PRETREF WORKSHOP

GHENT, 16TH OCTOBER 2019

TUTORIAL: Coke formation in 3D steam cracking reactors

Laurien Vandewalle

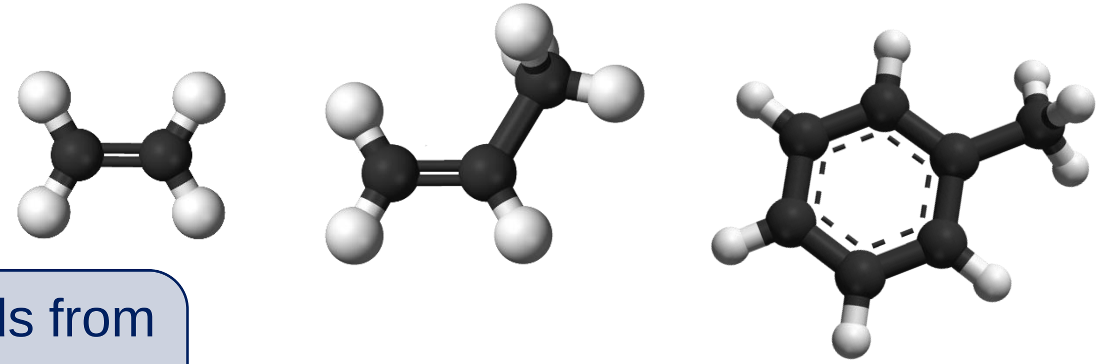
Laboratory for Chemical Technology

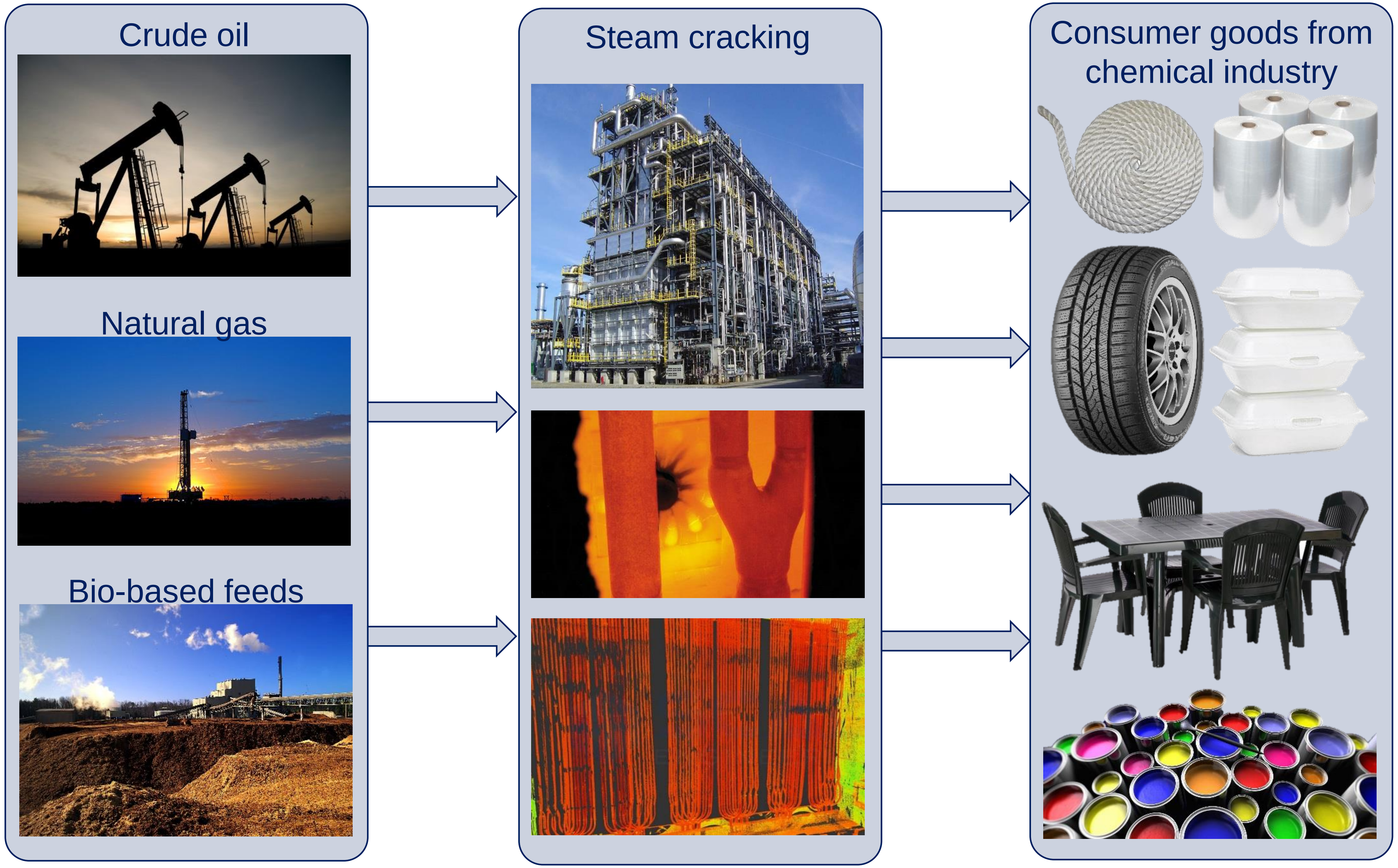
GHENT UNIVERSITY

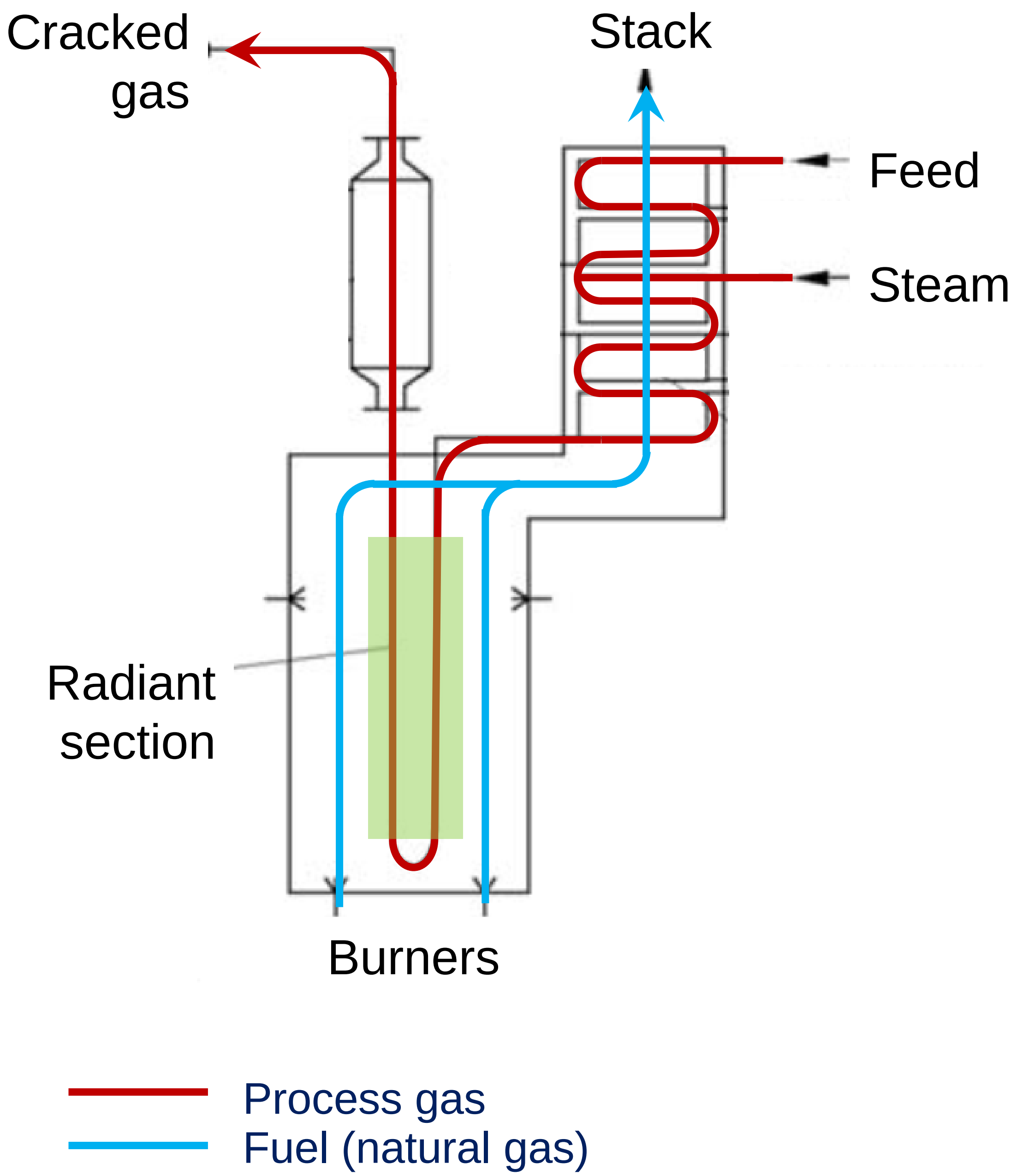
DRIVING CHEMICAL TECHNOLOGY

PRETREF

Introduction: steam cracking







GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

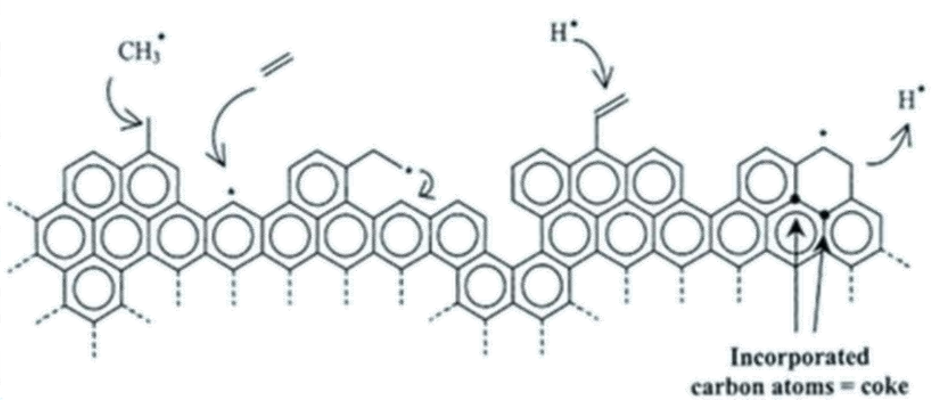
atozforex.com; pnnl.org; districtenergy.org; scade.fr; schmidt-clemens.de; Linde Group; IHS Chemical Insight

