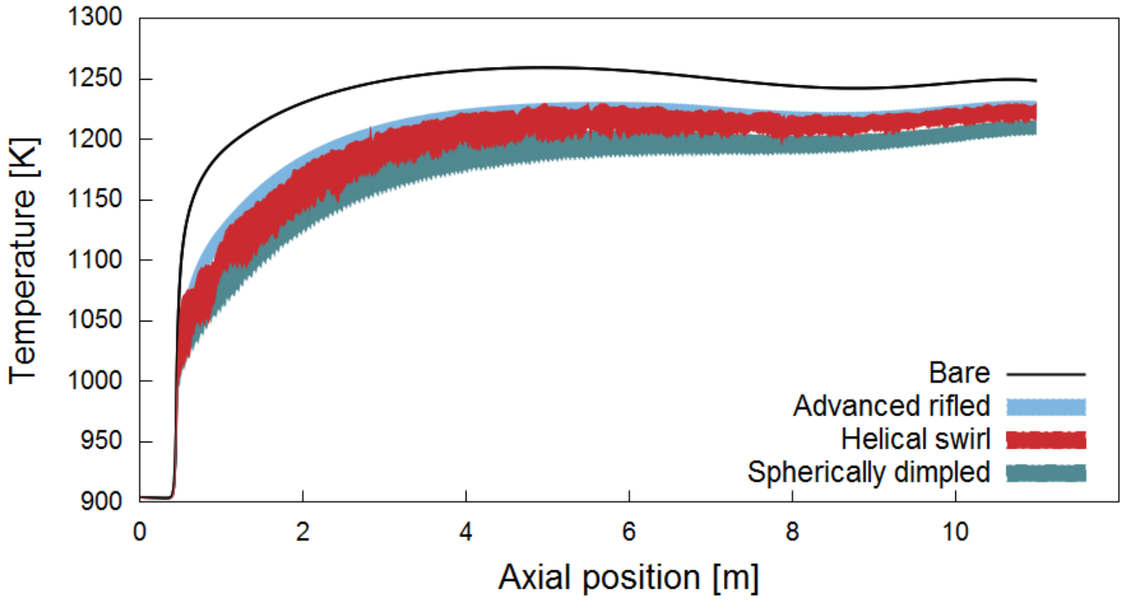
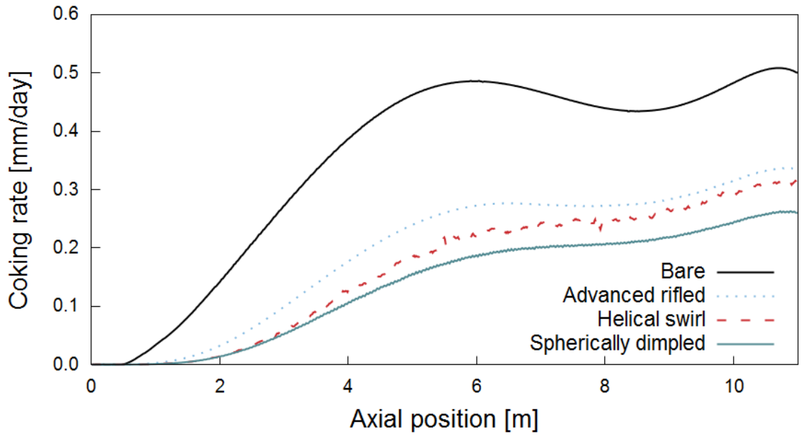
Reduced metal temperatures

Outside ~ TMT limitations



Inside ~ Coking rate





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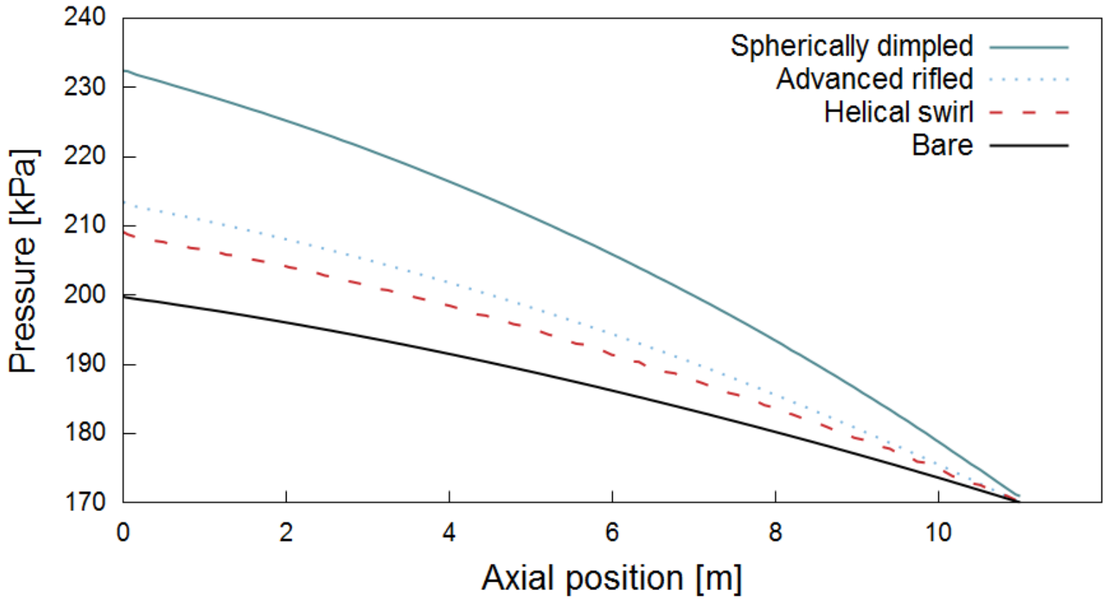
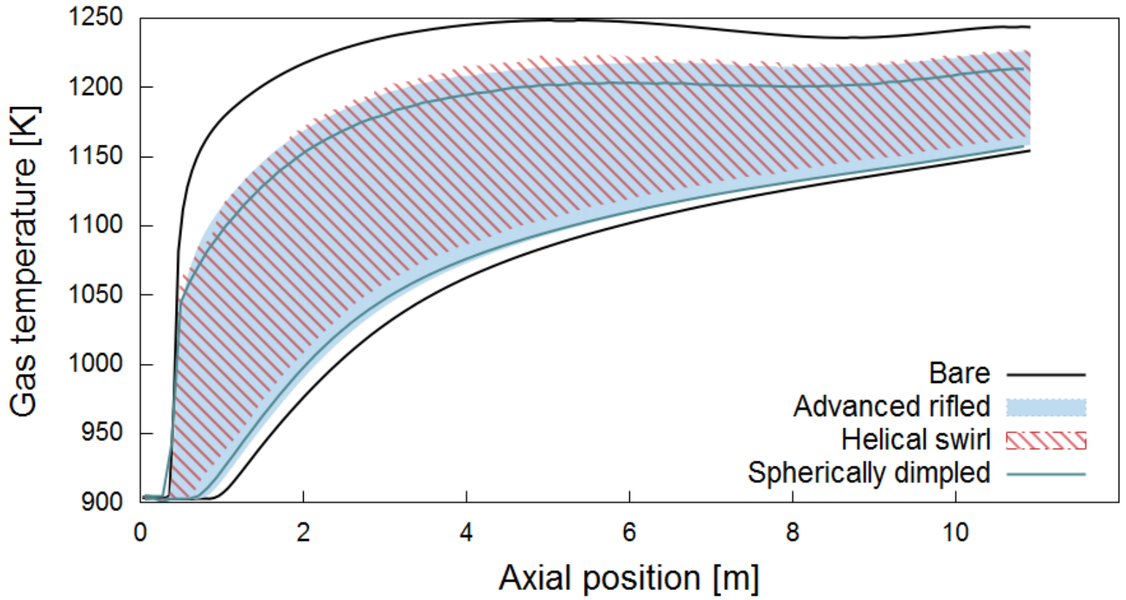
Higher Δp & more uniform T_{gas}





Substantial Δp due to relatively deep dimples
(e/D = 0.066)

