Computational fluid dynamics-based study of novel technologies in the steam cracking process

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INTRODUCTION

STEAM CRACKING

Hydrocarbon feed is cracked at high temperatures to produce light olefins
IMPROOF objective: improving the energy efficiency of the steam cracking process

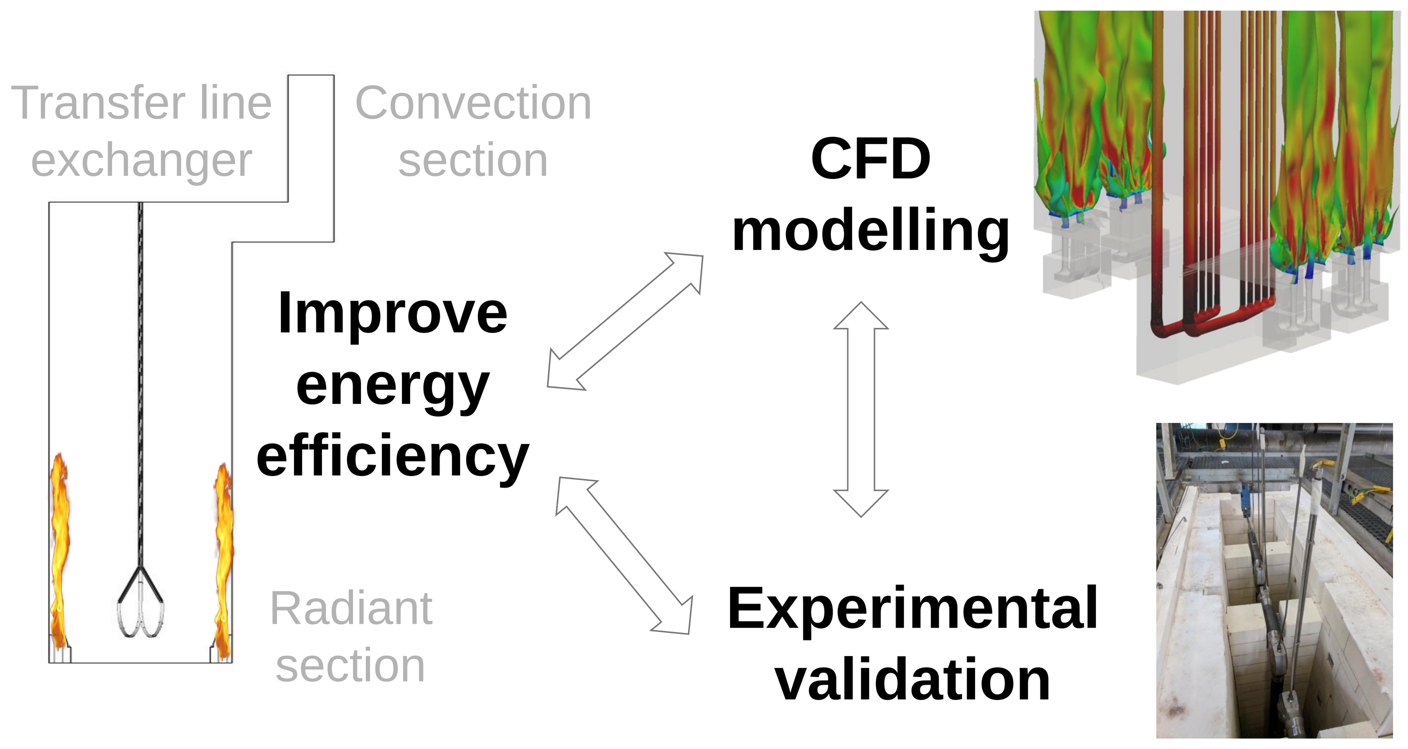
Novel technologies

reactor side

- 3D reactor design

furnace side

- high emissivity coatings
- oxy-fuel combustion



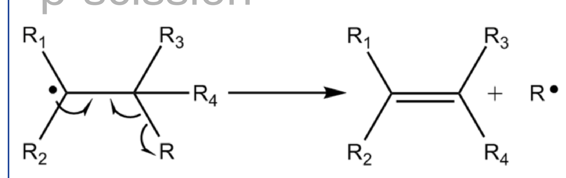
Hydrocarbon feedstock

- Crude oil → naphtha
- Bio-based feeds
- Propane, ethane

low value
no chemical functionality

Steam cracking

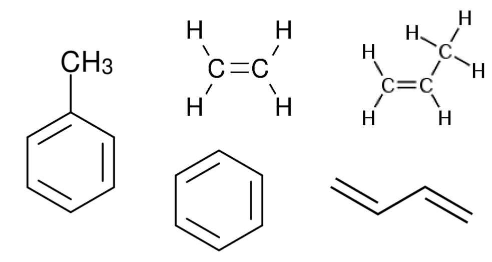
β-scission



low C-partial pressure
steam as diluent

Consumer goods

base chemicals



higher value
chemical functionality

NOVEL TECHNOLOGIES

3D REACTOR DESIGN

Enhanced heat transfer by modifying the reactor shape:

$$Q_{net} = U\,A\,(T_{reactor\ wall} - T_{fluid})$$

- increase tube surface A ↑
- increase heat transfer coefficient U ↑

↔

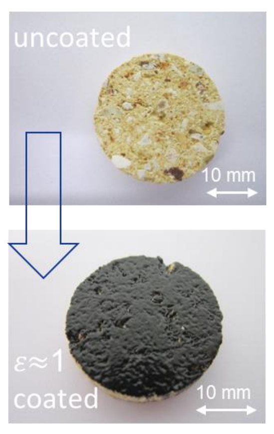
Increased pressure drop implies

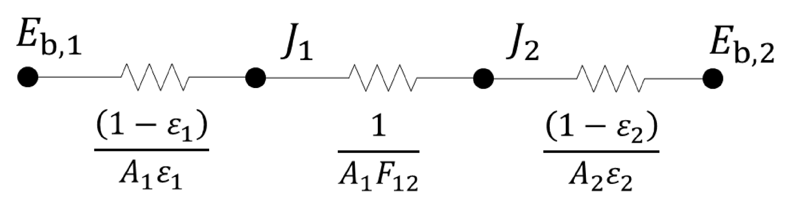
- loss in product selectivity

conventional bare reactor | industrial patented designs

HIGH EMISSIVITY COATINGS

Enhanced radiative heat transfer by tuning emissive properties
Electrical circuit analogy:





High emissivity coatings reduce the resistance and hence result in lower temperatures in the furnace → less firing

$$Q_{1,2} = \frac{E_{b,1} - E_{b,2}}{\frac{(1-\varepsilon_1)}{A_1\varepsilon_1} + \frac{1}{A_1F_{12}} + \frac{(1-\varepsilon_2)}{A_2\varepsilon_2}}$$

OXY-FUEL COMBUSTION

Oxygen is separated from air prior to combustion
Combustion of fuel in the presence of oxygen diluted with recycled flue-gas

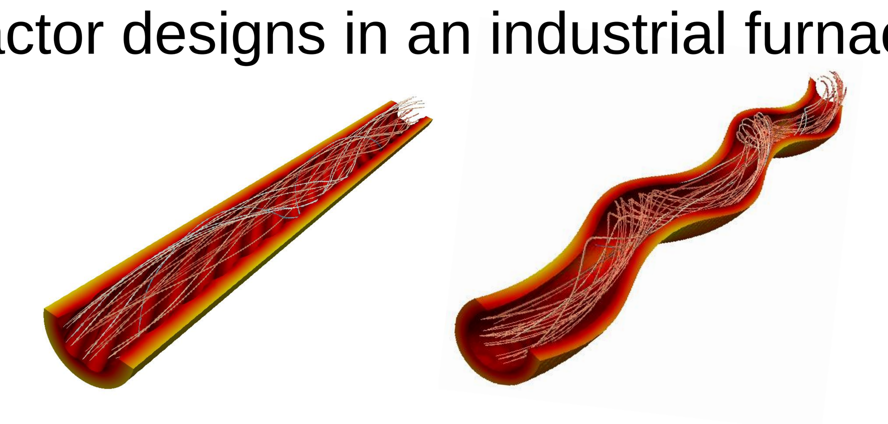
$CH_4 + 2O_2 + 8N_2 \rightarrow CO_2 + 2H_2O + 8N_2 + \text{HEAT}$