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



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

Coke reduction method: 3D reactor technology

Coil cracking due to differences in thermal expansion rate

Hot spots due to inhomogeneous coke formation

GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Nova Chemicals, **2002**; Linde Group; Muños et al., **2013**; Albright et al., **1988**; Muños et al., **2014**

Long term behavior

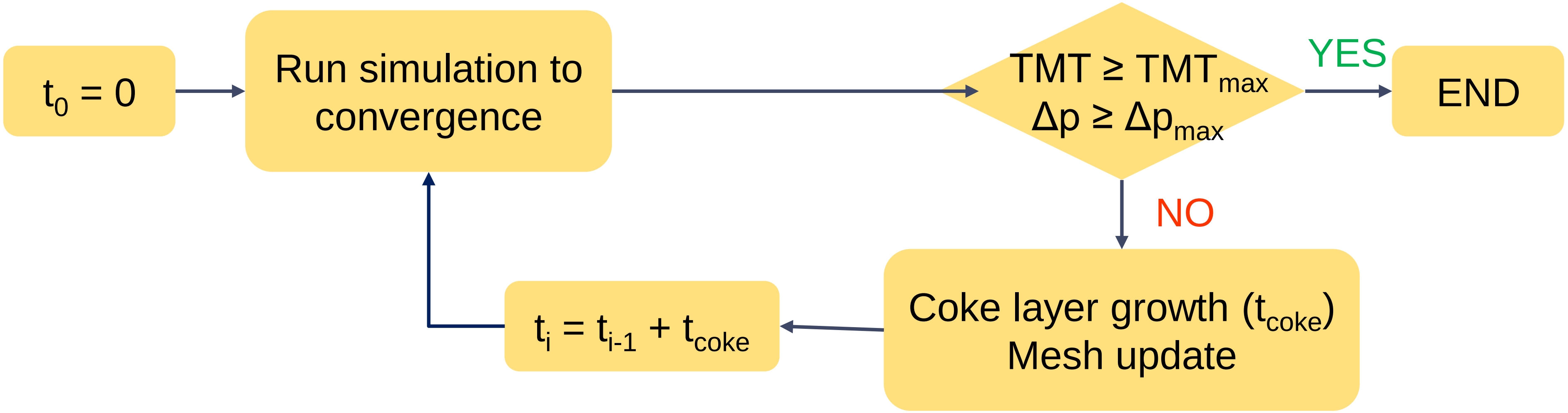
3D elements lead to non-uniform coking

Shape of 3D element + cokes change over time

Flow field (and heat transfer) is altered

Position of local hot spots changes

➔ Run length simulations



GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

OpenFOAM applications

chtQSSAFoam solver

- Multi-region reactive solver (with solid-fluid heat transfer)
- Steam cracking chemistry implemented directly in the code, including quasi-steady state approximation (QSSA) to reduce stiffness

crackerCokeSim utility

- Create structured multi-region (fluid, cokes, metal) grids of 3D steam cracking reactor tubes
- Simulate coke layer growth in a post-processing step

Before we start

Open X2Go or VNC connection to HPC

Copy and unpack case files

```
tar -xzvf steam_cracking_tutorials.tar.gz
```

Start an interactive job on HPC

```
qsub -I --pass=reservation=PRETREF -l nodes=1:ppn=4 -l walltime=02:00:00
```

Load OpenFOAM

```
module load OpenFOAM/2.2.x-intel-2019a
source $FOAM_BASH
```

Compile the necessary solvers and utilities

In the folder `steam_cracking_tutorials/solvers_utilities:` `./Allwmake`

GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Tutorial part 1
Meshing

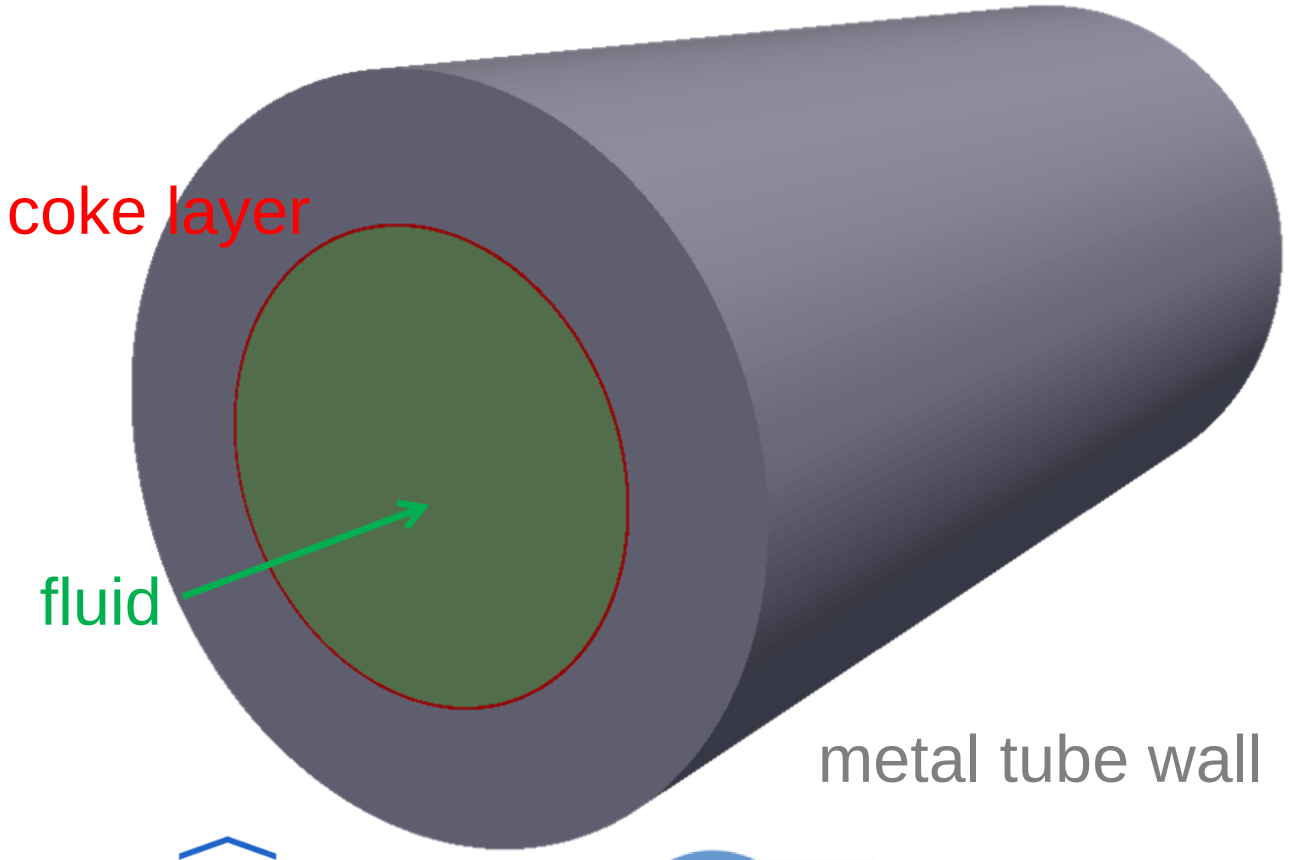
GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

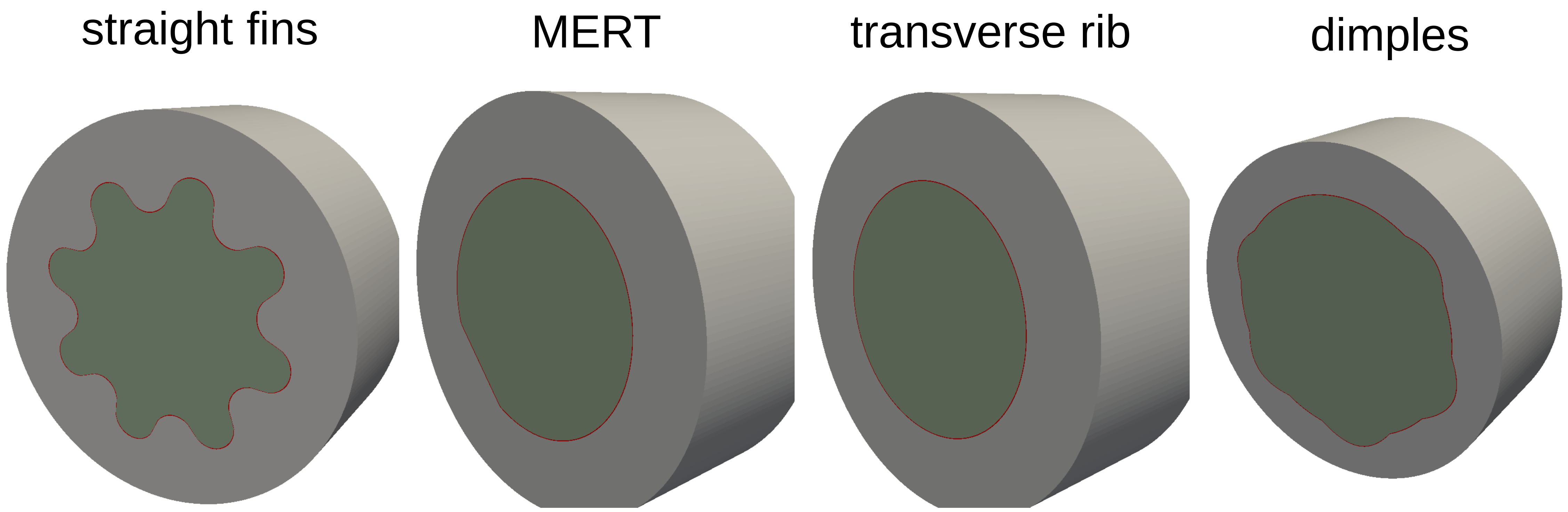
Meshing: introduction

Goal: create multi-region (fluid, cokes, metal) grid of 3D steam cracking reactor geometries

