Numerical Simulation of a Biogenic Fluid Catalytic Cracking (BFCC) Regenerator with MFIX-Exa

NATIONAL ENERGY TECHNOLOGY LABORATORY

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The 2024 Multiphase Flow Science Workshop

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Disclaimer

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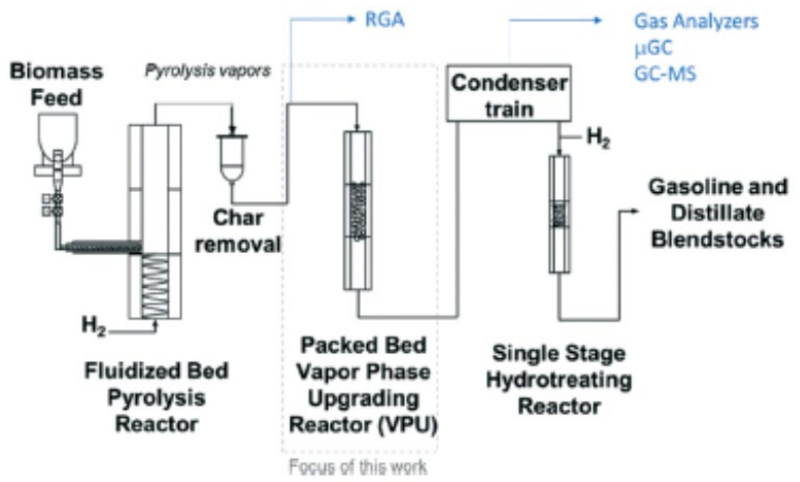
Goals of this Research

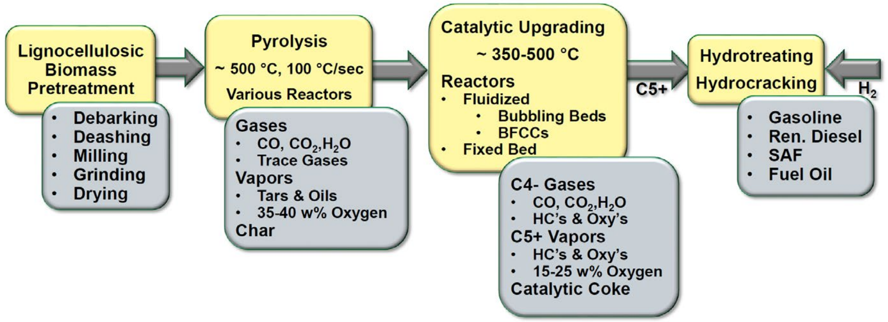
- Develop a Biogenic Coke Oxidation Kinetic for Biogenic Fluid Catalytic Cracking (BFCC) Catalyst Regeneration in MFiX.
- Validate the model based on experimental results.
- Design of a 2,500 metric ton per day (mTPD) BFCC regenerator.
- Investigate key parameters regarding the reactor performance.

Background

Renewable Energy through Catalyst Fast Pyrolysis



Catalytic Fast Pyrolysis (CFP)



- The full CFP process has been experimentally studied at National Renewable Energy Laboratory (NREL).
- Biomass was pyrolyzed for biofuel.
- Low molecular weight hydrocarbon was formed in pyrolysis vapors.
- Low molecular weight hydrocarbon can be upgraded with the catalyst.
- A packed bed Vapor Phase Upgrading Reactor (VPU) was used.
- Catalyst needed to be regenerated.
- A fixed bed has been used for catalyst regeneration.
- Different sectors have been studied thoroughly with MFiX.
- New systems need to be designed for continuous operation and industrial applications!

Background

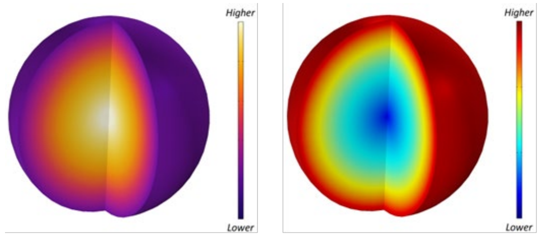
Biogenic Coke Oxidation Kinetics for Catalyst Regeneration

ChemCatBio
Chemical Catalysis for Bioenergy

Catalytic Fast Pyrolysis (CFP)	**CCPC** Reactor	**CDM**

Kinetics Extraction via COMSOL

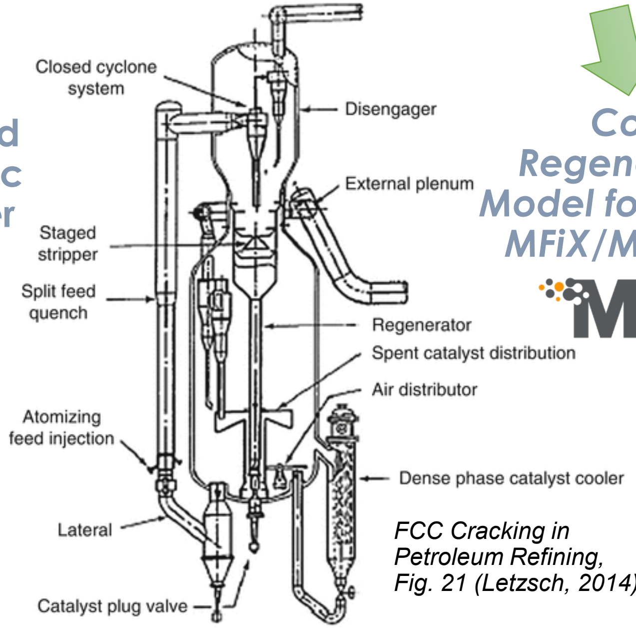
COMSOL



Temperature ***O2 Concentration***

- Project Background
  - Zeolite based catalyst regeneration and BFCC optimization
  - Biogenic FCC coke is very different than petroleum FCC coke
  - Combined particle scale (simplified) and reactor scale
  - Two spent catalysts: (a) Geldart B (~700 µm) from 2FBR for method development, and (b) FCC (80 µm) catalyst from Davison Circulating Riser (DCR)
- Consortium for Computational Physics and Chemistry (CCPC) Toolset Applied:
  - COMSOL bed models for deconvolution of combustion kinetics and mass/heat transport effects from Temperature Programmed Oxidation (TPO) data complimented by spent and partially regenerated particle/coke characterization
  - MFiX models for pilot- and commercial-scale regenerators, with afterburn (freeboard combustion), catalyst cooler, etc.
- Impact and Relevance:
  - First R&D program specifically aimed to understand nature of biogenic coke and consequences for BFCC design

Fluidized Catalytic Cracker (FCC)



FCC Cracking in Petroleum Refining, Fig. 21 (Letzsch, 2014)