Lower coking rate will reduce this difference over time

T_{gas} much more uniform for dimpled coils

Spherical dimples realize the most narrow distribution

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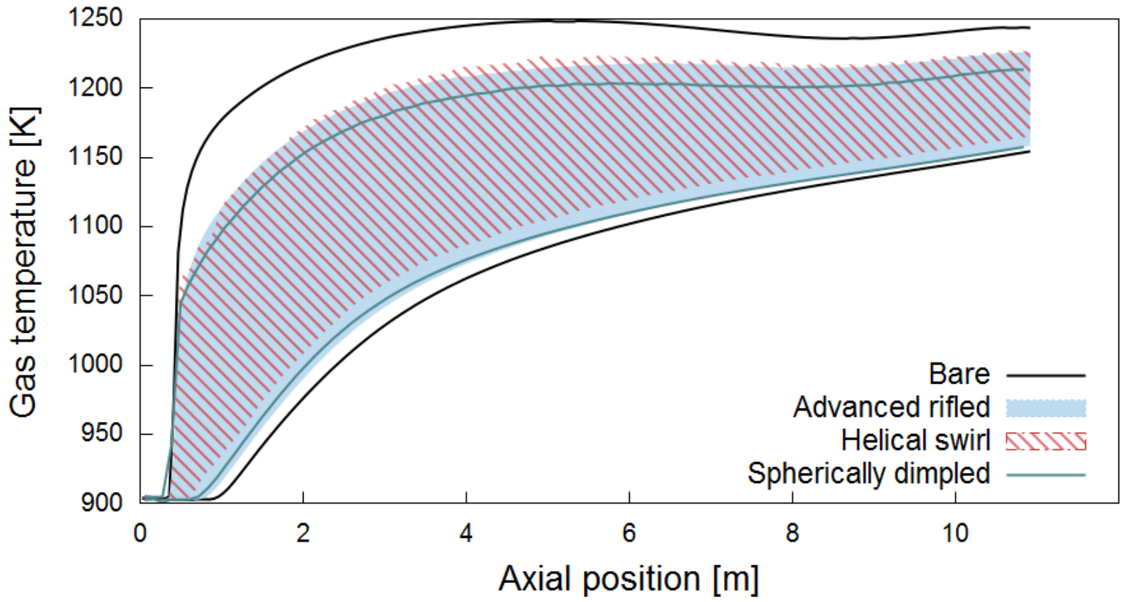
Reactor technology – P/E



Lower peak temperatures

➔ Less overcracking = higher propylene selectivity

➔ 3D reactors result in higher P/E at same X

Yields [wt%]	C3H6	C2H4	C4H6	CH4	C3H4	Benzene
Bare	17.41	34.02	1.66	19.27	0.65	1.54
Helical Swirl	17.99	33.71	1.60	19.30	0.65	1.48
Advanced Rifled	18.32	33.54	1.57	19.21	0.65	1.45
Spherically Dimpled	18.33	33.55	1.58	19.33	0.63	1.43

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Impact of dimple shape

TRUTH DIGEST
MYGOLFSPY

#DIMPLEGATE — TITLEIST SUES 10 SMALL BALL COMPANIES

BY JOHN BARBA

MAY 21, 2015 | 88 COMMENTS

Back in April Acushnet filed suit in Federal Court in Boston, claiming that ten *competitors* are violating Acushnet's patented "triangular dipyramid dimple pattern" with their offerings.

How to come up with the best shape?

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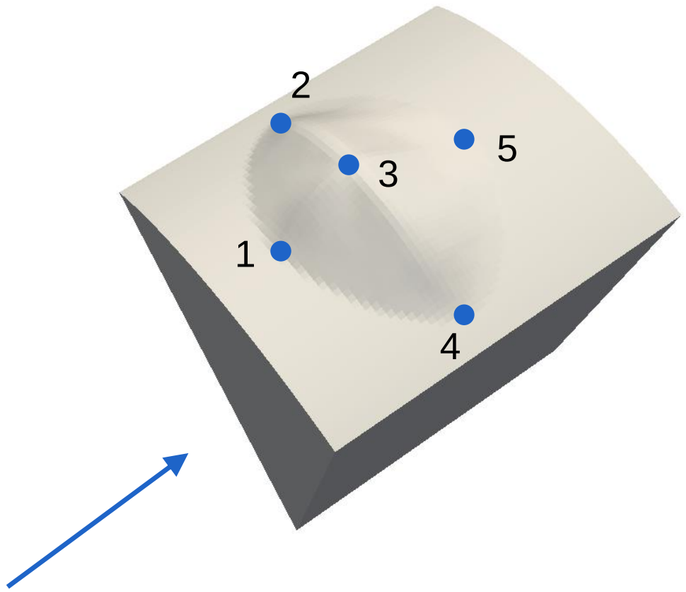
Shape parameters

Best shape = best combination of geometrical parameter values

5 important surface points



1: most upstream point of dimple

2 & 4: Determining maximum dimple width

3: Determining max dimple depth

5: most downstream point of dimple

Large variety of geometries possible with these parameters

However: no control over slope of surface

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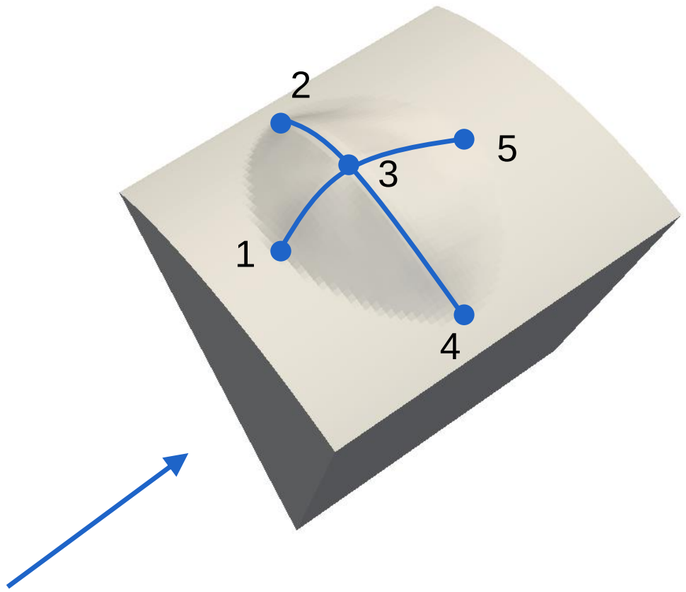
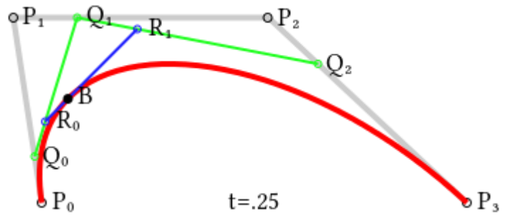
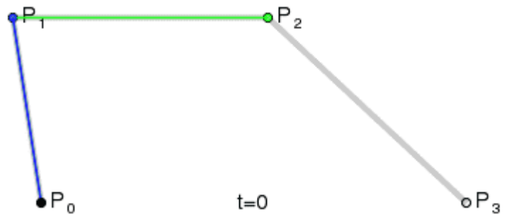
Shape parameters

Best shape = best combination of geometrical parameter values

5 important surface points connected via 4 quadratic Bézier curves







Easy to calculate, parametric curves

Wide range of smooth curves possible

Used in animation, robotics, automobile design, …

Curvature completely described by 4 points/parameters

➔ Start and end points defined by 2 surface points

➔ 2 additional points (weights) describing slope of curve

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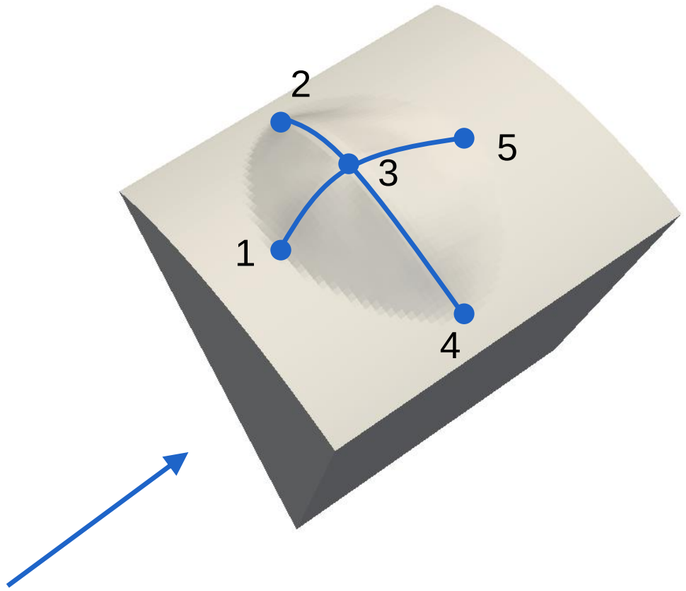
Shape parameters

Best shape = best combination of geometrical parameter values

5 important surface points connected via 4 quadratic Bézier curves



Degrees of freedom

- Position of surface points (5 points x 3 coordinates = 15)
- Curvature of slope (4 curves x 2 points x 3 coordinates = 24)

Optimization of 39 parameters too demanding

➔ Imposed rules

- Points 1, 2, 4 and 5 on cylinder with fixed radius
- Point 1 completely fixed
- Tangential position of 1, 3 and 5 identical
- Curve 2-3 & 4-3 are symmetrical.
- Axial position of 2, 3 and 4 identical