Multi-region



3D reactor geometries

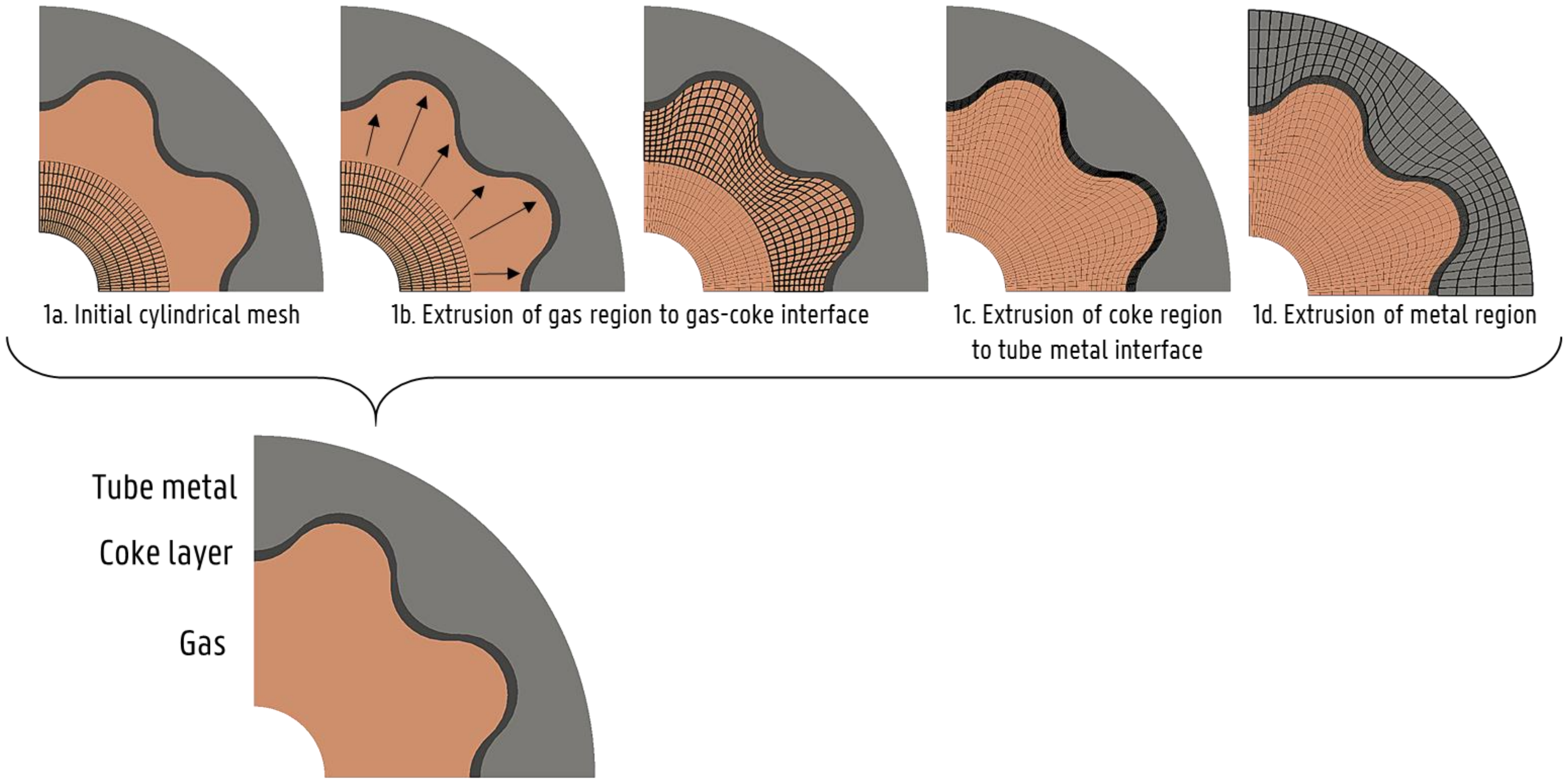


GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

crackerCokeSim utility

Initial meshing



Tutorial instructions

Base case files are available in ‘meshing_geometryModels’ folder

Required OpenFOAM commands

```
./Allclean
./Allrun
```

- **blockMesh24x -dict system/blockMeshDict**

  after executing blockMesh, move polyMesh to subfolder ‘cylinder’

- **crackerCokeSim –createMesh**

Adjust crackerCokeDict to create the geometry of your choice

GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Tutorial part 2
Reactive simulation

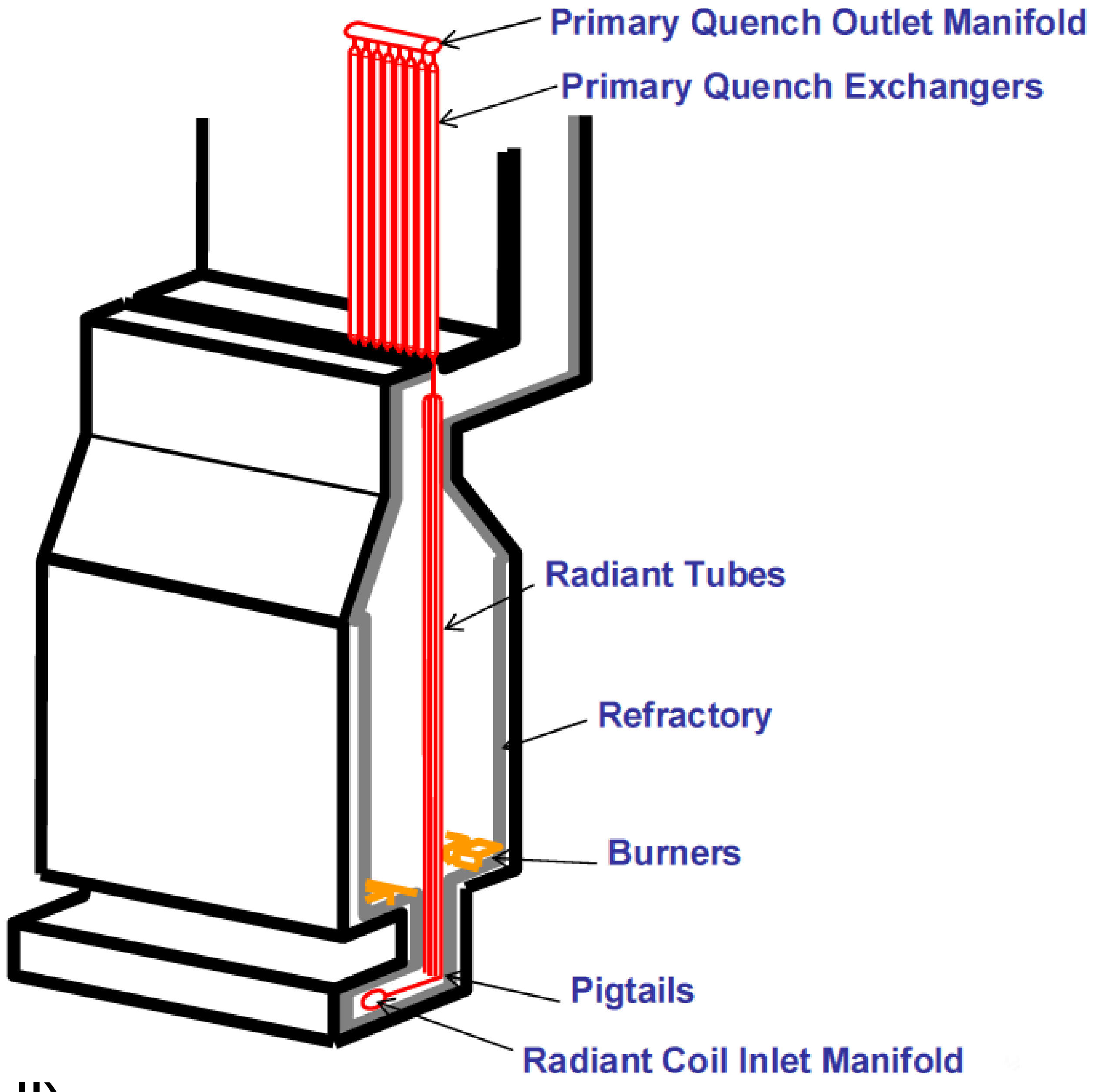
GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Test case: Millisecond propane cracker

Bare cylindrical tube (2D wedge grid)

ID / OD	30 mm / 40 mm
Length	10 m



<u>Operating conditions</u>

– Feedstock	118.5 kg/h propane
– Steam dilution	0.326 kg/kg
– CIT	903.7 °C
– COP	170 kPa
– Uniform heat flux	69.625 kW/m^2 (on metal wall)

Note: In reality, the heat flux is non-uniform

GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Tutorial instructions

Base case files are available in ‘propane_cracker_bare_wedge’ folder

Required OpenFOAM commands

`./Allclean`

`./Allrun`

- **blockMesh**

  after executing blockMesh, move polyMesh to subfolder ‘cylinder’