Coke Regeneration Model for BFCC in MFiX/MFiX-Exa

MFiX

Bruce Adkins (ORNL), Mehrdad Shahnam (NETL)

Biogenic Coke Combustion Kinetic Model

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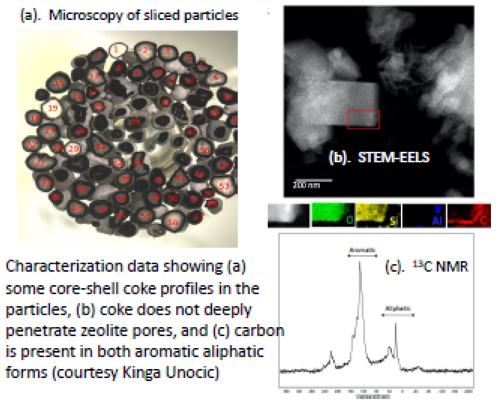
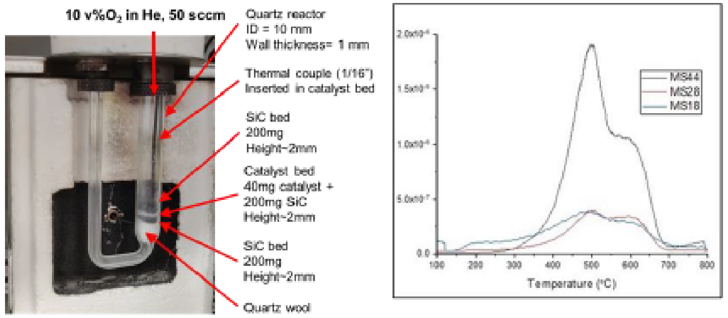


Characterization data showing (a) some core-shell coke profiles in the particles, (b) coke does not deeply penetrate zeolite pores, and (c) carbon is present in both aromatic aliphatic forms (courtesy Kinga Unocic)



TPO set-up and typical MS spectra showing evolution of CO, CO2 and H2O (courtesy Huamin Wang)

Rate Equations

	Reaction	Rate Equation	Units
1	Low temperature CO_2 formation on surface	$R_{CO2\_low} = a_{CO2\_low}\, cC_{low}\, cO_2^{b_{CO2\_low}}\, e^{\frac{-Ea_{CO2\_low}}{RT}}$	$mol/(m^2.s)$
2	High temperature CO_2 formation on surface	$R_{CO2\_hi} = a_{CO2\_hi}\, cC_{hi}\, cO_2^{b_{CO2\_hi}}\, e^{\frac{-Ea_{CO2\_hi}}{RT}}$	
3	Low temperature CO formation on surface	$R_{CO\_low} = a_{CO\_low}\, cC_{low}\, cO_2^{b_{CO\_low}}\, e^{\frac{-Ea_{CO\_low}}{RT}}$	
4	High temperature CO formation on surface	$R_{CO\_hi} = a_{CO\_hi}\, cC_{hi}\, cO_2^{b_{CO\_hi}}\, e^{\frac{-Ea_{CO\_hi}}{RT}}$	
5	CO oxidation	$R_{CO\_CO2} = a_{CO\_CO2}\, \rho_p\, cCO\, cO_2^{b_{CO\_CO2}}\, e^{\frac{-Ea_{CO\_CO2}}{RT}}$	$mol/(m^3.s)$

Parameters

Parameter	Units	Solver Value
a_{CO_CO2}	$m^3/(kg.s)$	0.2925
a_{CO2_low}	1/s	1,087
a_{CO2_hi}		5,102
a_{CO_low}		33,881
a_{CO_hi}		594,715
b_{CO_CO2}	-	0.0695
b_{CO2_low}		0.5384
b_{CO2_hi}		0.4793
b_{CO_low}		0.6650
b_{CO_hi}		0.9739
Ea_{CO_CO2}	J/mol	14,680
Ea_{CO2_low}		88,103
Ea_{CO2_hi}		118,197
Ea_{CO_low}		109,677
Ea_{CO_hi}		143,340