Underlying assumption: asymmetric dimple shape not optimal

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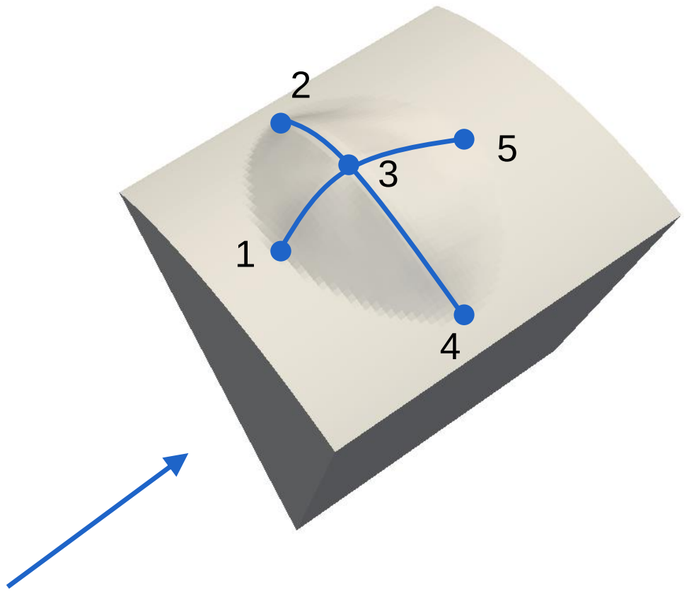
Shape parameters

Best shape = best combination of geometrical parameter values

5 important surface points connected via 4 quadratic Bézier curves



Actual degrees of freedom

- 1 for axial position of 2, 3, 4
- 1 for radial position of 3
- 1 for tangential position of 2, 4
- 1 for axial position of 5
- 2 for curvature of 1-3
- 2 for curvature 3-5
- 2 for curvature 2-3, 4-3

➔10 parameters to define shape

= 10 parameters to tune for optimization

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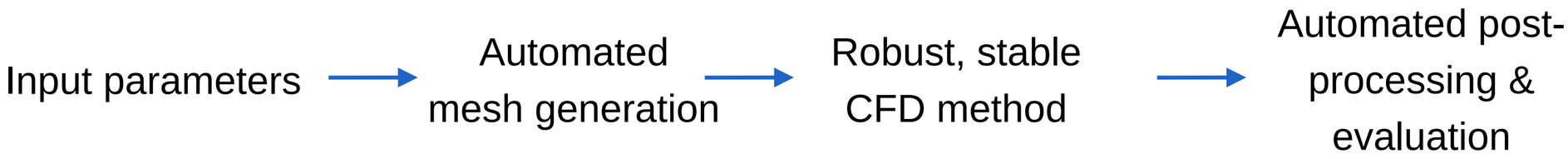
Optimization of 10 parameters

10 times 1D optimization ⇔ 1 time 10D optimization

Parameters could be dependent on each other ➔ 1 x 10D optimization for accurate results

This requires a very high number of CFD evaluations

➔ Automation of evaluations



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Automation of evaluations

Scripted grid generation

+ Excellent grid control
+ Lots of design options available
- Scripting language is bloated and cumbersome
+ Journaling option makes scripting easier

CFD evaluations

OpenFOAM

The OpenFOAM Foundation

+ Open source
+ Wide range of applications
- User experience required for complex cases
+ Start from previously converged similar case

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Optimization of 10 parameters

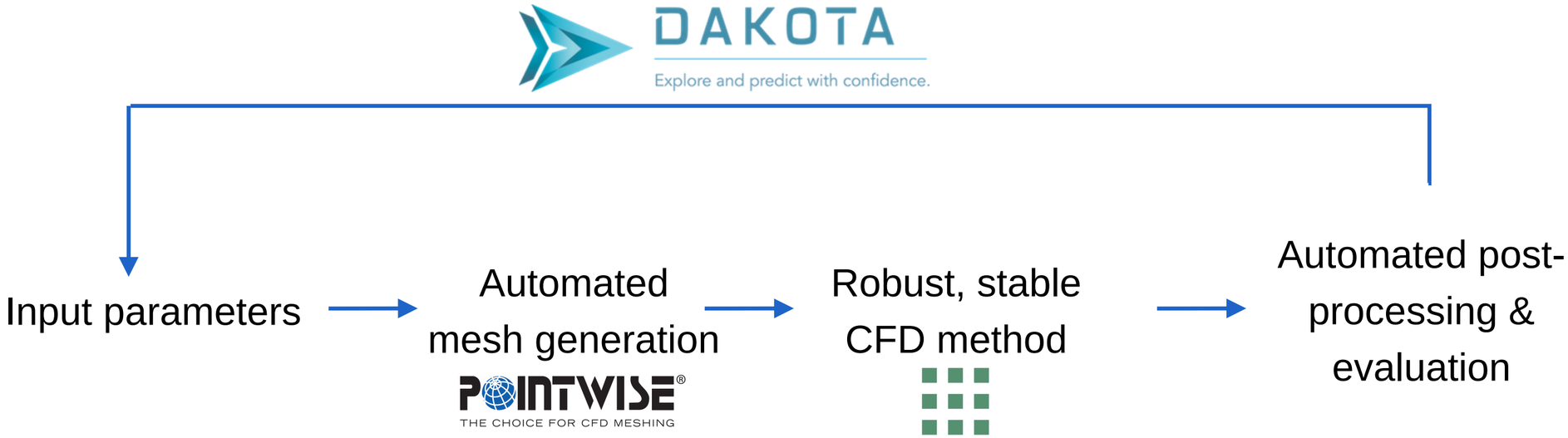
10 times 1D optimization ⇔ 1 time 10D optimization

Parameters could be dependent on each other ➔ 1 x 10D optimization for accurate results

This requires a very high number of CFD evaluations

➔ Automation of evaluations

➔ Smart selection of designs to evaluate



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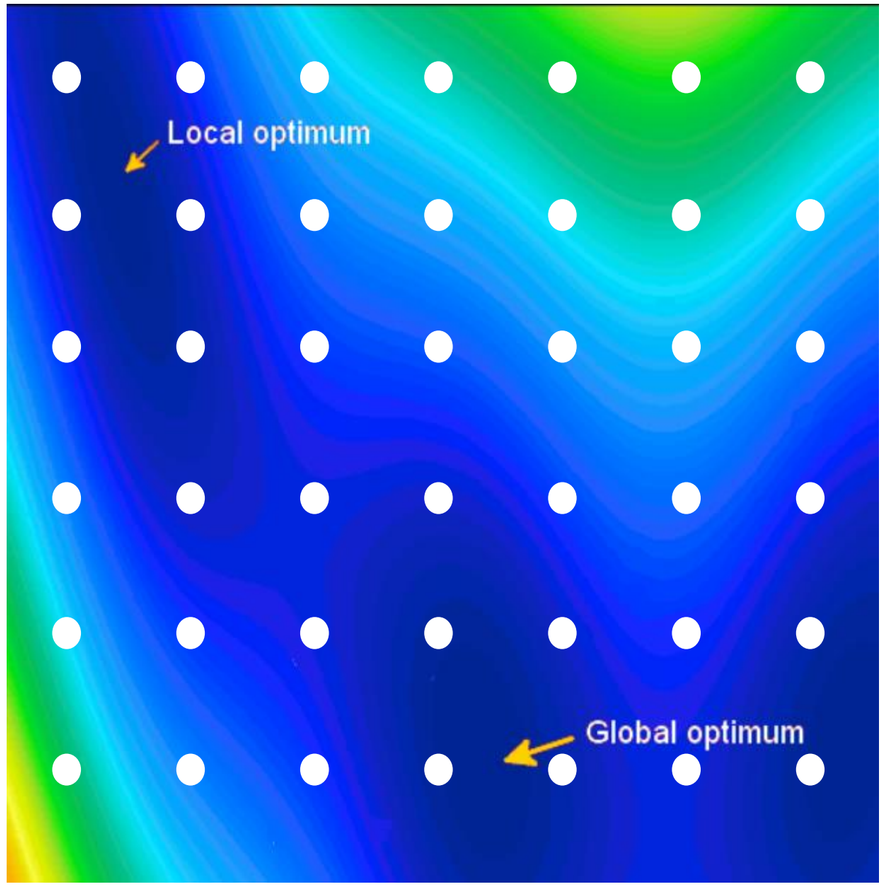
Smart selection of designs