- **crackerCokeSim –createMesh**
- **chtQSSAFoam**

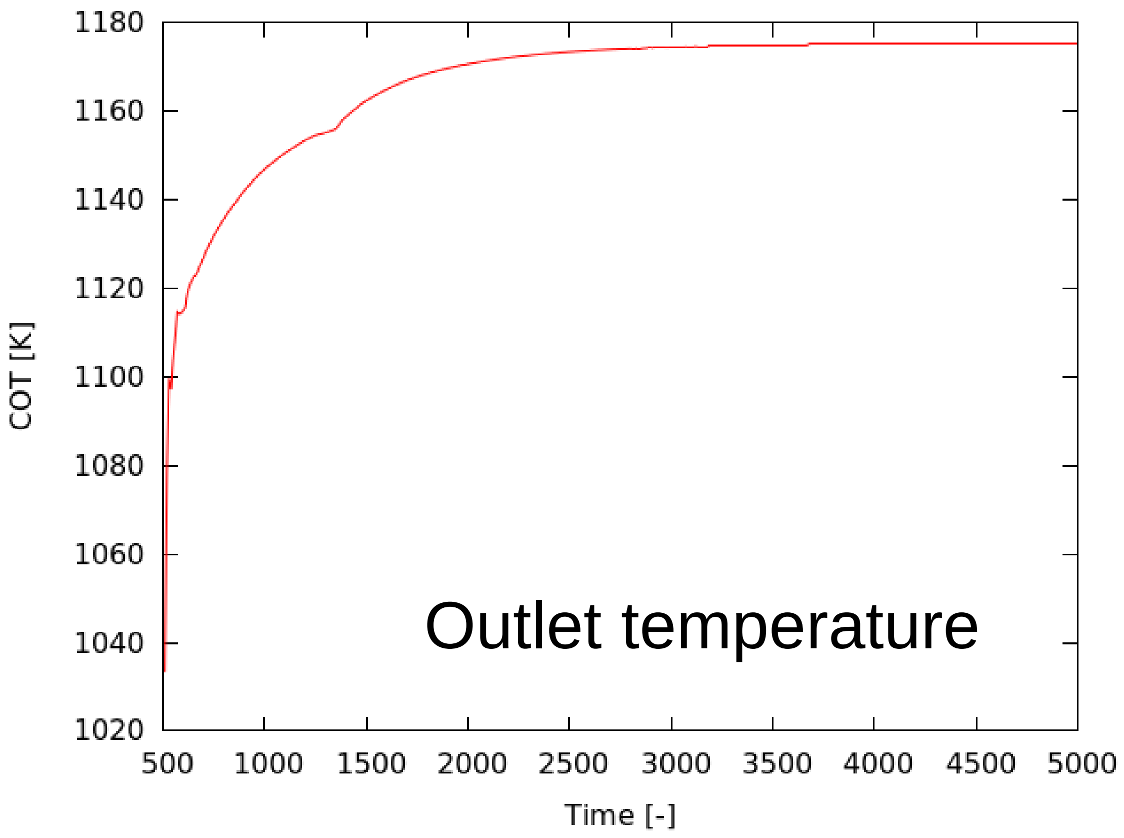
GHENT UNIVERSITY

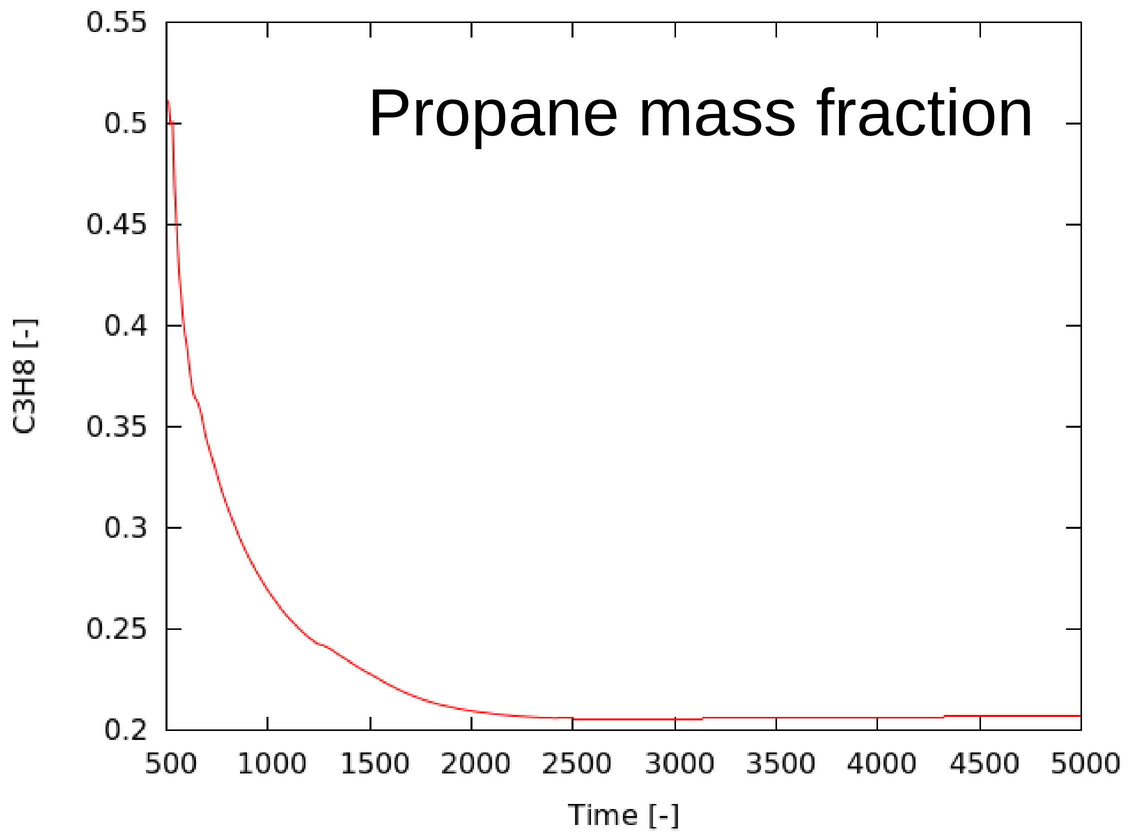
LCT DRIVING CHEMICAL TECHNOLOGY

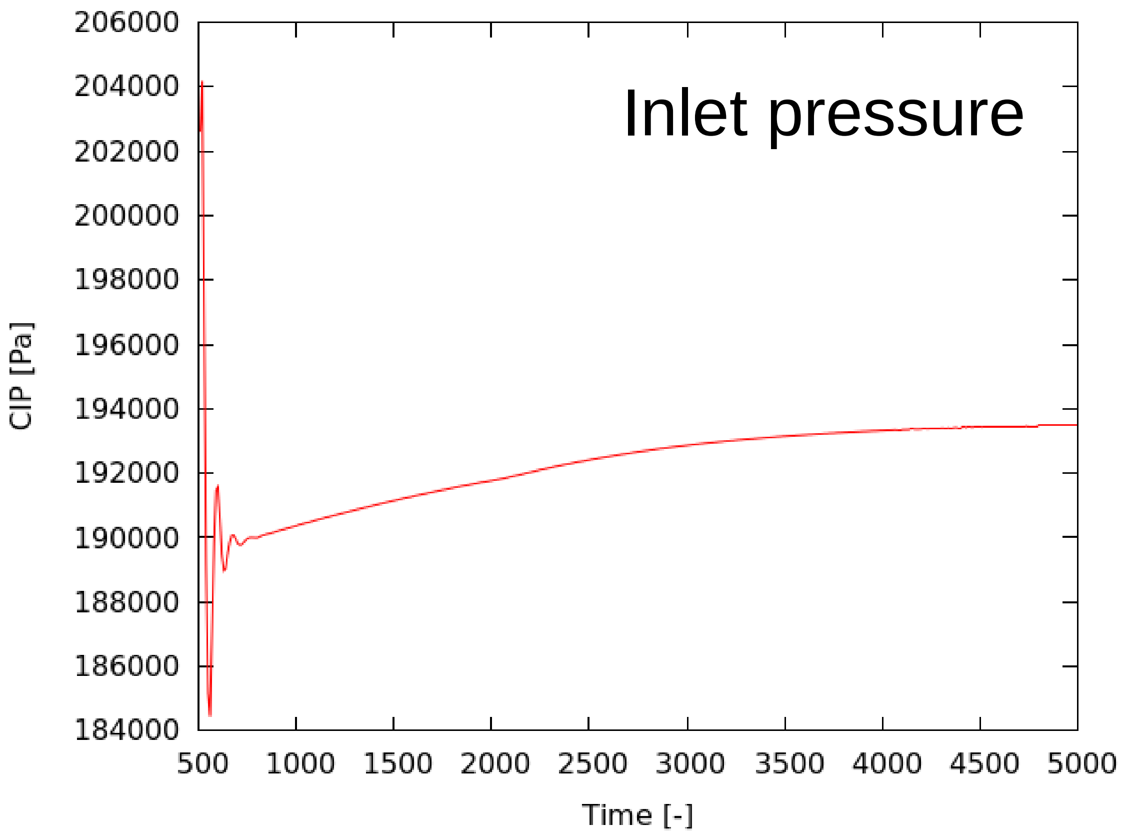
Run-time post-processing

See controlDict: functions

Plot mixing-cup averages at outlet to check convergence







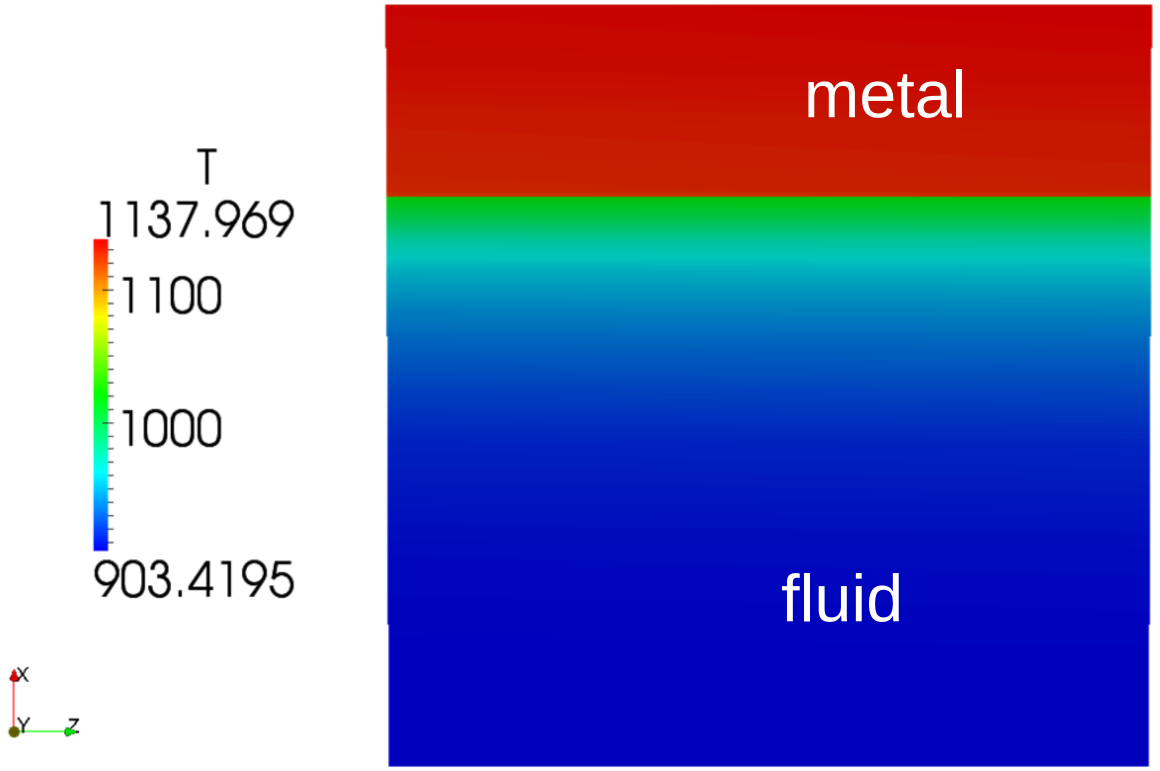
GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