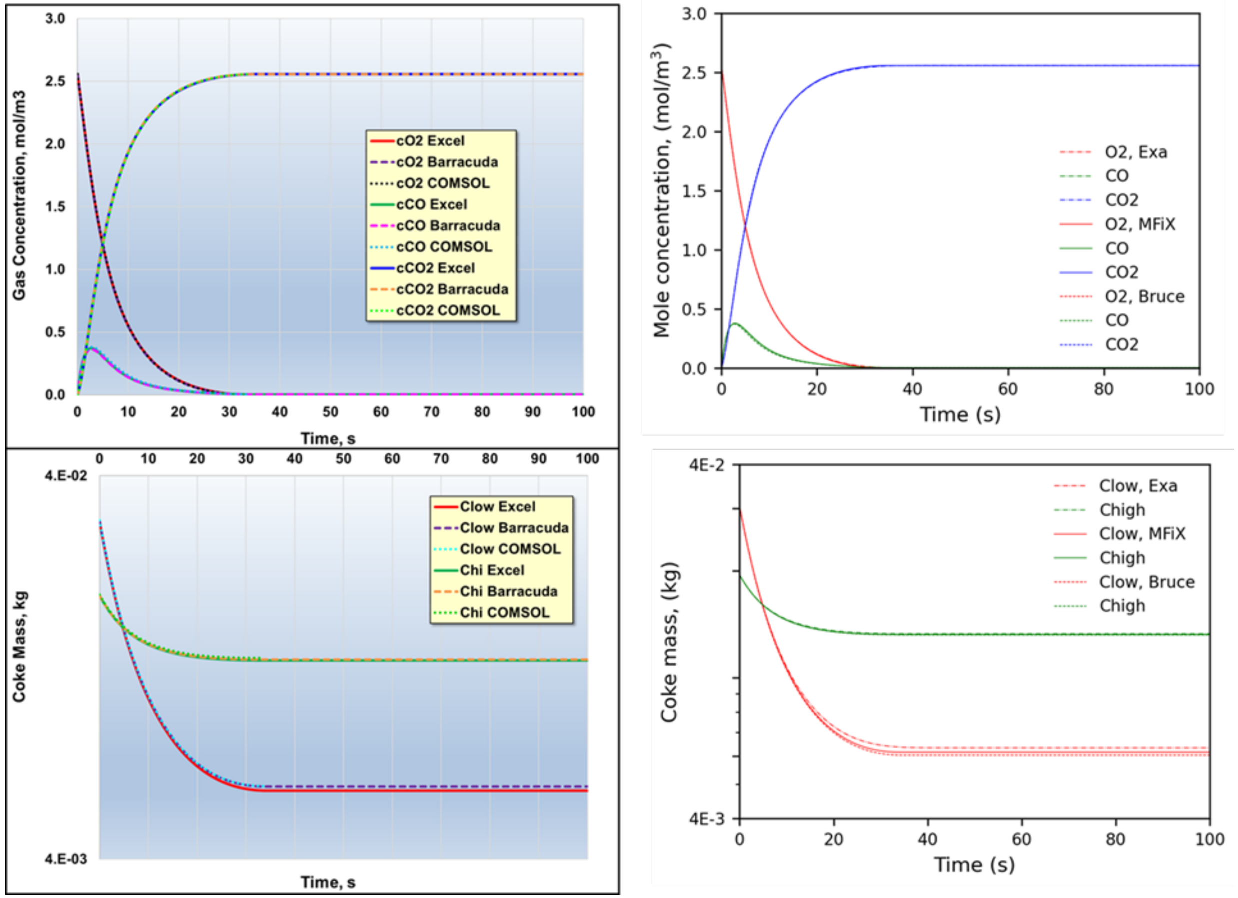
Kinetics Comparison

Excel, Barracuda, COMSOL, MFiX, MFiX-Exa

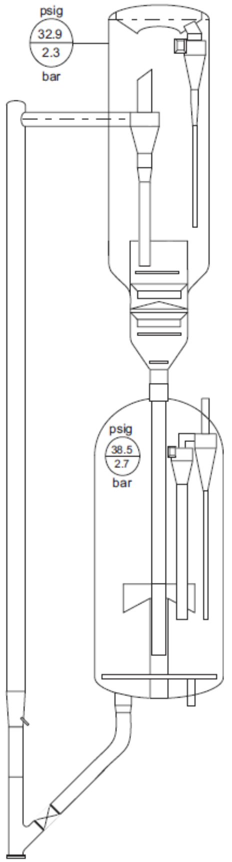
- Assumed no internal transfer resistances in the FCC particles, and converted the rate constants to use mass basis for carbon concentration
- Single cell simulation
- Domain: 1 m x 1 m x 1 m (1 m^3 volume)
- No flow, isothermal
- MSA 60 m^2/g, particle density 1,380 kg/m^3
- Four C oxidation reactions
- (Catalytic) CO oxidation

CoC = 0.5 w% Clow = 61% Chi = 39%

BCT1-23 1000K 10 kg cat 21v% O2



Typical Commercial FCC Reactor Operation Conditions



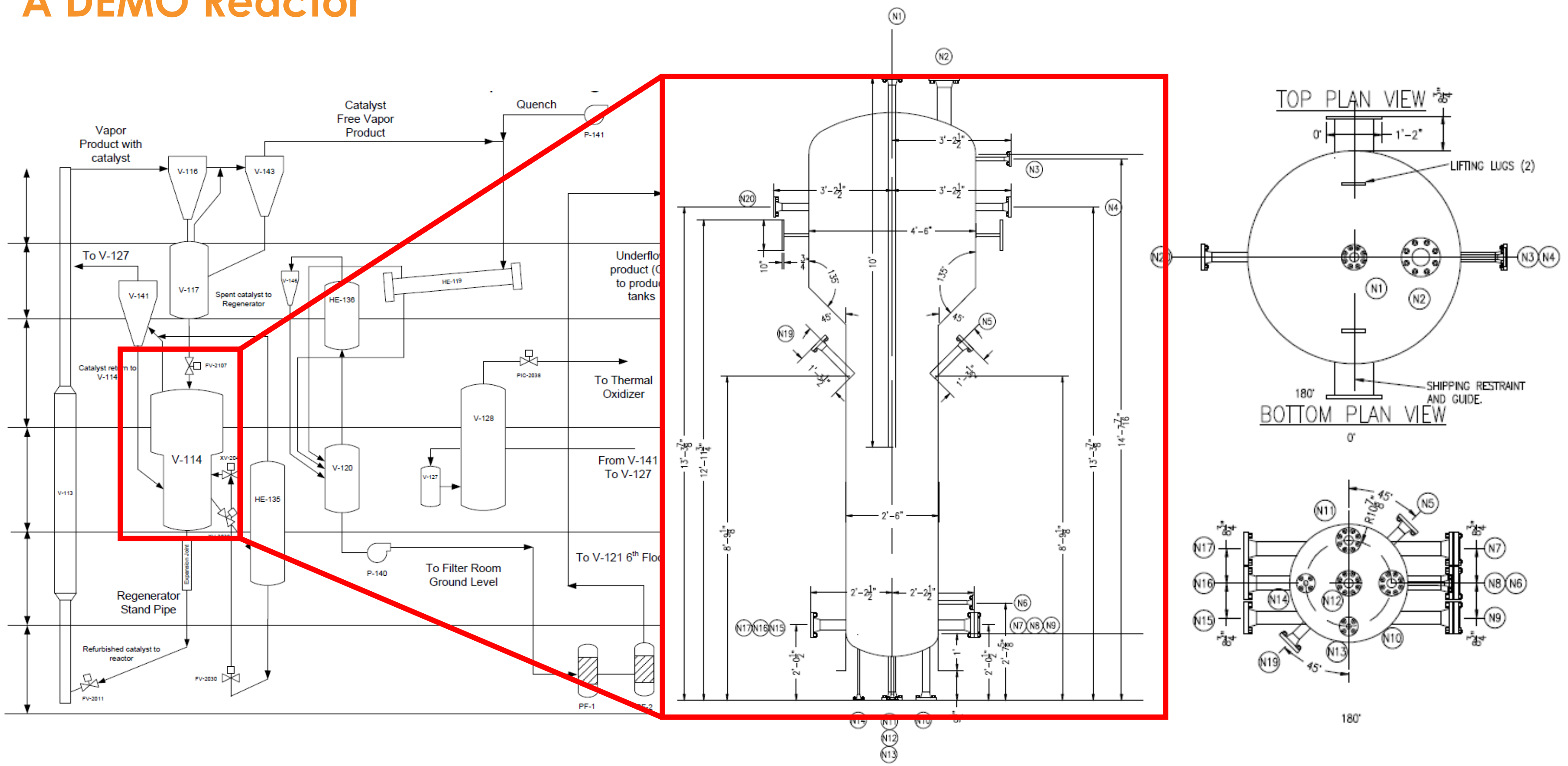
Example of KBR Orthoflow design FCC unit.