Systematic sampling

time consuming



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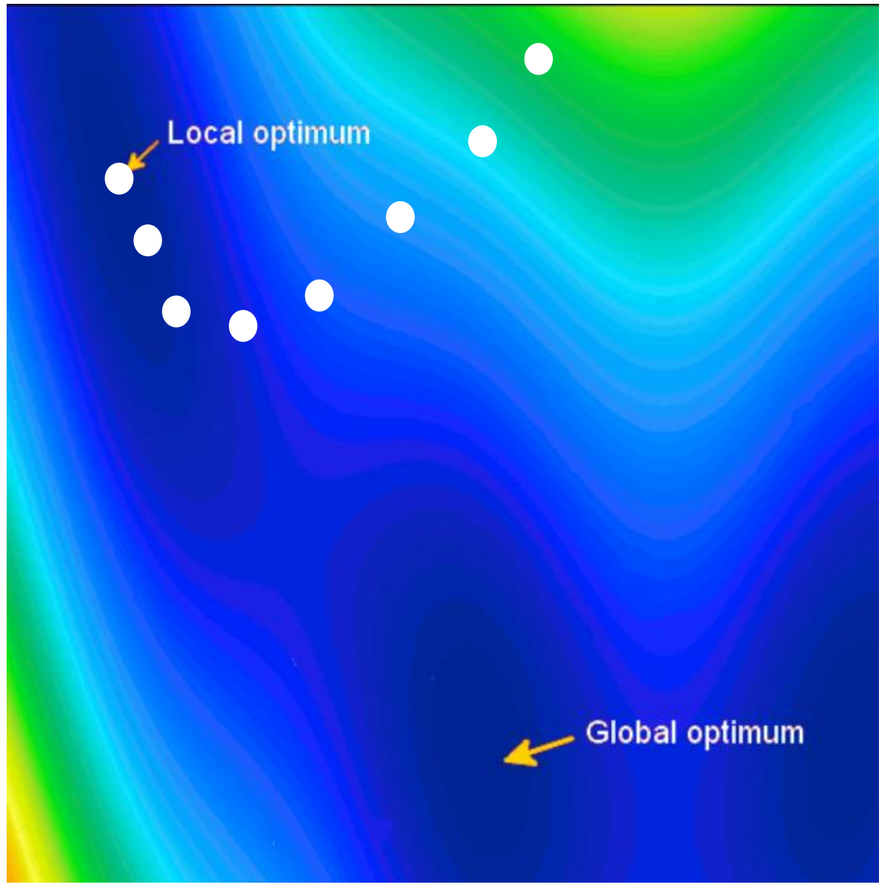
Smart selection of designs

Systematic sampling

time consuming

Sampling towards improved solution

risk of local optimum
result depending on initial case



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Smart selection of designs

Systematic sampling

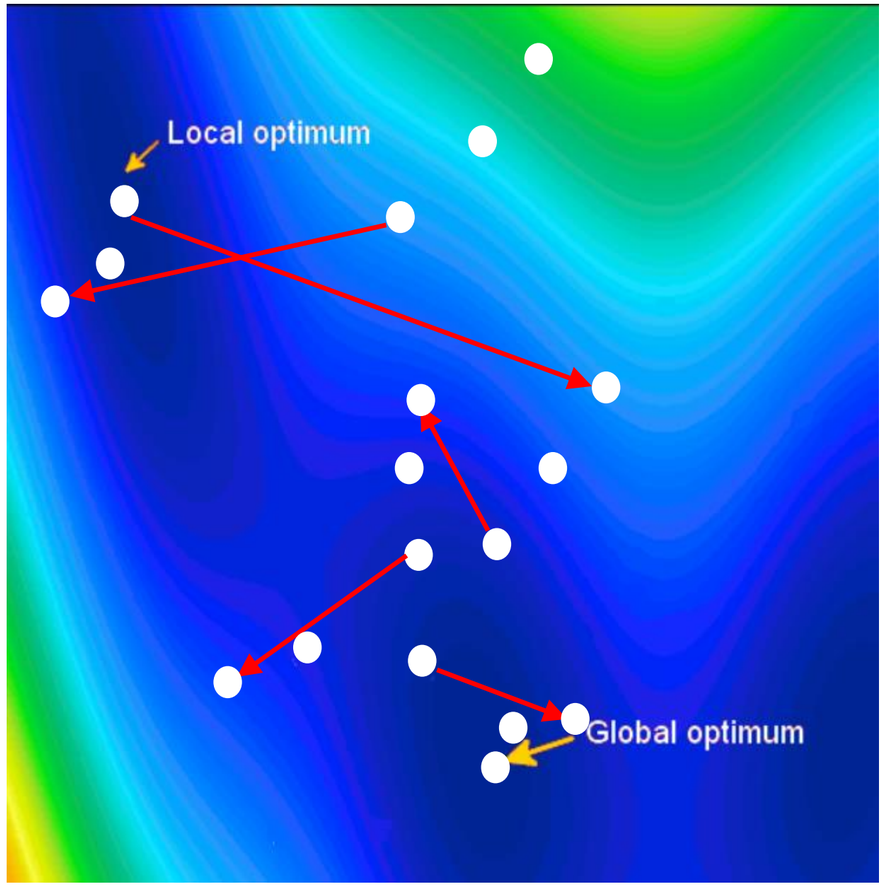
time consuming

Sampling towards improved solution

risk of local optimum
result depending on initial case

Sampling towards improved solution with randomization

given sufficient time always reaches global optimum
delicate balance between order and chaos
High order: waste time near local optima
High chaos: previously information “lost”



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Smart selection of designs

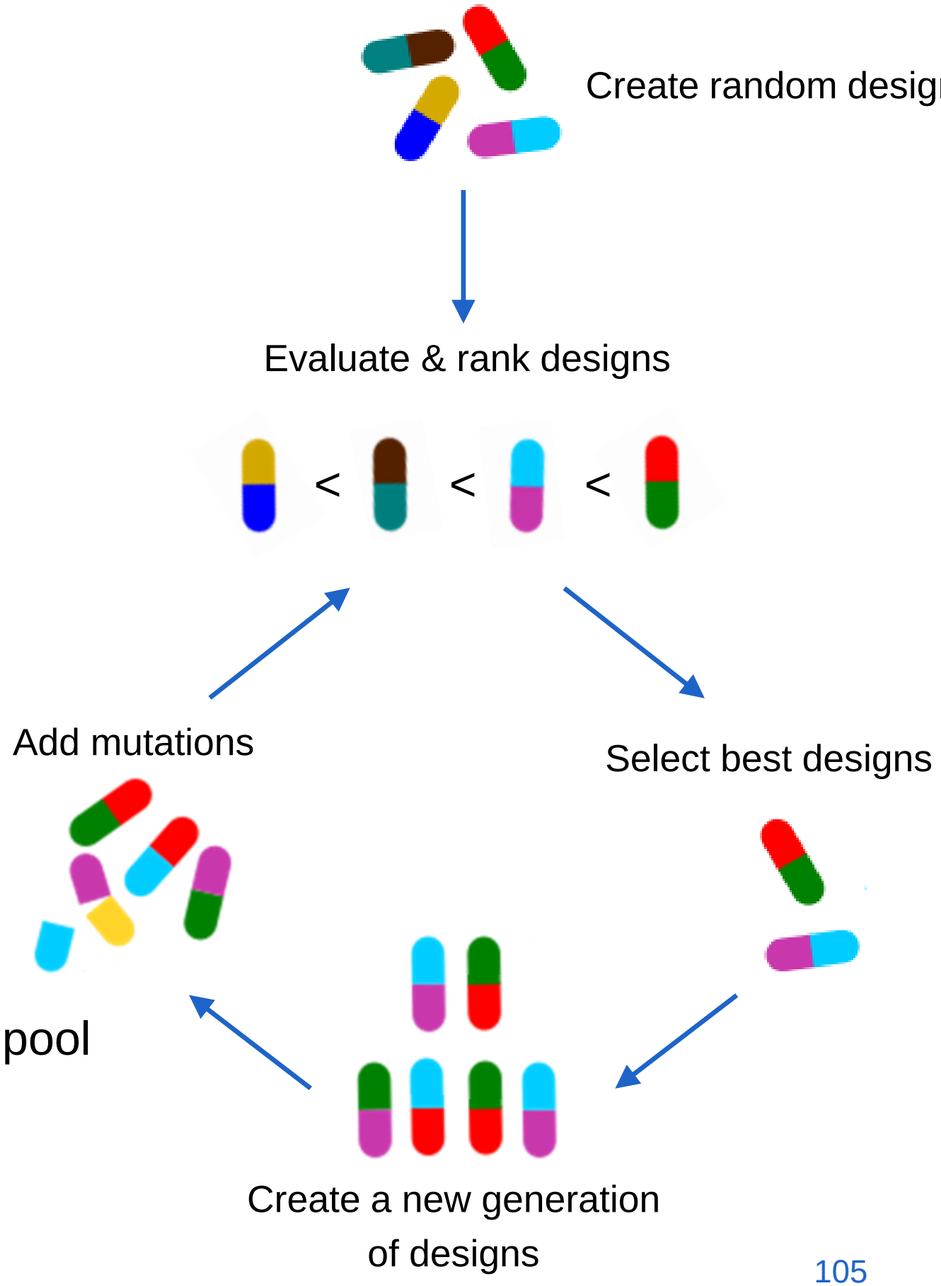
Genetic algorithm = theory of evolution

Parameter values = genes

Best designs pass their genes to next generation

How to determine what are the best designs?