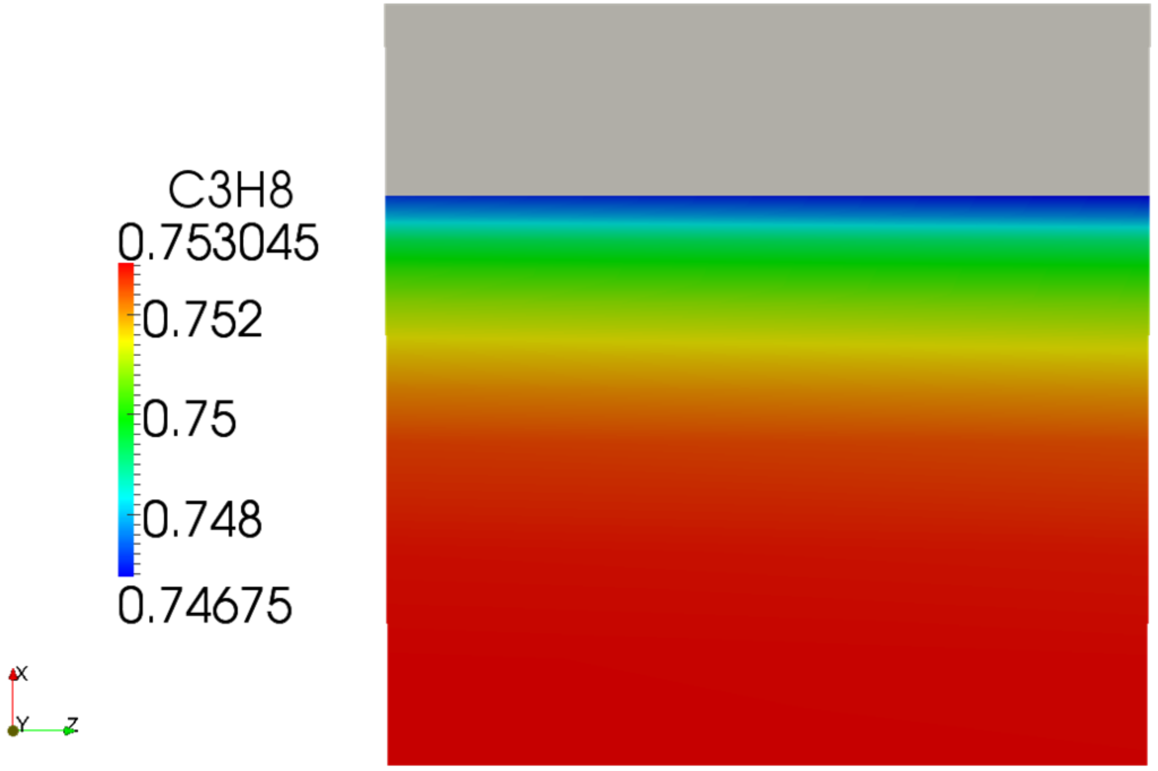
Post-processing

Visual postprocessing using ParaView

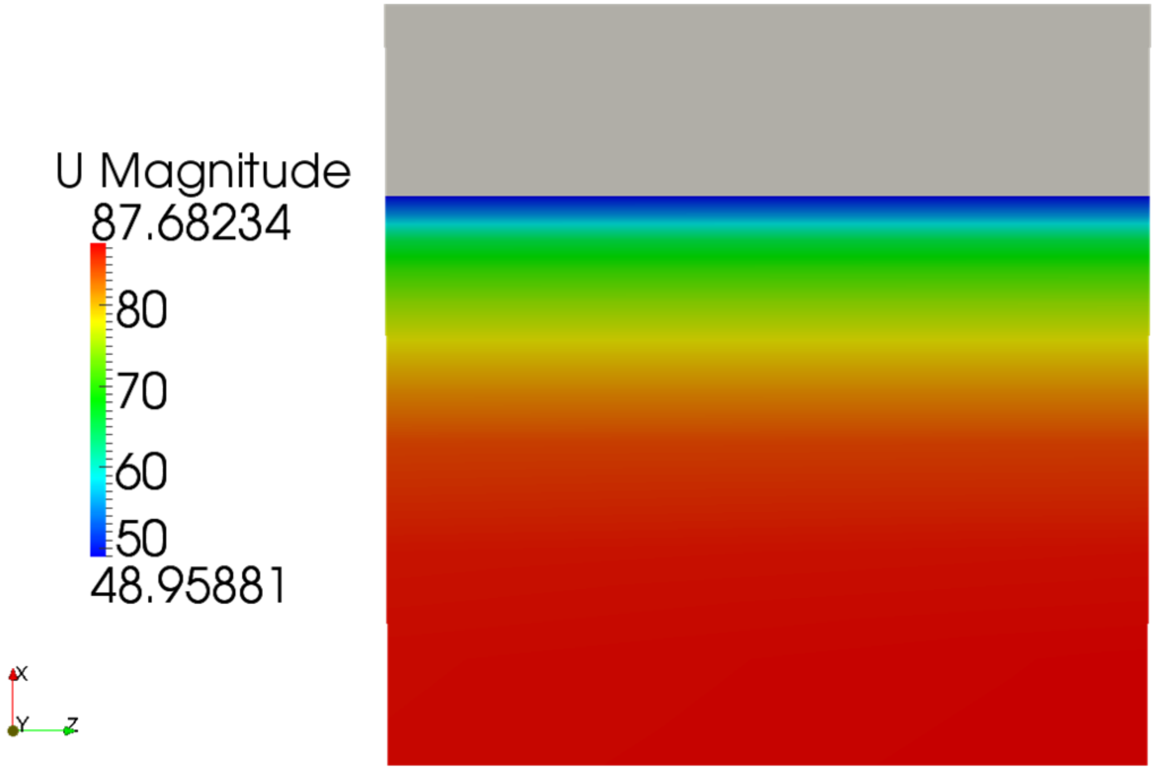
Temperature



Species mass fraction

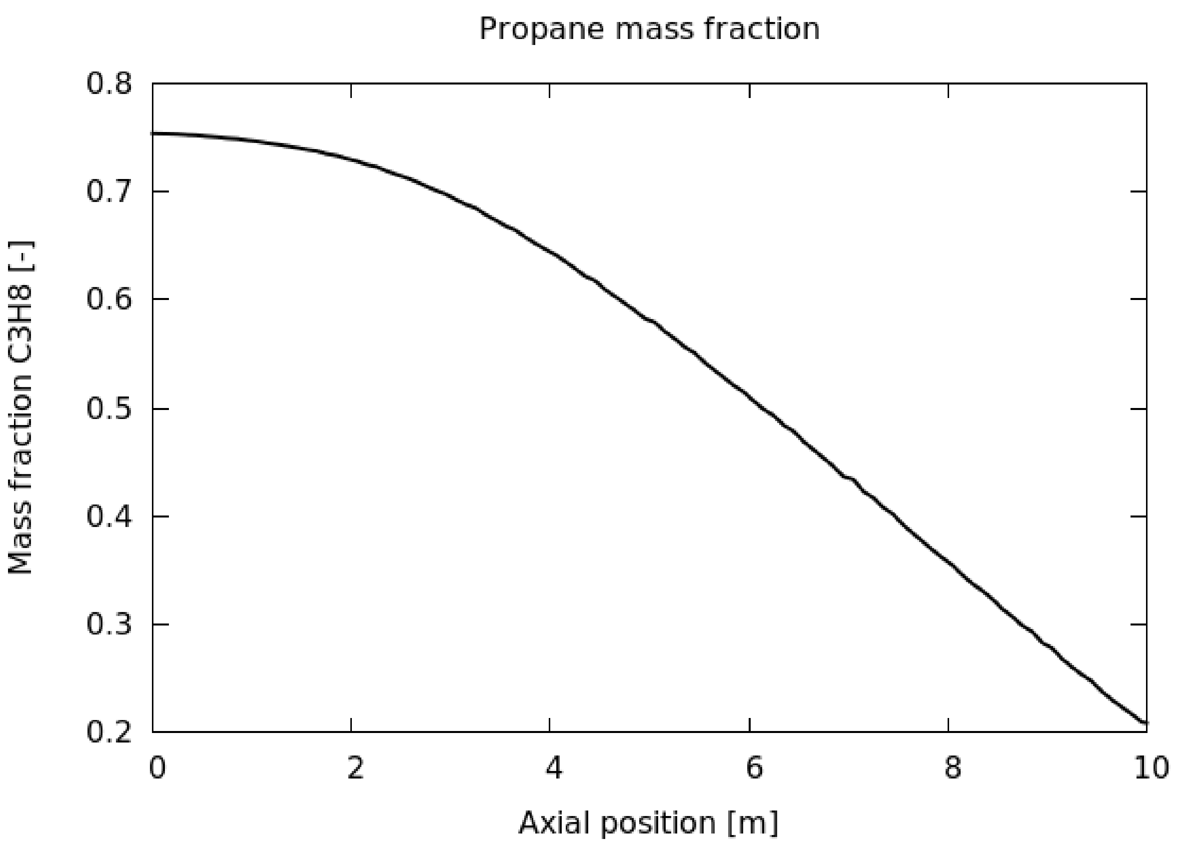


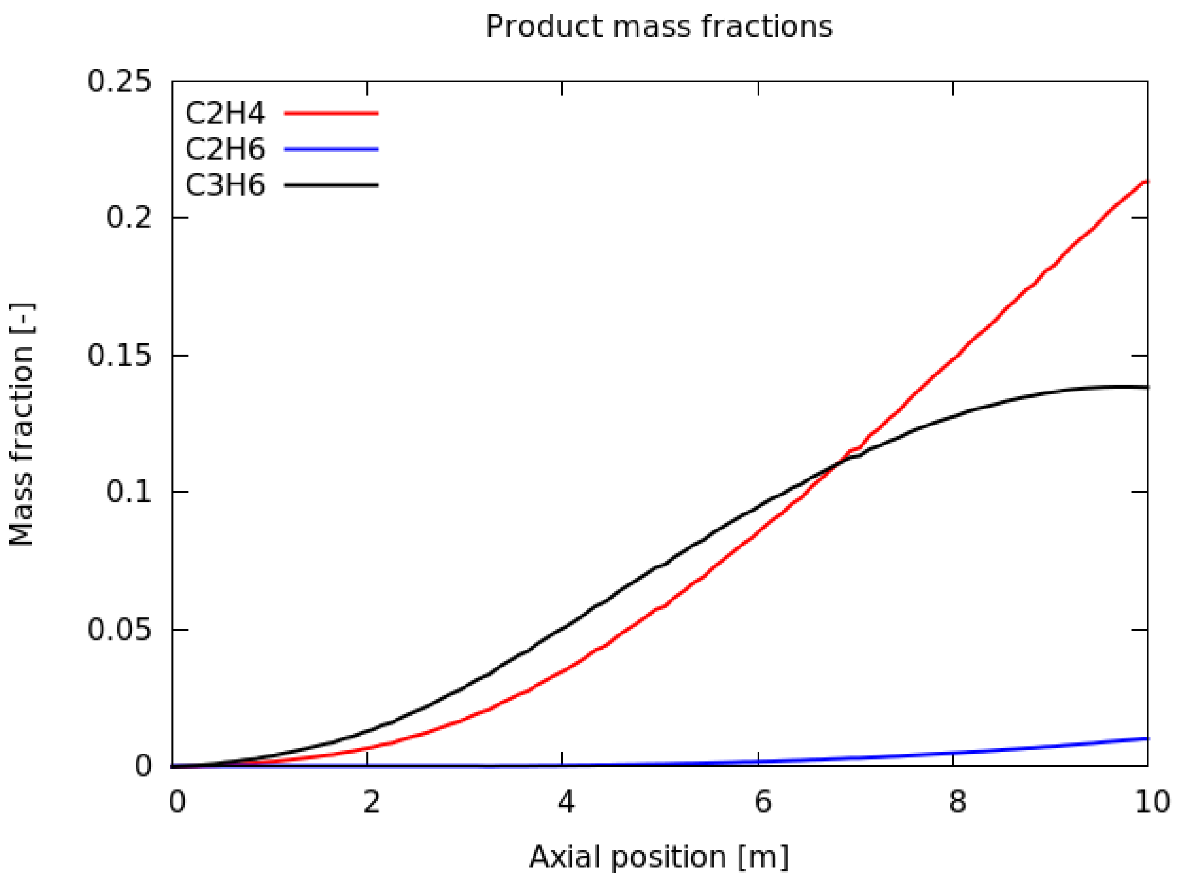
Velocity

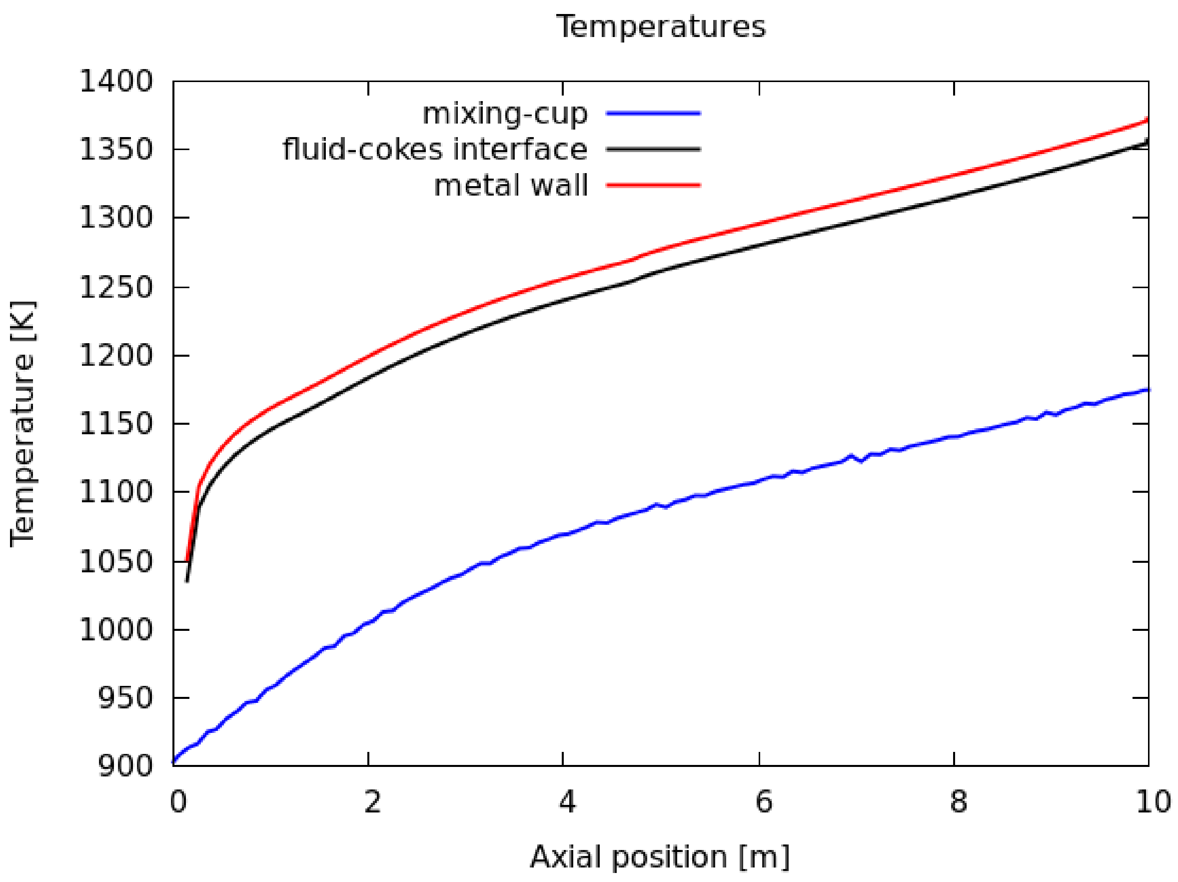


Post-processing

Plot mixing-cup averages as a function of axial position







GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Tutorial part 3

Coke formation in a finned steam cracking reactor

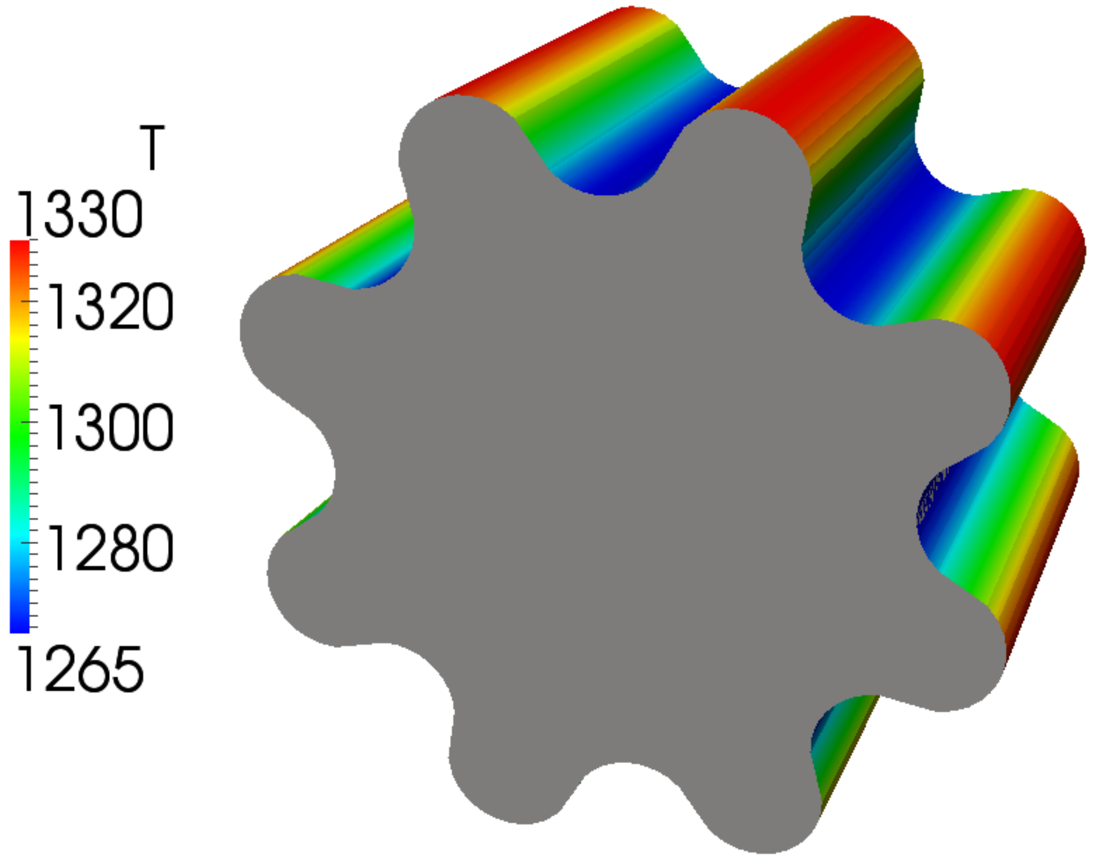
GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Case description

The rate of coke formation is a function of temperature, C_2H_4 and C_3H_6 at the fluid-coke interface

- An artificial non-uniform temperature field is applied to a finned steam cracking reactor to illustrate the usage of the `crackerCokeSim` utility.
- C_2H_4 and C_3H_6 are specified as constants (using the 'coldFlow' option of the utility).



$$T = 1230 + 100 \cdot \frac{R - 0.01}{0.0073}$$

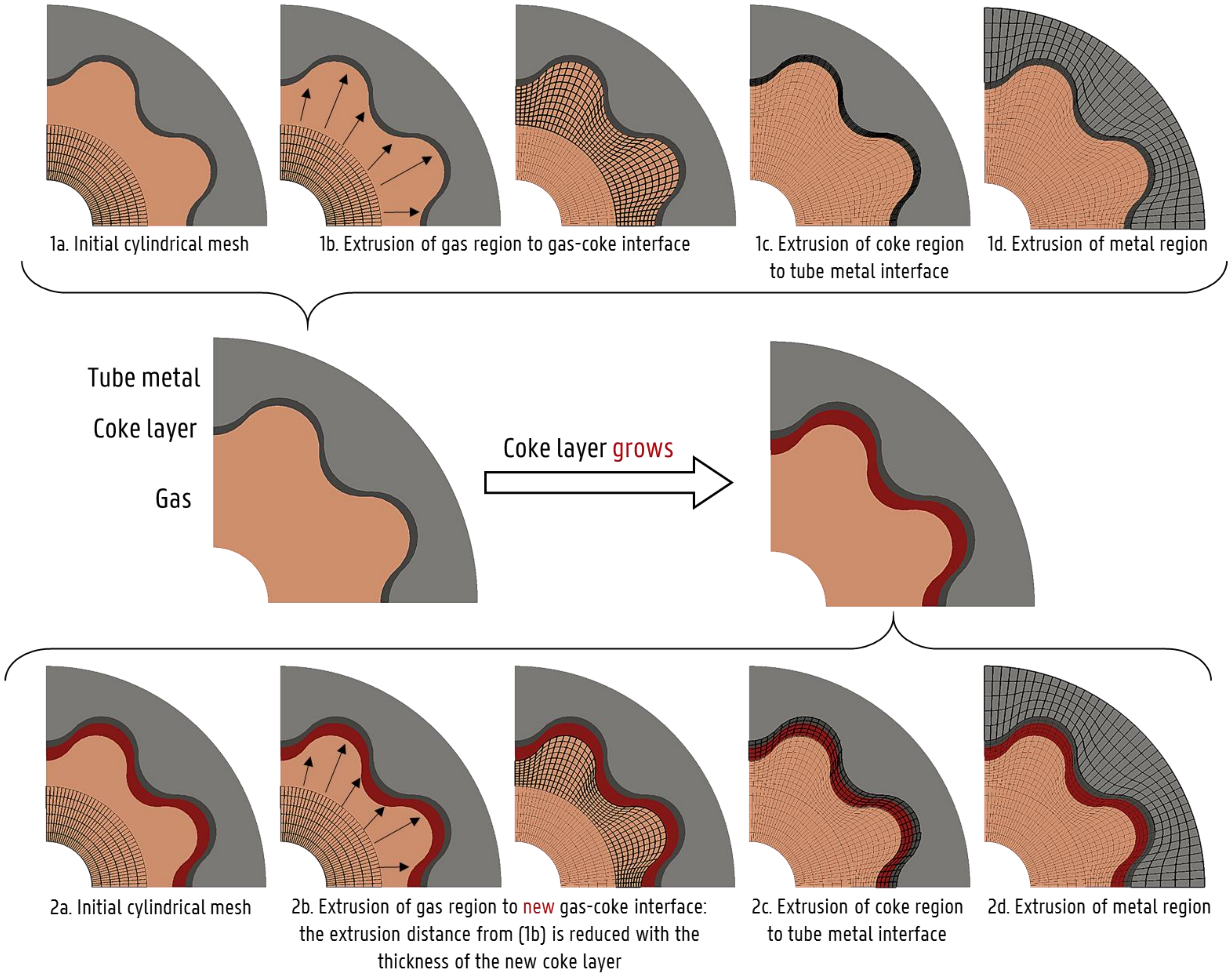
GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