- The cracking reactions take place in **3 seconds or less**.
- Depending on the feed preheat, regenerator bed, and riser outlet temperatures, the ratio of catalyst to oil is normally in the range of **4:1 to 10:1** by weight.
- The typical regenerated catalyst temperature ranges between 1,250 °F and 1,350 °F (**677-732 °C**).
- The cracking or reactor temperature is often in the range of 925-1,050 °F (**496-565 °C**).
- Typical risers are 2 to 7 feet (61 to 213 cm) in diameter and 75 to 120 feet (**23 to 37 m**) long.
- Risers are normally designed for an outlet vapor velocity of 40-60 ft/s (**12-18 m/s**).
- The spent catalyst entering the regenerator usually contains between **0.5 and 1.5 wt.% coke**.
- Components of coke are C, H, and trace amounts of S and organic nitrogen molecules.
- Air distributors are often designed for a 1.0- to 2.0-psi (7-15 kPa) pressure drop to ensure positive air flow through all nozzles.
- In traditional bubbling bed regenerators, there are two regions: the dense phase and the dilute phase. At velocities common in these regenerators, 2-4 ft/s (**0.6-1.2 m/s**), the bulk of catalyst particles are in the dense bed, immediately above the air distributor.
- During regeneration, the coke level on the catalyst is typically reduced to, **0.10%**.

Sadeghbeigi, Reza. Fluid catalytic cracking handbook: An expert guide to the practical operation, design, and optimization of FCC units. Butterworth-Heinemann, 2020.

Proof-of-Concept of a BFCC Regenerator

A DEMO Reactor



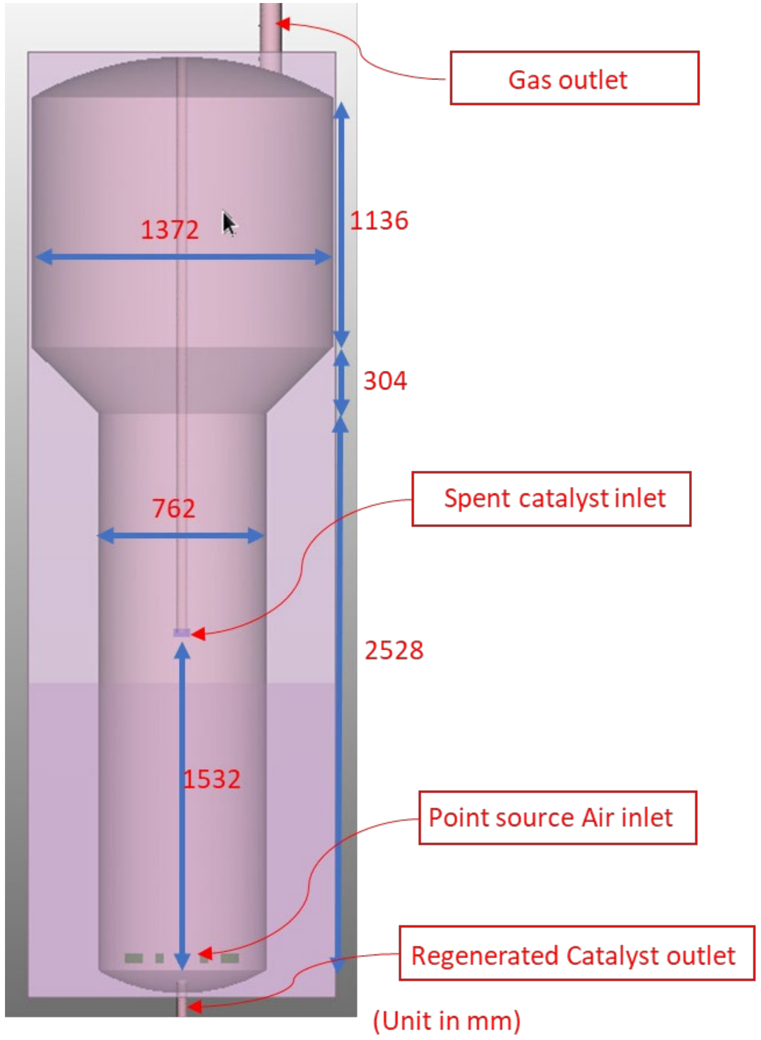
NOZZLE SCHEDULE

MARK	DESCRIPTION	SIZE
N1	FROM STRIPPER	2"
N2	GAS EXIT	4"
N3	TEMPERATURE	3/4"
N4	GAS FROM REGENERATOR COOLER	2"
N5	CATALYST FROM REGENERATION	2"
N6	TEMPERATURE	3/4"
N7	DISTRIBUTOR SUPPORT	3"
N8	DISTRIBUTOR SUPPORT	3"
N9	DISTRIBUTOR SUPPORT	3"
N10	CATALYST TO REGENERATOR COOLER	2"
N11	CATALYST TO HOPPER	2"
N12	CATALYST TO CATALYST COOLER	2"
N13	SAMPLING	1/2"
N14	NATURAL GAS	1/2"
N15	DISTRIBUTOR SUPPORT	3"
N16	DISTRIBUTOR SUPPORT	3"
N17	DISTRIBUTOR SUPPORT	3"
N18		
N19	FRESH CATALYST FEED	2"
N20	GAS FROM CATALYST COOLER	2"

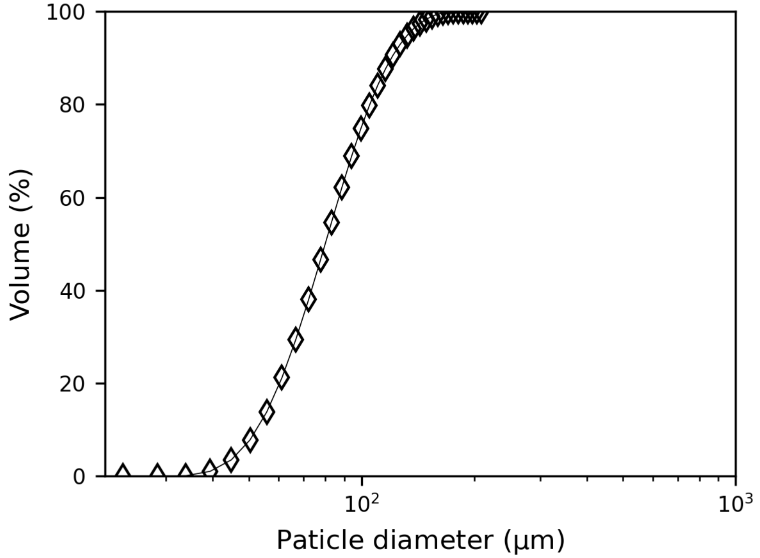
A DEMO FCC regenerator: geometry, dimensions and other parameters.

- A 5 t/day DEMO unit is used as a proof-of-concept.
- Reactor dimensions were available.