1. Select an appropriate **objective function**
2. **Evaluate** the objective function value for all designs
3. **Rank** designs according to objective function value
4. Highest ranks are the best designs



Mutations can occur and introduce a random element in the gene pool

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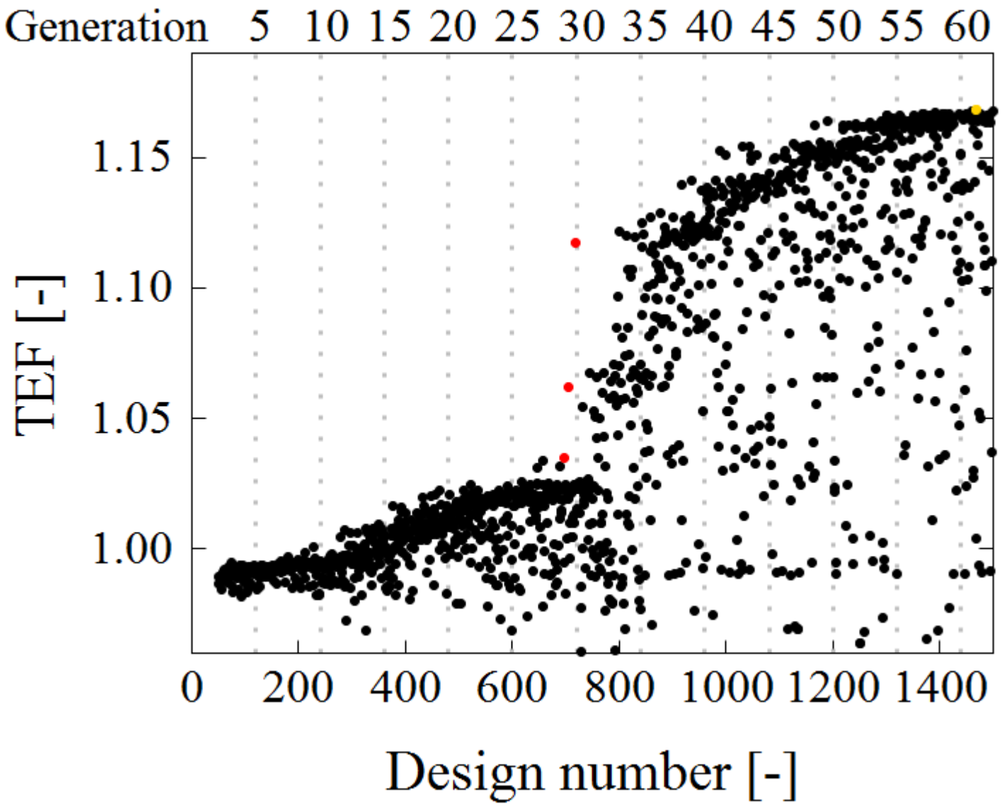
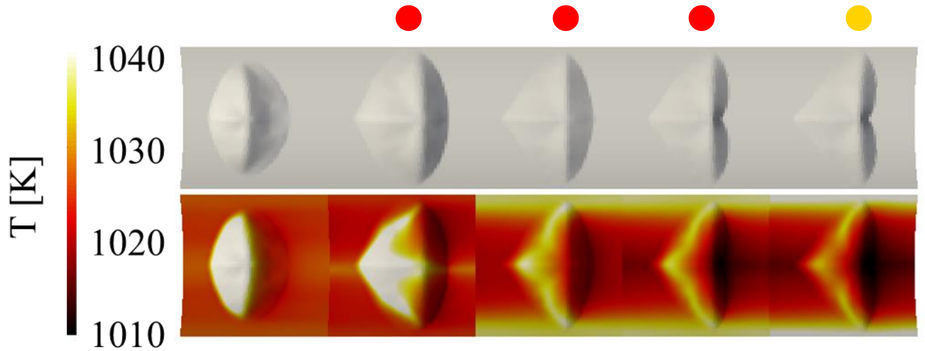
Optimization results - TEF





- Upstream part elongated & flattened
- Downstream part compressed
- Formation of cusp at downstream edge

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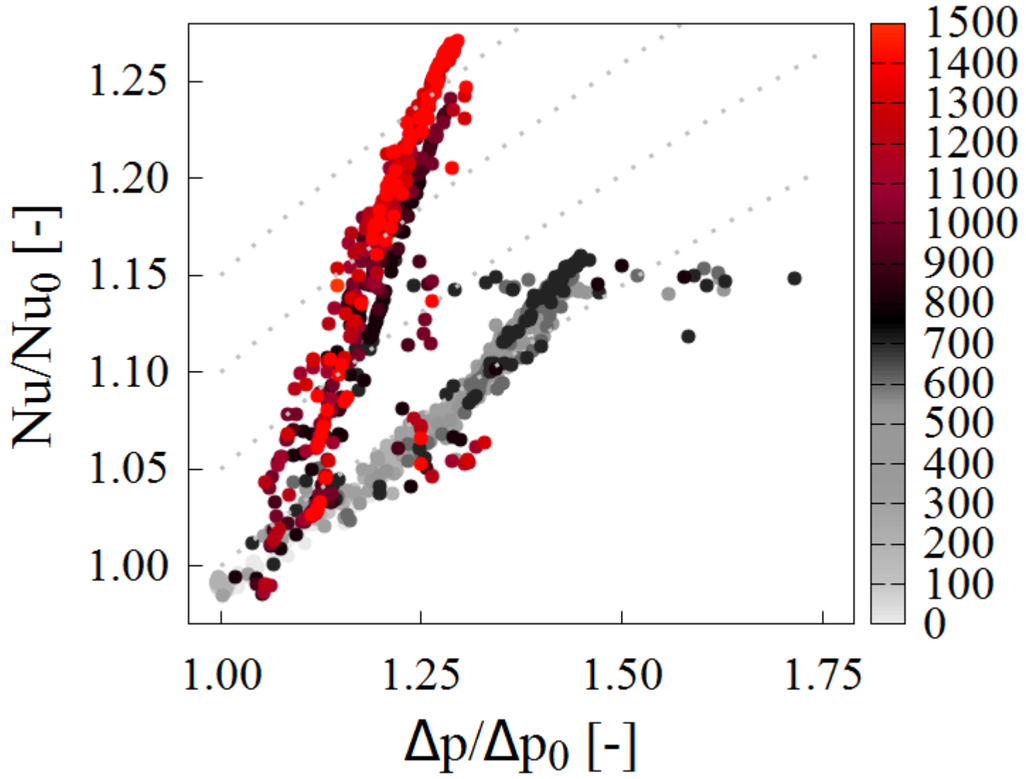
Close up to optimization results

Objective function can be debated.

Constituting elements can give a more detailed impression



Rapid change in TEF due to rapid decrease in Δp
= flattening & elongating upstream section

Final increase in TEF due to improved heat transfer
= cusp formation

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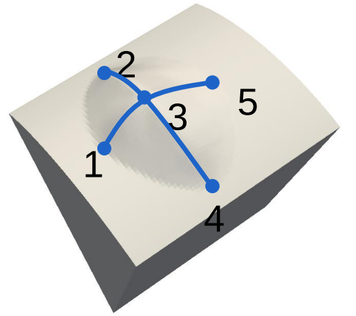
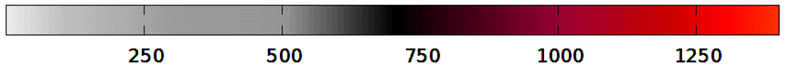
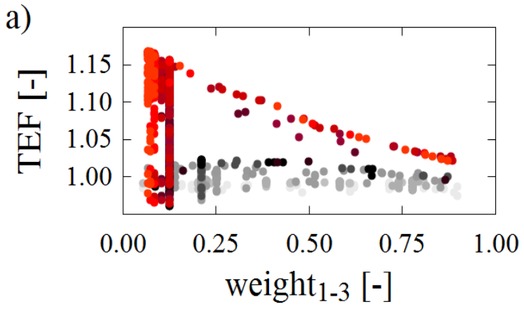
Deep dive

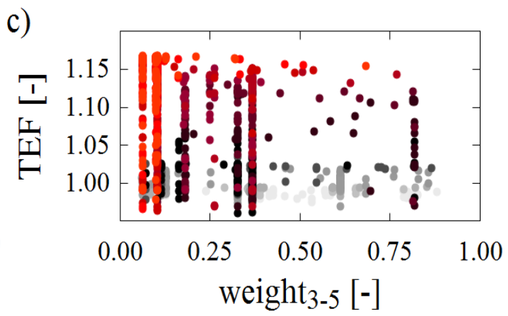


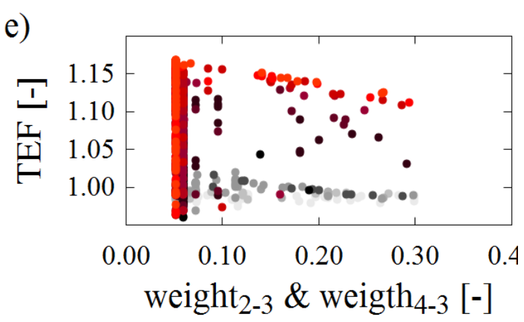
What is the impact of each geometric parameter on performance?