crackerCokeSim utility

Initial meshing

Coke formation



GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Tutorial instructions

Base case files are available in ‘coke_growth_finned’ folder

Required OpenFOAM commands

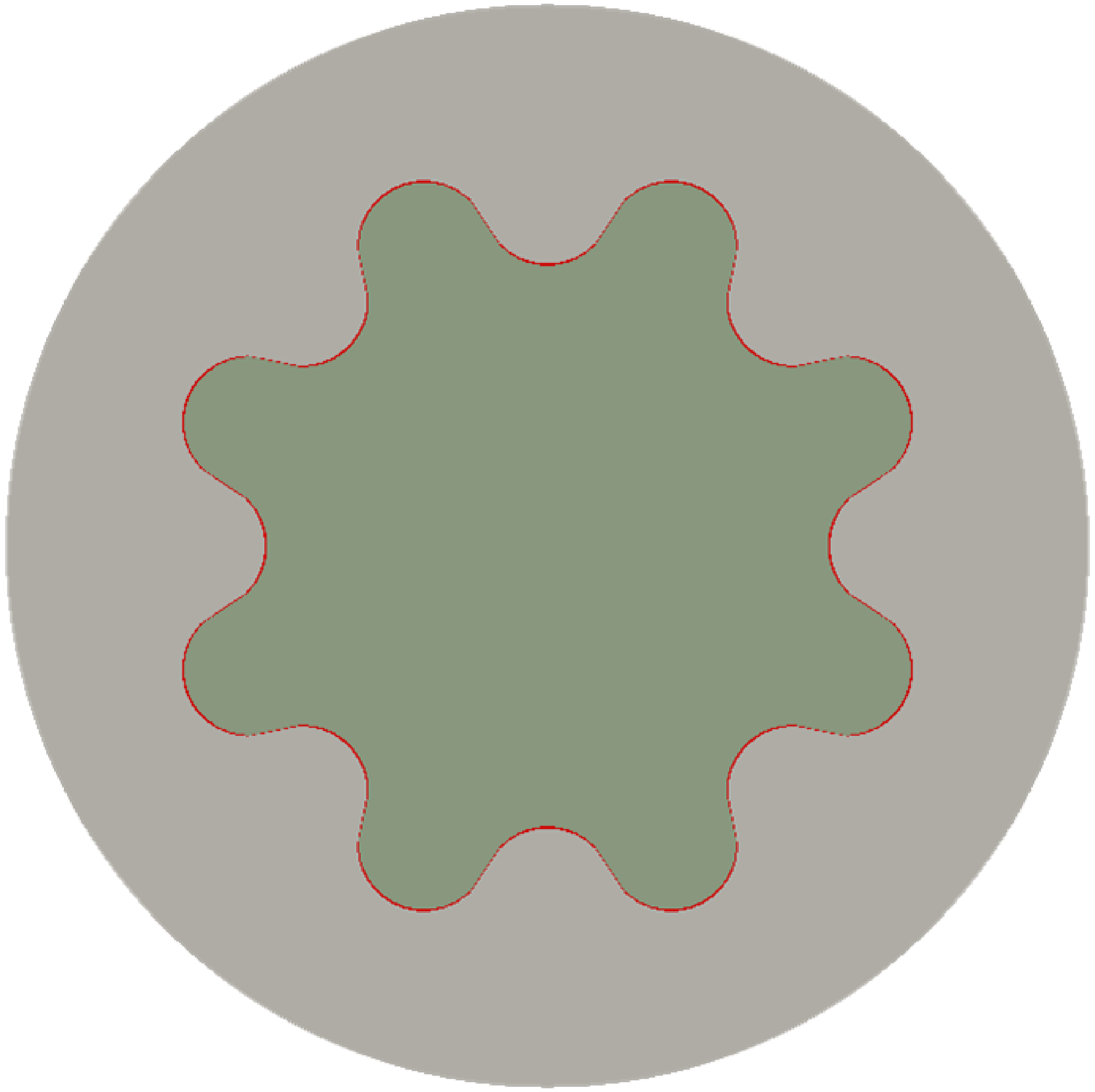
- `crackerCokeSim`

```
./Allclean
./Allrun
```

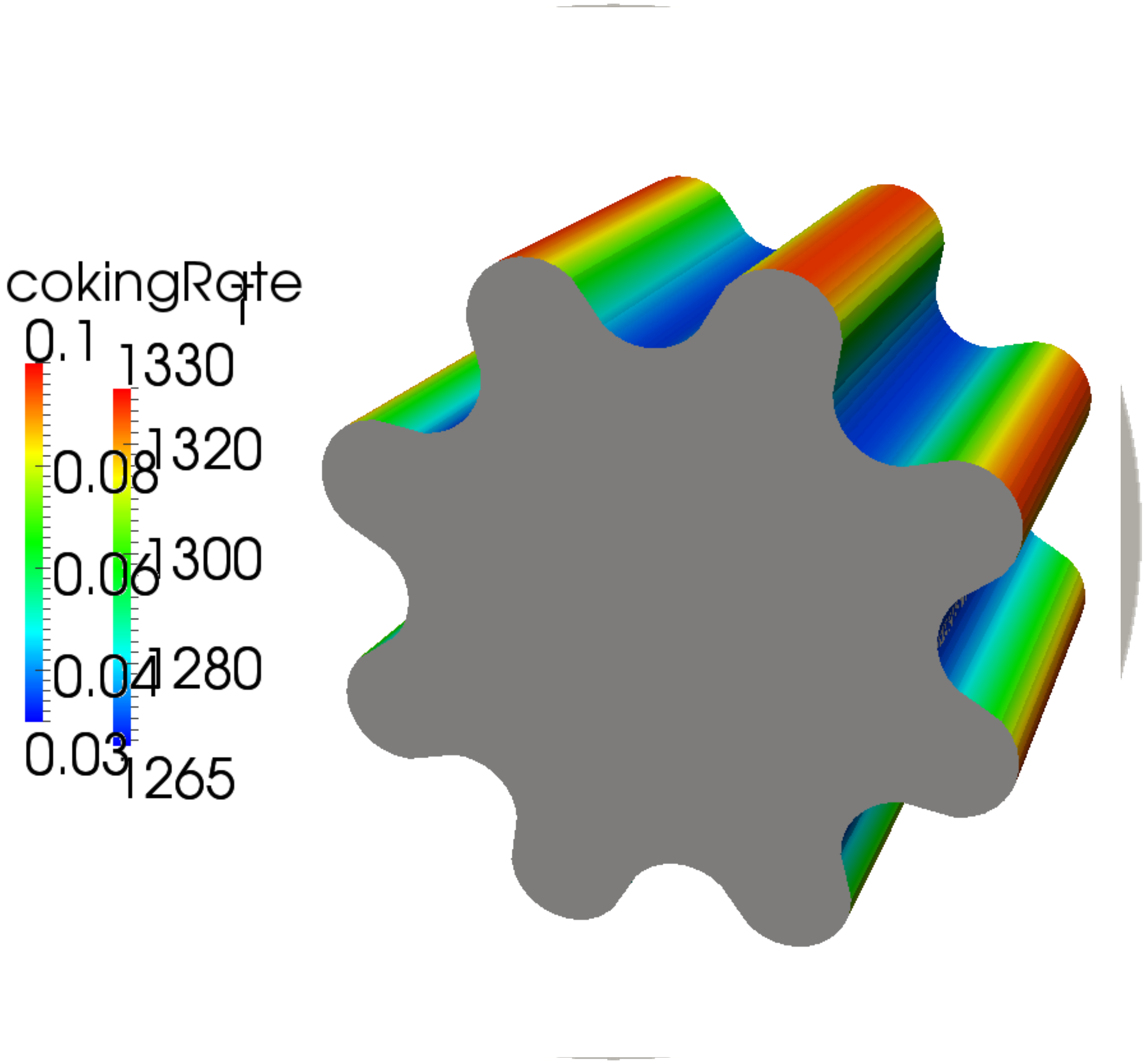
Have a look at the required parameters in crackerCokeDict (e.g. values for C_2H_4 and C_3H_6 mass fractions)