MFiX-Exa Settings and BFCC Properties



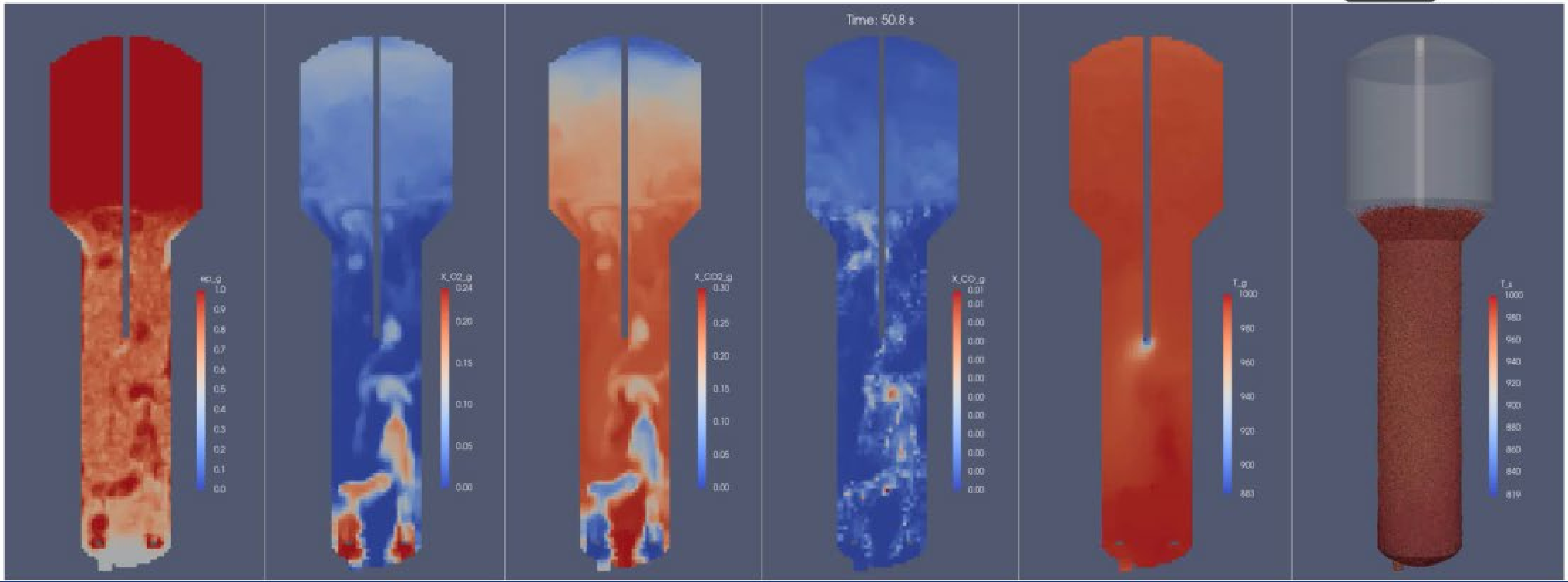
- Reactor type: FCC Catalyst regeneration
- Reactor size: 1.5 x 4.5 x 1.5 m
- Domain cells: 48 x 48 x 144 (331776)
- Drag closure: Wen_Yu
- Convective heat transfer correlation: Gunn
- Initial bed inventory: ~327.8 kg
- Particle tracking method: Particle-In-Cell (PIC)
- Parcel number: > 510,000
- pic.parcels_per_cell_at_pack = 36.0
- Circular point source for air inlet
- Biomass feed rate = 5 mTPD
- Catalyst to Biomass (CTB) = 9
- Spent catalyst flow rate: 0.5208 kg/s
- Coke on catalyst: 1.0%
- Stoichiometric airflow (AF = 1): 0.0598 kg/s
- A real E-catalyst was simulated
- Catalyst Particle Size Distribution (PSD)/density were provided
- Initial Temperatures 711°C (984 K)
- Gas inlet = 711°C (984 K) and Spent catalyst inlet = 544°C (817 K)
- 274,000 Pa



Properties of FCC catalyst

- Coke on spent catalyst: 1.0%
- Mass Fraction C in LOW species: 61.00%
- Mass Fraction C in HIGH species: 39.00%
- Spent catalyst density (kg/m^3):1,380.95
- Catalyst D50 (μm): 80.0

Results of 5 Ton Per Day DEMO Reactor with MFiX-Exa

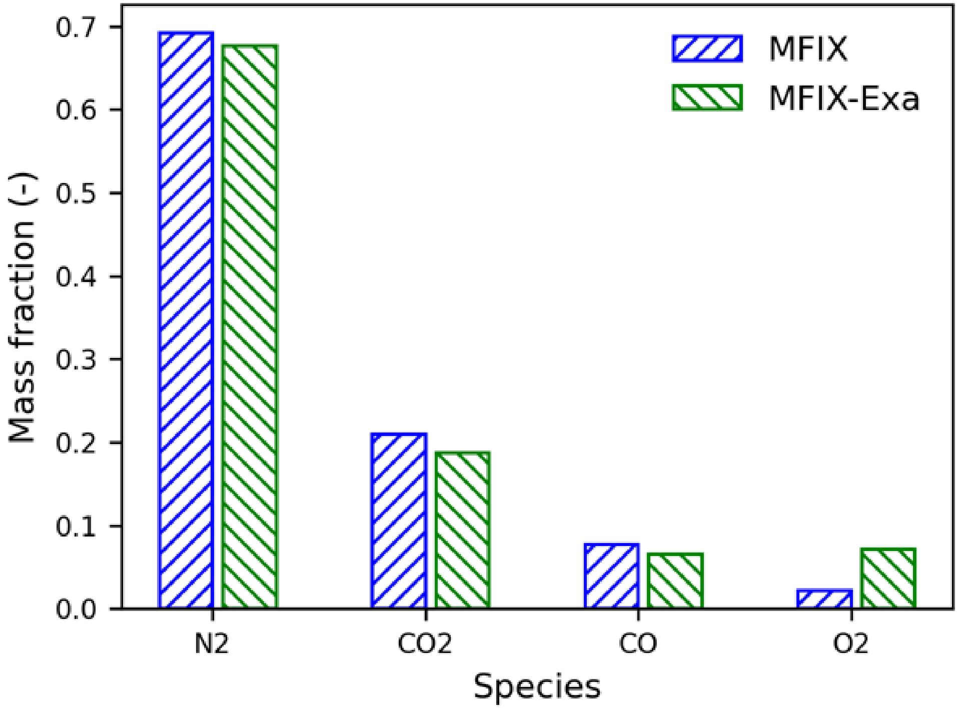


Ep_g | $X\_O_2\_g$ | $X\_CO_2\_g$ | X_CO_g | Tg (K) | Catalyst Temperature (K)