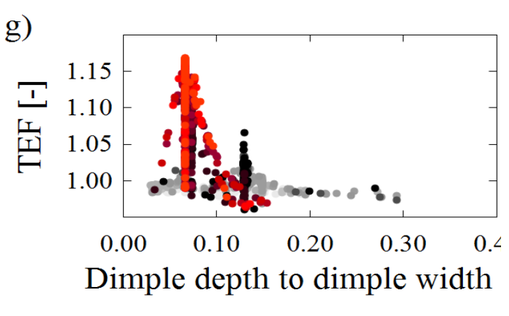
Design number

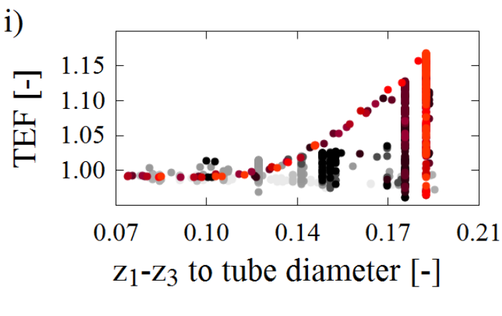


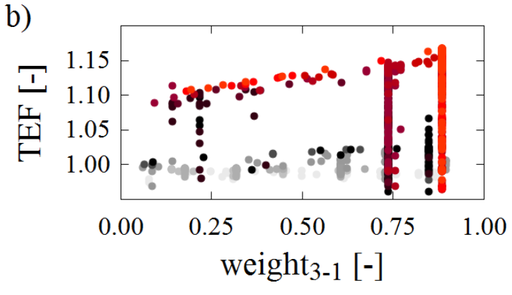


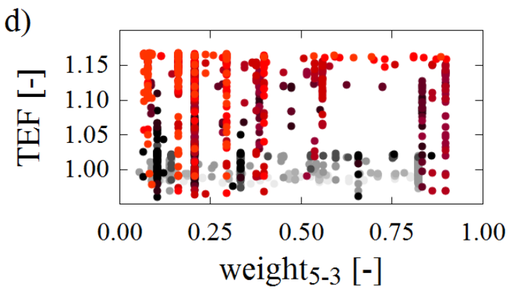


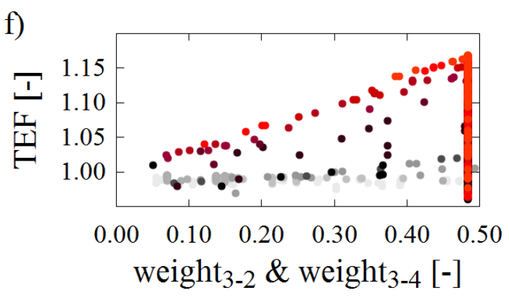


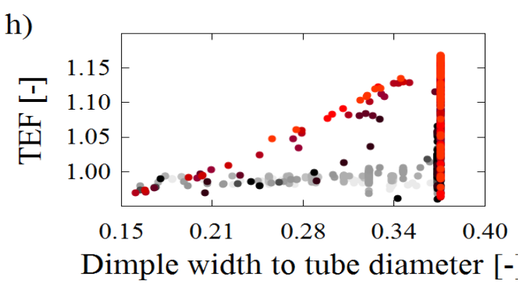


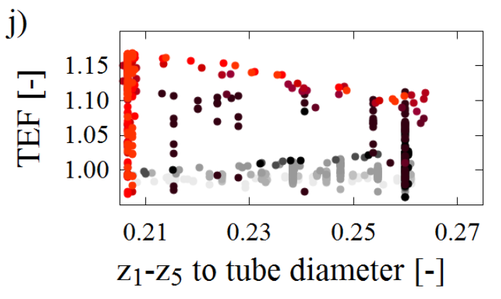












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Objective function

What is the immediate impact of 3D reactors?

+ Change in olefin yield

Requires time-consuming reactive simulations

Assess difference between base case and optimal case

+ Improved heat transfer
- Increased pressure drop

Can be assessed with fast non-reactive simulations

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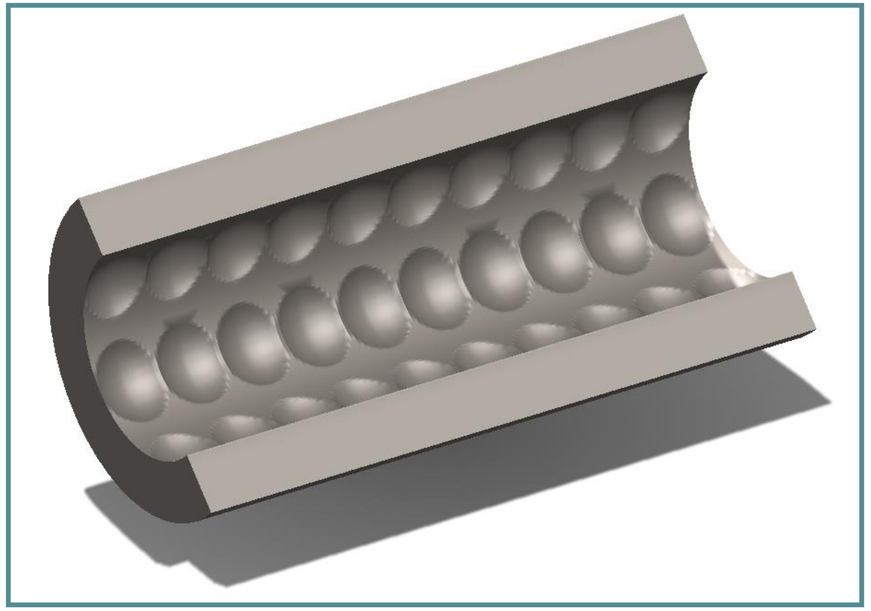
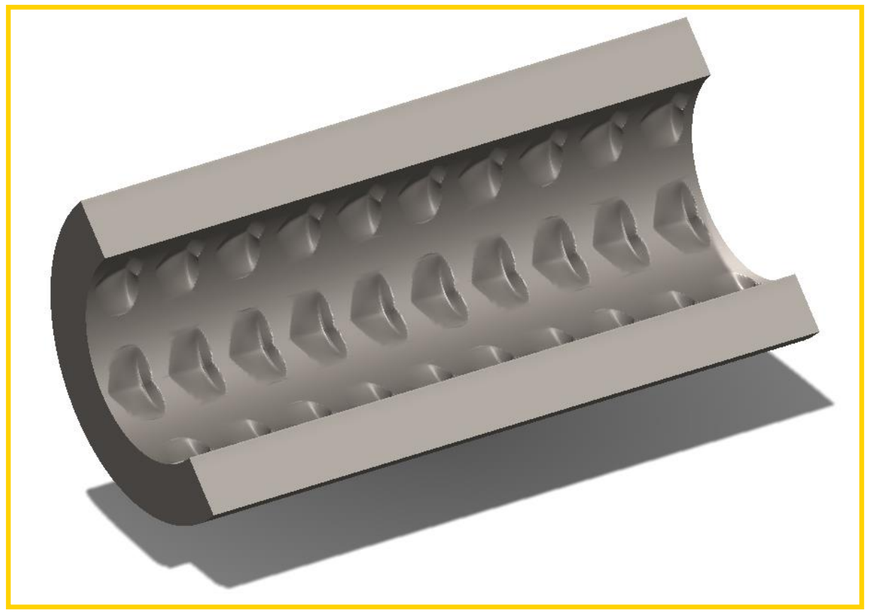
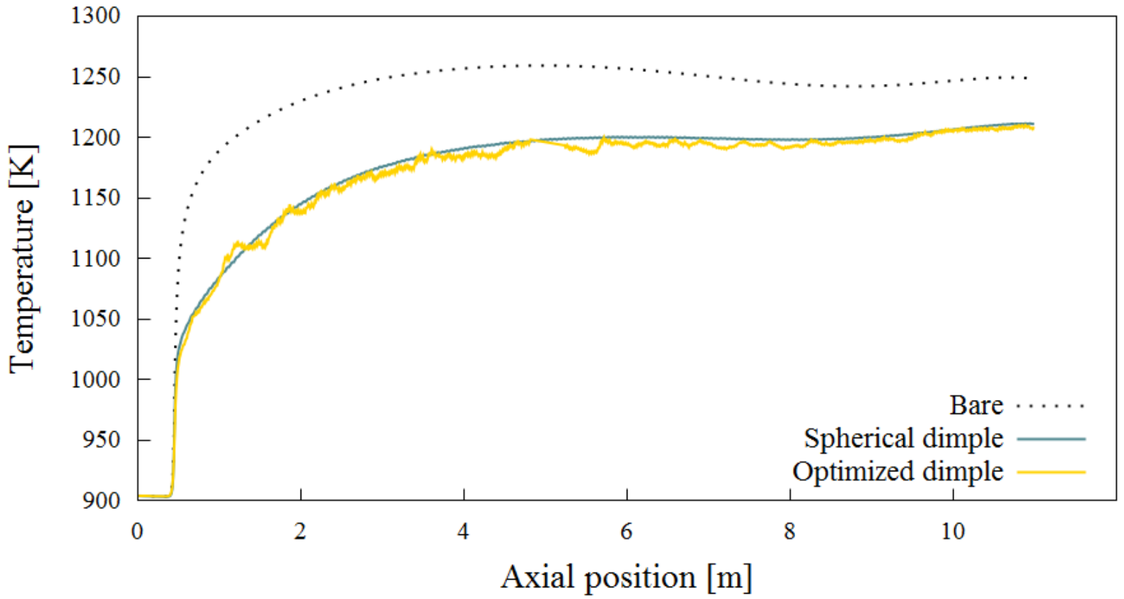
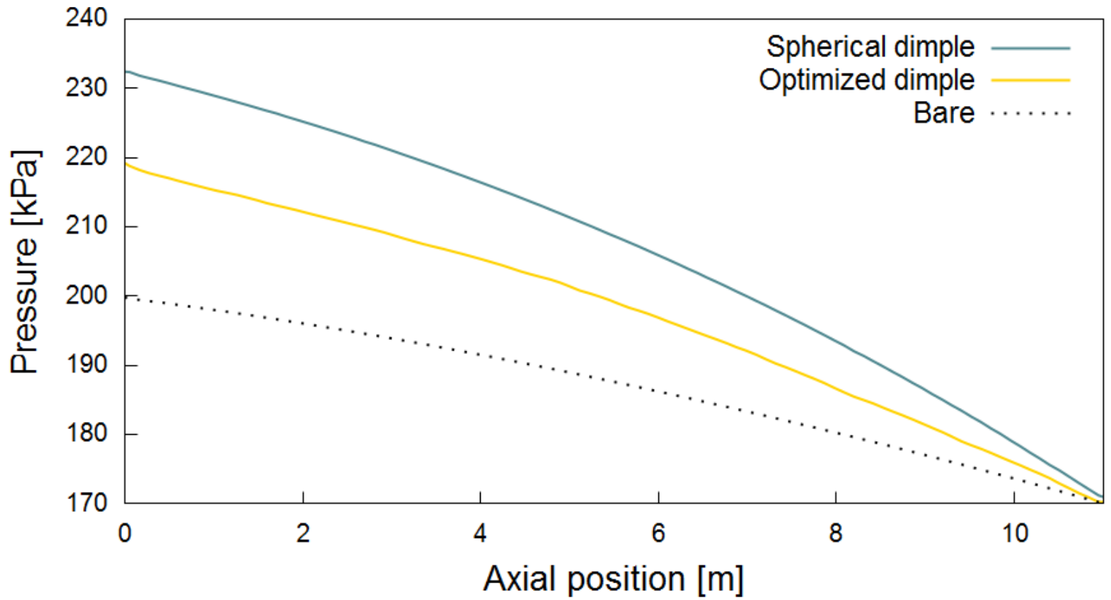
Optimized shape reduces pressure drop …