Results

Before coke layer growth



After coke layer growth

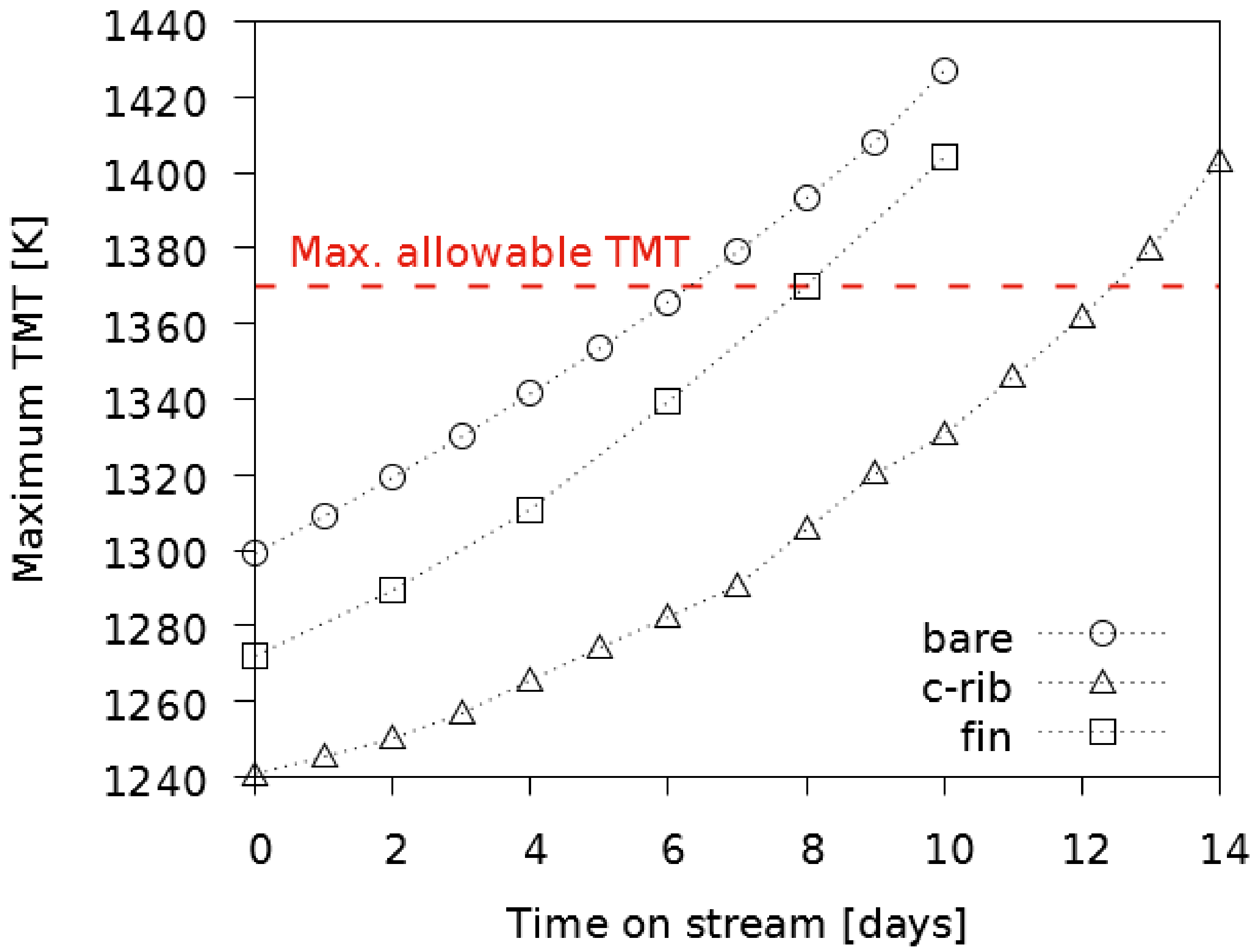


More advanced simulation results

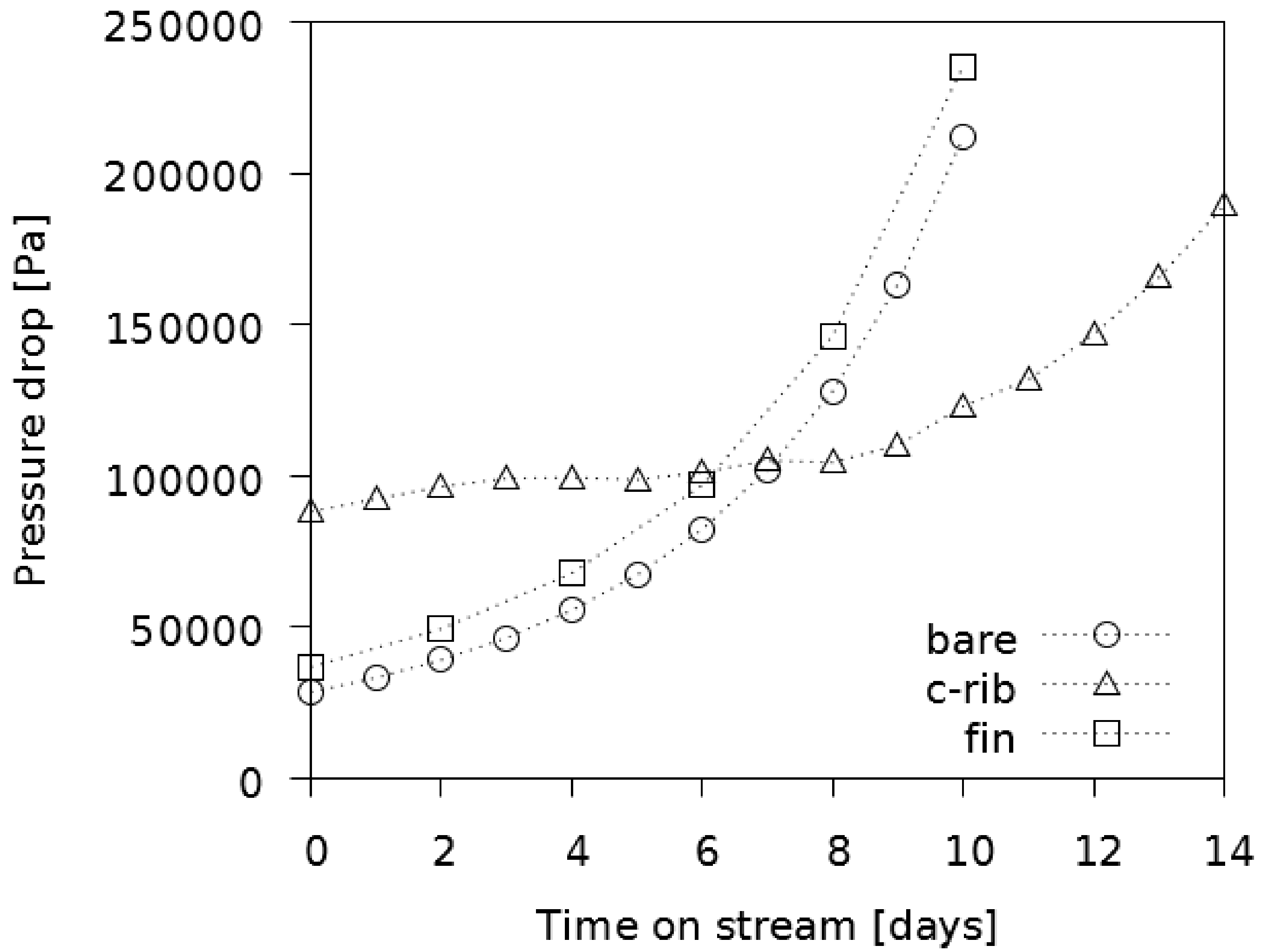
GHENT UNIVERSITY

DRIVING CHEMICAL TECHNOLOGY

Run length



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



Pressure drop increases because of reduction in cross-sectional flow area during coke formation

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

GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Vandewalle, L. A.; Van Cauwenberge, D. J.; Dedeyne, J. N.; Van Geem, K. M.; Marin, G. B. Dynamic Simulation of Fouling in Steam Cracking Reactors Using CFD. *Chem. Eng. J.* **2017**, *329*, 77–87.

Coke formation and velocity fields

Fin

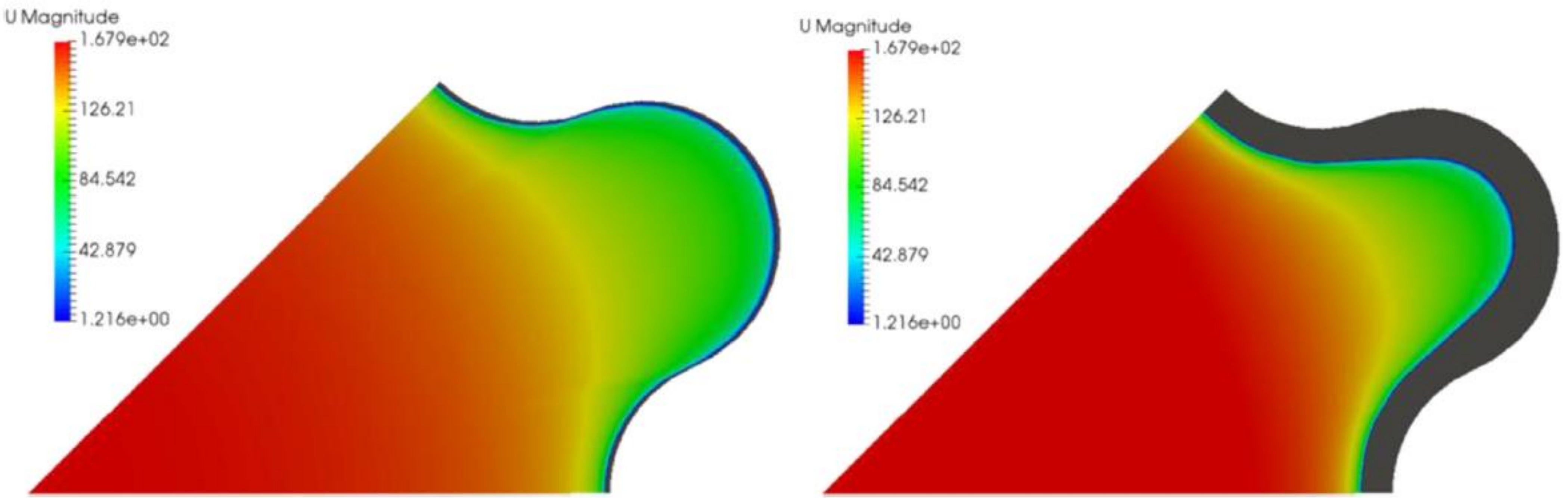


Fig. 11. Fields of velocity magnitude [m s^{-1}] in the finned reactor geometry: (left) at start-of-run, and (right) after 48 h of coke layer growth (for operating conditions as described in Section 3.1).

c-Rib

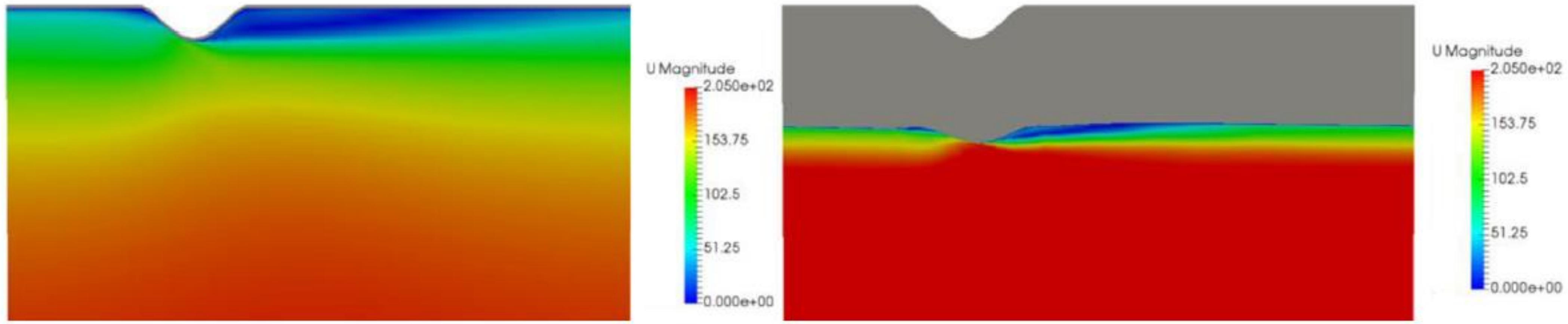


Fig. 12. Fields of velocity magnitude [m s^{-1}] in the continuously ribbed reactor geometry: (left) at start-of-run, and (right) after 10 days of coke layer growth (for operating conditions as described in Section 3.1).

GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY

Vandewalle, L. A.; Van Cauwenberge, D. J.; Dedeyne, J. N.; Van Geem, K. M.; Marin, G. B. Dynamic Simulation of Fouling in Steam Cracking Reactors Using CFD. *Chem. Eng. J.* **2017**, *329*, 77–87.