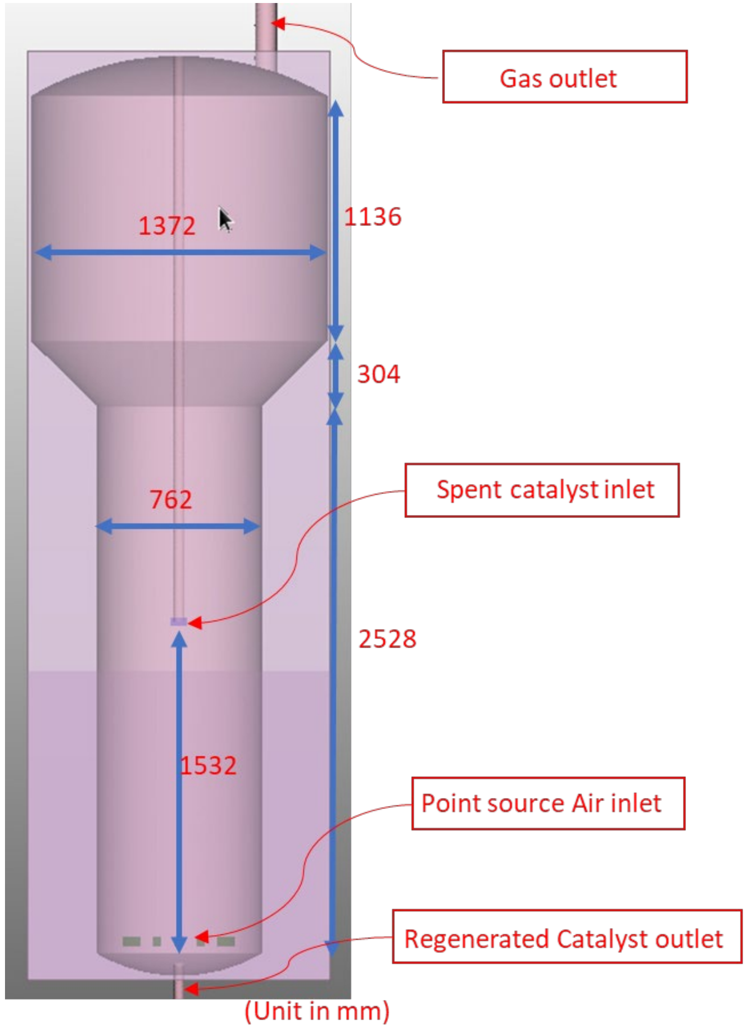
- The gas volume fraction, O_2, CO_2, CO, T_g of the central cross-section are shown together with the catalyst temperature.

Comparison Between MFIX and MFIX-Exa

- Both MFIX-Exa and MFIX predicted similar exit gas composition.
- The MFIX-Exa can reach > **140 s of simulation time per day** with 1 GPU node on Joule 3 (8 NVIDIA Hopper H100 using NVLink). (Only 1 GPU node is allowed for each user.)
- The MFIX-Exa can reach > **300 s of simulation time per day** with 6 CPU nodes (648 CPU Cores) on Joule 3 (**128 cores with AMD EPYC 9534 64-Core Processor per node.**)



Scale-up from 5 mTPD to 2,500 mTPD



Khartoum Refinery Company

Table 1. Dimensions of the FCC regenerator

Parameters	
Length of the regenerator (m)	26.19
Length of the top section (m)	12.69
Length of the middle section (m)	3.89
Length of the bottom section (m)	9.61
Diameter of the top section (m)	9.6
Diameter of the bottom section (m)	8
Diameter of air inlet (m)	1.95
Diameter of catalyst inlet (m)	1.1
Diameter of outlet(m)	3.51

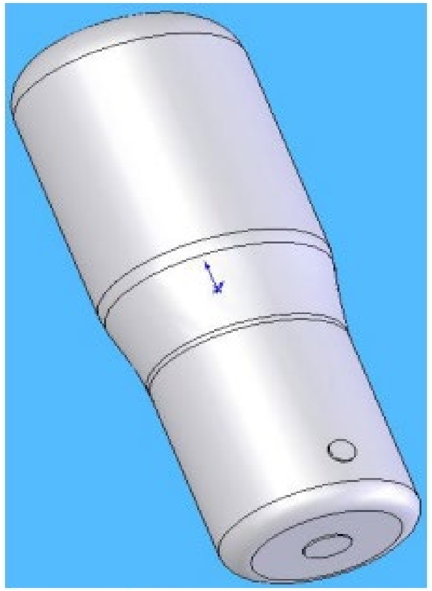


Fig.1. Complete geometry of the Regenerator

Table 2. The data for the regenerator air inlets the for the three cases

	Base Case	Case (1)&(2)
Mass flow rate (kg/s)	147.5	29.5
Pressure (kPa)	300	300
Hydraulic diameter (m)	1.95	0.78
Temperature (K)	473	473

Table 3. The data for the regenerator catalyst inlet for the three cases

Mass flow rate (kg/s)	288.89
Pressure (kPa)	240
Hydraulic diameter(m)	1.1
Temperature (K)	973