$CH_4 + 2O_2 + \text{flue gas} \rightarrow CO_2 + 2H_2O + \text{flue gas} + \text{HEAT}$

Reduce thermal NO_x emissions
Produced concentrated CO_2 flue gas stream easier captured and stored

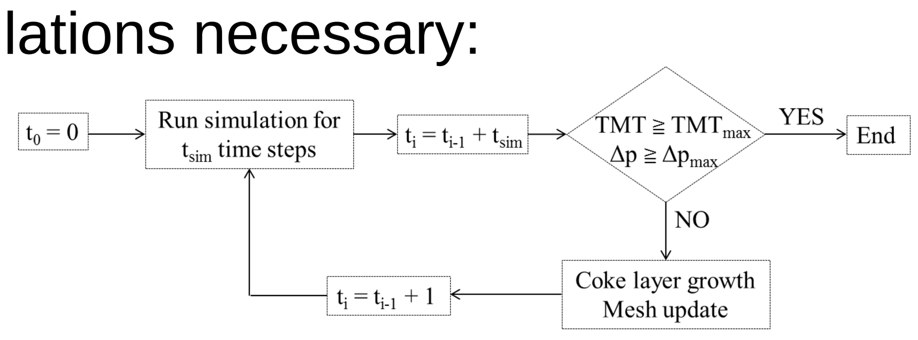
COMPUTATIONAL FLUID DYNAMICS SIMULATIONS

Reactive CFD modelling of different reactor designs in an industrial furnace:



SCOPE | **SFT**

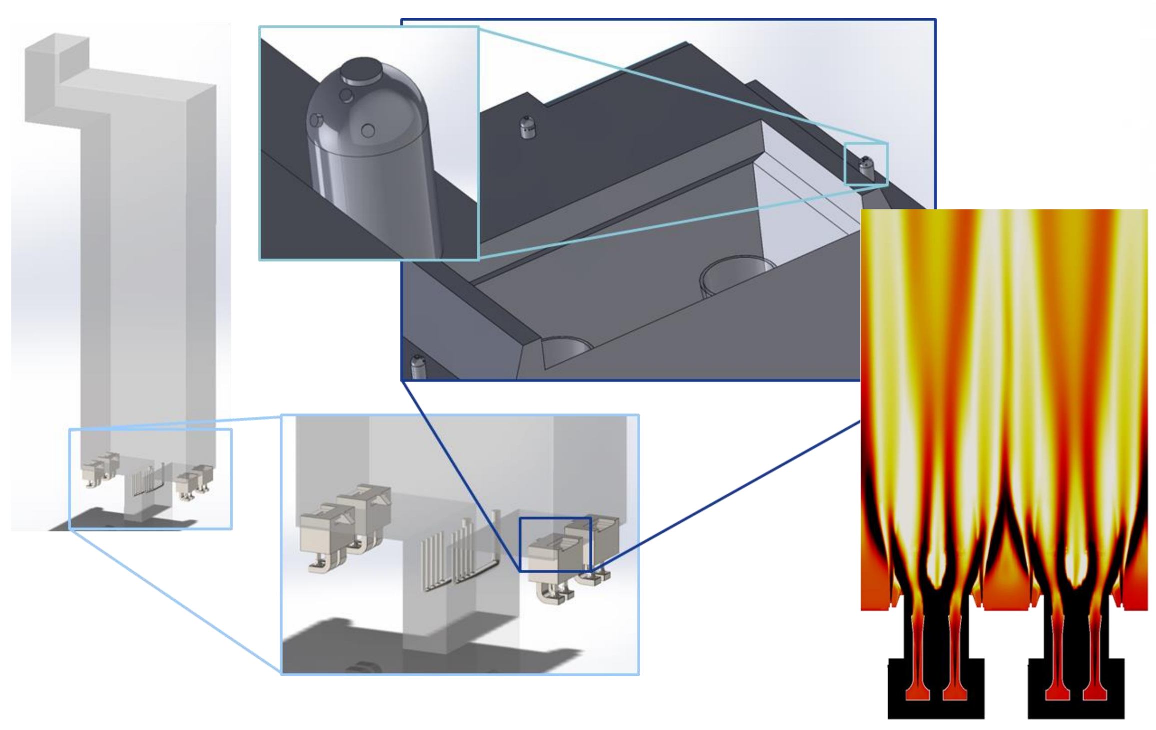
Coke formation is the nemesis of the steam cracking process, dynamic simulations necessary:



Exponential wide band CFD modelling (EWBM) to account for non-grey:

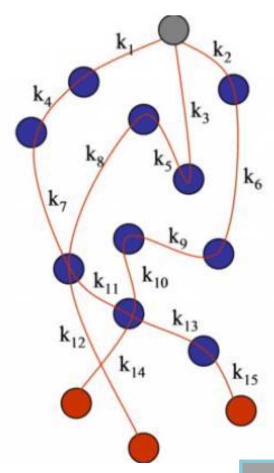
- gas phase absorption
- boundary wall emission

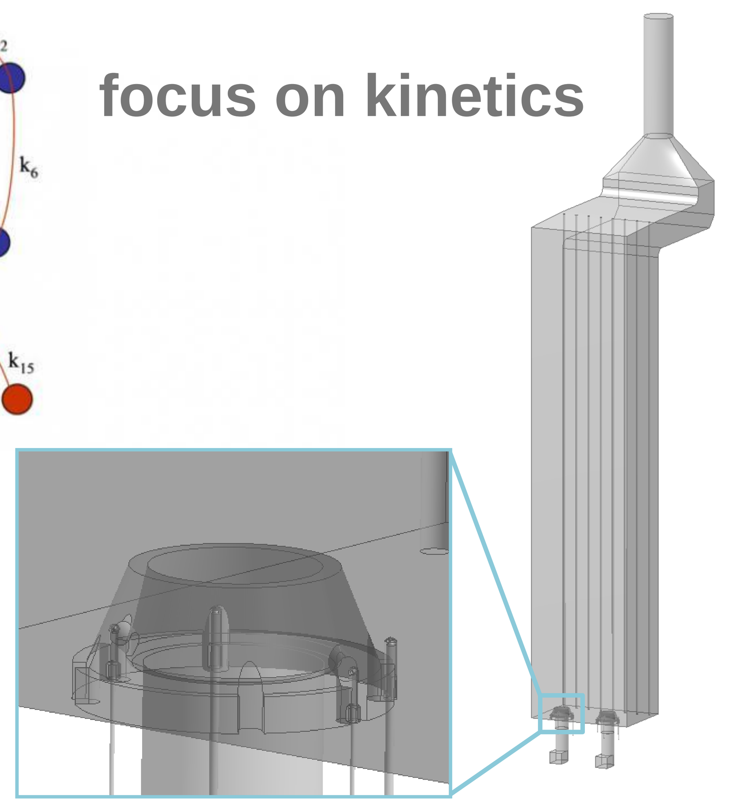
focus on radiation



Kinetic network required that is suitable for CFD

focus on kinetics





CONCLUSIONS AND FUTURE RESEARCH

3D reactor technologies outperform bare reactors
→ research ongoing to develop new geometries
→ experimental validation: pilot plant & cold flow experiments (VKI)

Emissive properties of both coated and uncoated materials typically used in steam cracking furnaces have been determined
→ applicable in CFD models
→ experimental validation: pilot plant & emissivity measurements

Compare reactive CFD simulations to experiments performed by industrial partner

Define kinetic network based on laboratory scale experiments

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