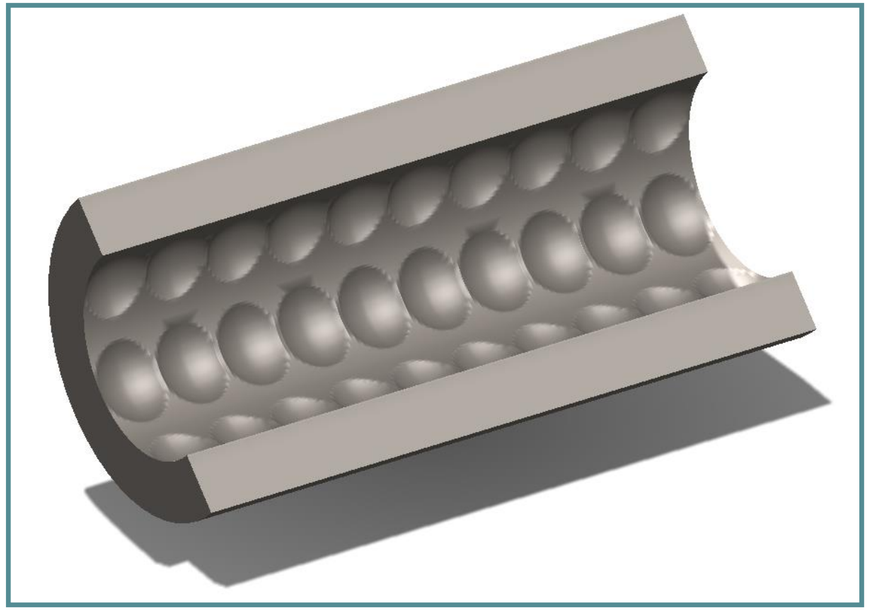


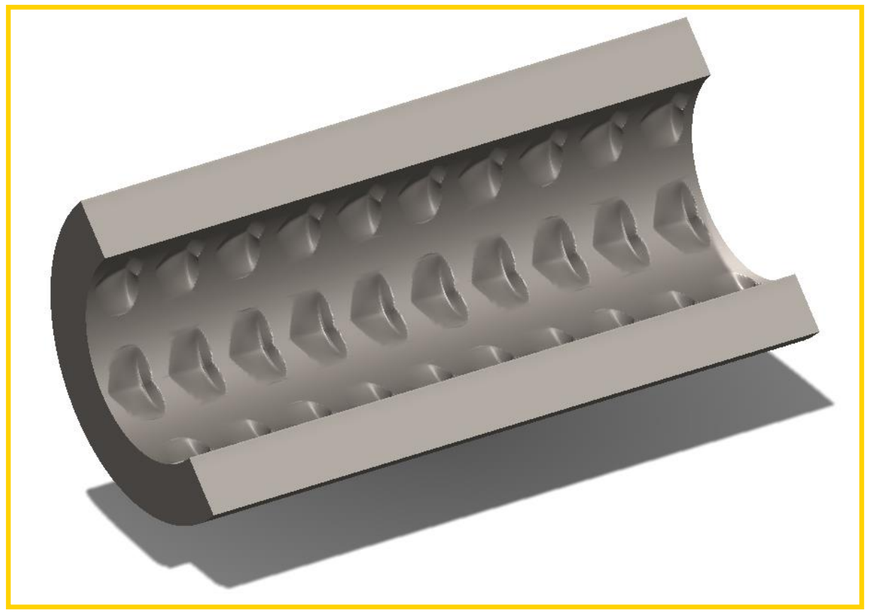


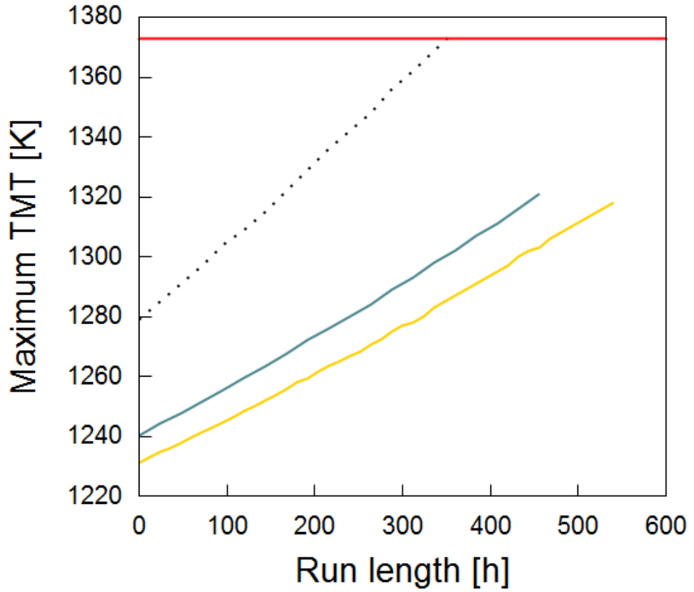


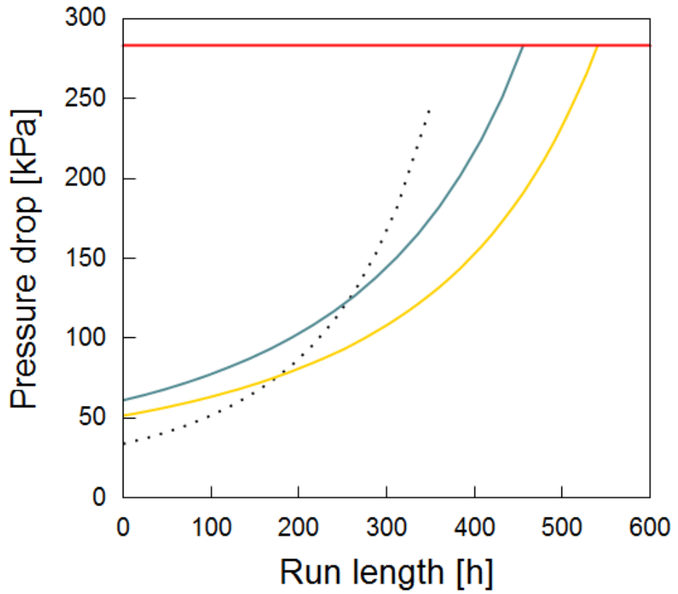


… leads to a longer run length …

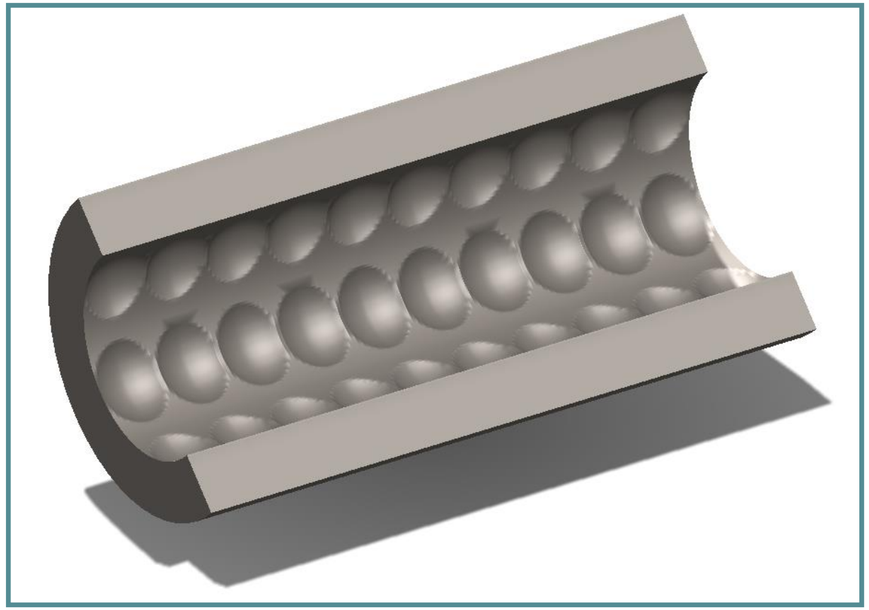


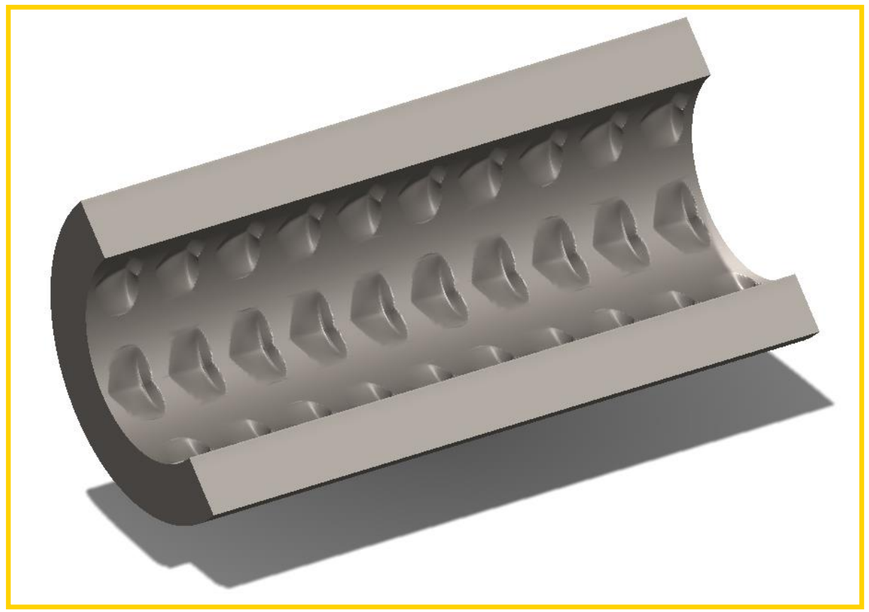


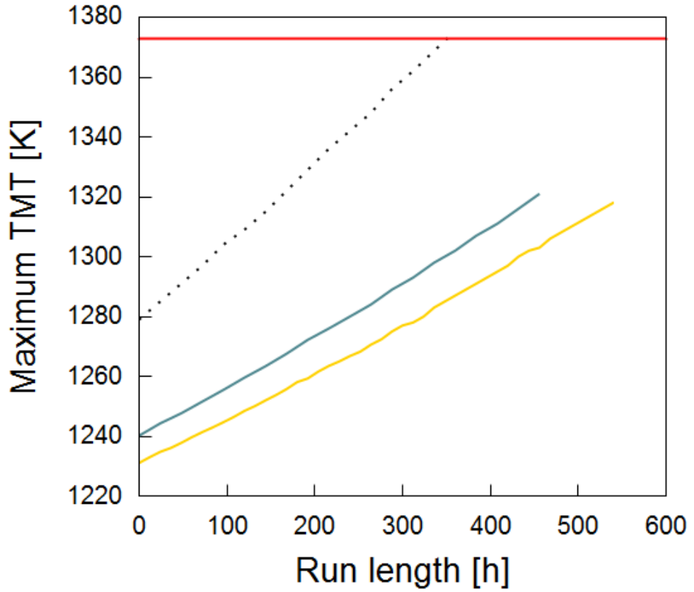


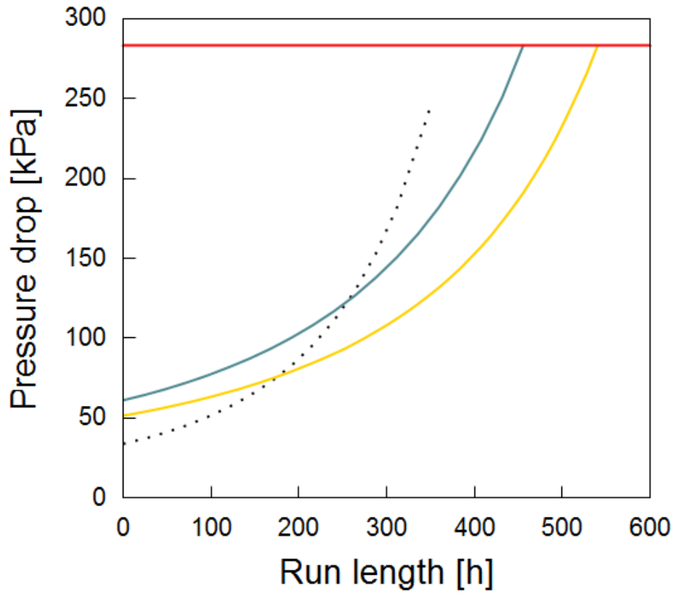


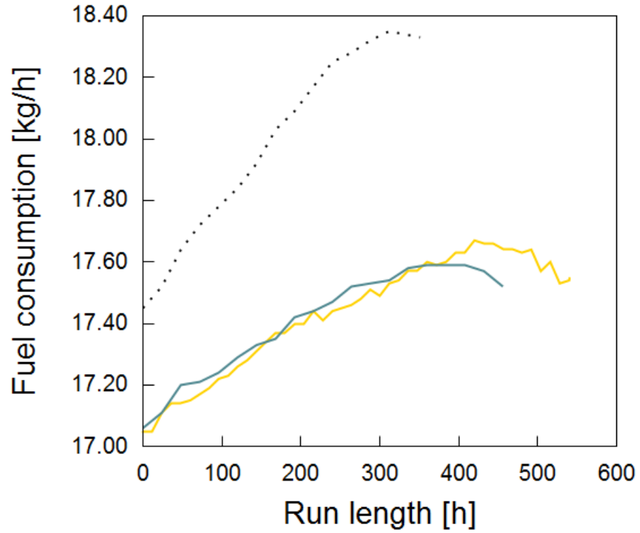
… and reduces fuel consumption.











Conclusions

- Experiments show promising flow behavior

- Minimal dimple depth required to sustain vortices
- Reduced wall temperature can extend run length
- Uniform gas temperature results in a higher propylene yield

- Shape optimization via genetic algorithm leads to
  - ➢ Lower pressure drop penalty
  - ➢ Additional run length extension
  - ➢ Reduced fuel consumption and reduced emissions

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- Marie-Françoise Reyniers
- …

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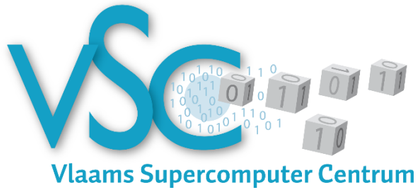

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