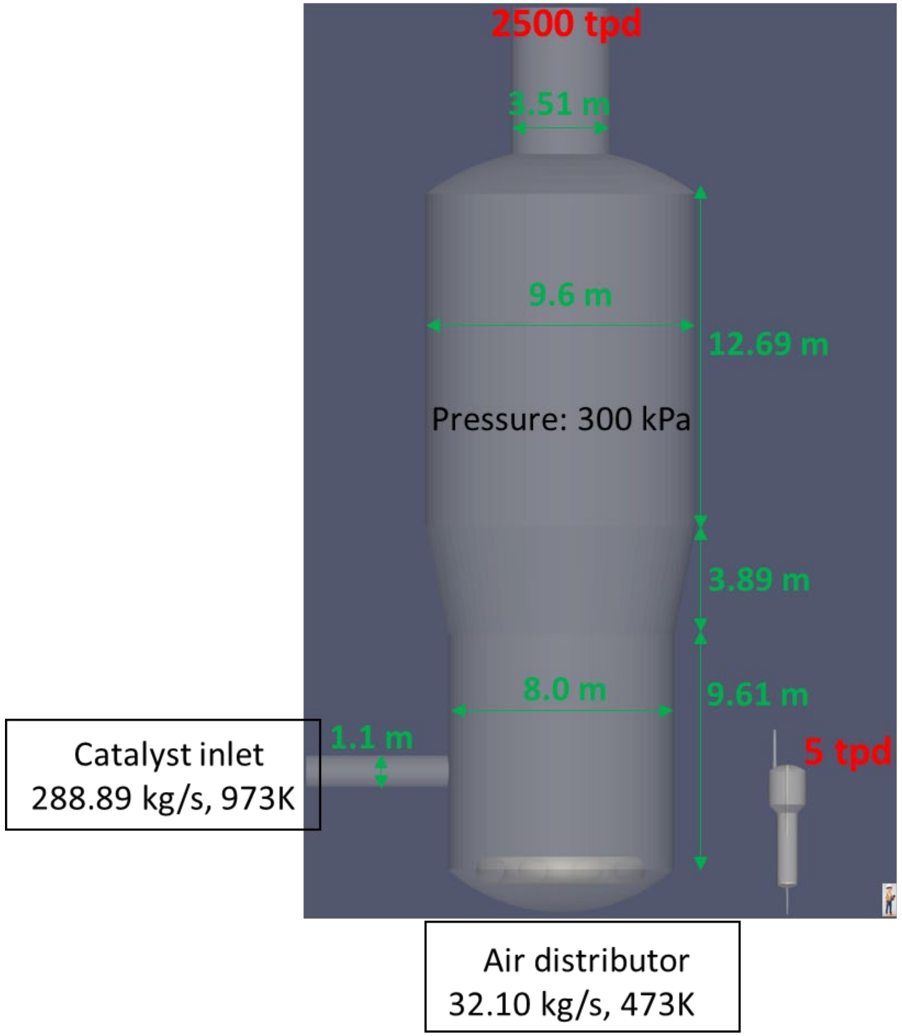
Catalyst flow rate = 288.29 kg/s

= 25,000 mTPD (of catalyst)

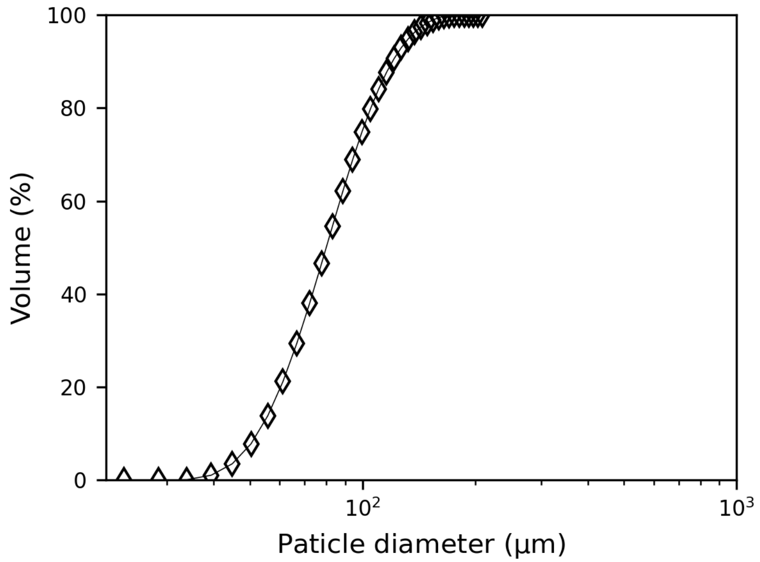
With the **Catalyst to Biomass = 10**,
this reactor is the perfect match.

Ahmed, N. A. M., Mustafa, M. A., & Seory, A. M. A. (2016). Computational fluid dynamics simulation of a fluid catalytic cracking regenerator. University Of Khartoum Engineering Journal, 5(1).

Numerical Settings

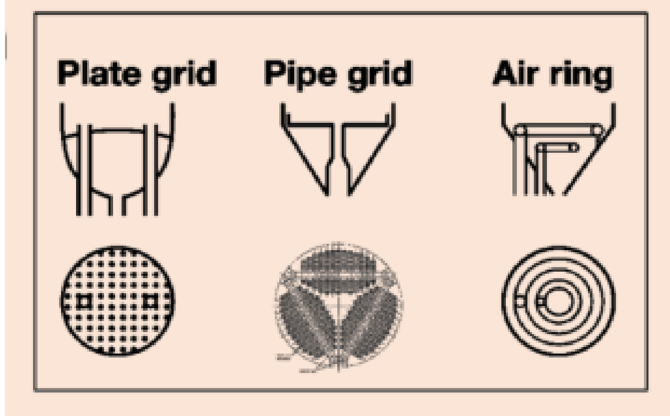


- Reactor type: 2500 mTPD FCC Catalyst regeneration
- Reactor size: 10 x 10 x 30 m
- Domain CFD cells: 64 x 64 x 192 (786,432)
- Drag closure: Wen_Yu
- Convective heat transfer correlation: Gunn
- Initial bed inventory: ~150,700 kg
- Particle tracking method: Particle-In-Cell (PIC)
- Parcel number: ~ 1,260,000
- pic.parcels_per_cell_at_pack = 24.0
- Circular point source for air inlet
- Biomass feed rate = 2,500 mTPD
- Catalyst to Biomass (CTB) = 10
- Spent catalyst flow rate: 288.89 kg/s
- Coke on catalyst: 1.0%
- Air flow rate: 32.10 kg/s
- A real E-catalyst was simulated
- Catalyst PSD/density were provided



- Coke on spent catalyst: 1.0%
- Mass Fraction C in LOW species: 61.00%
- Mass Fraction C in HIGH species: 39.00%
- Spent catalyst density (kg/m^3): 1,380.95
- Catalyst D50 (μm): 80.0

Air distributor ring configuration study



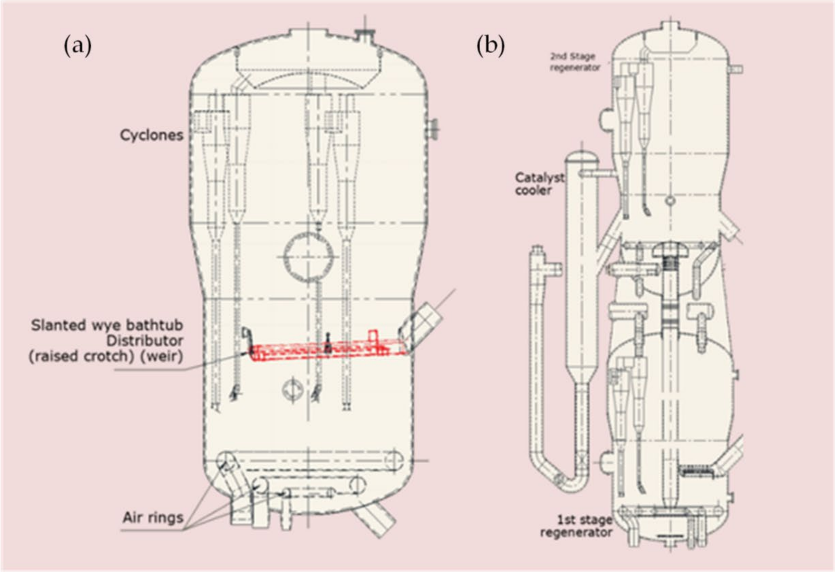


Figure 3. FCC regenerator full combustion designs: (**a**) single-stage regeneraator; (**b**) TechnipFMC two-stage regenerator (adapted from Singh and Gbordzoe [88]).

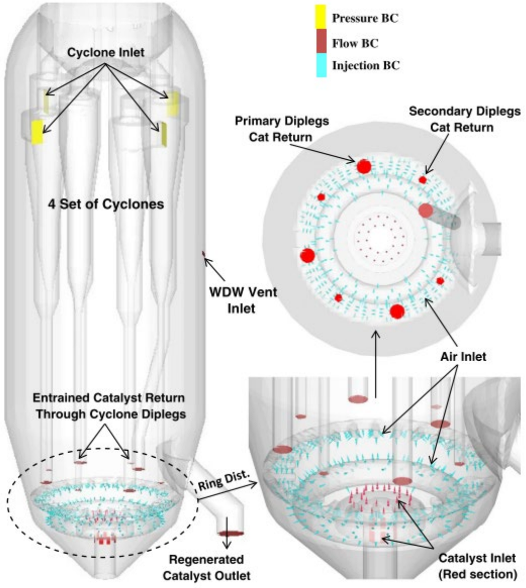


Fig. 3. Regenerator model – boundary conditions.

"… the air ring is the most effective, since the cantilever arms of pipe grid due to their geometry suffer from arms cyclic oscillations and fatigue resulting in low mechanical life and more downtime, while the ring grid, on the other hand, could sit concentrically, providing maximum coverage of the entire cross-section of the catalyst bed, providing excellent gas distribution in the annulus of the regenerator. They further argued that the jet penetration from the ring nozzles enhances uniform mixing and combustion with high resistance to erosion of internals and catalyst attrition."

Oloruntoba, A., Zhang, Y., & Hsu, C. S. (2022). State-of-the-art review of fluid catalytic cracking (FCC) catalyst regeneration intensification technologies. Energies, 15(6), 2061.
RAJ SINGH, PAUL MARCHANT and STEVE SHIMODA. (2019) Improved distribution of spent catalyst
Singh, R., & Gbordzoe, E. (2017). Modeling FCC spent catalyst regeneration with computational fluid dynamics. Powder Technology, 316, 560-568.

Air distributor ring configuration study

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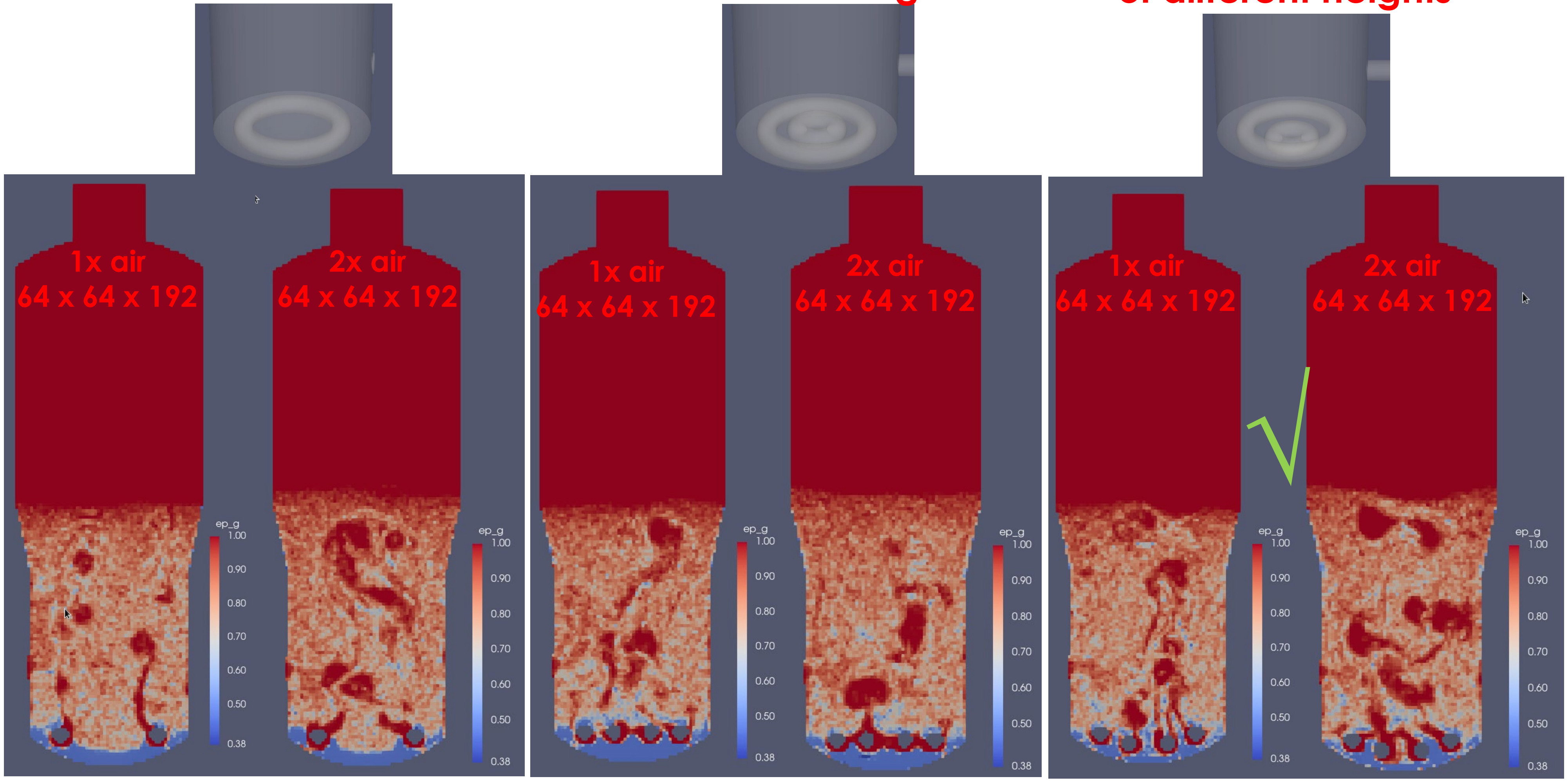
1 air distributor ring

2 air distributor rings of same height

2 air distributor rings of different heights

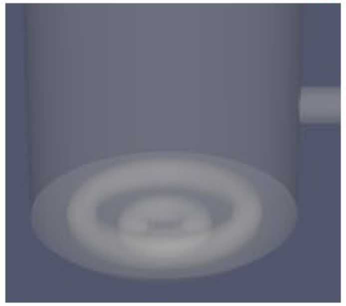


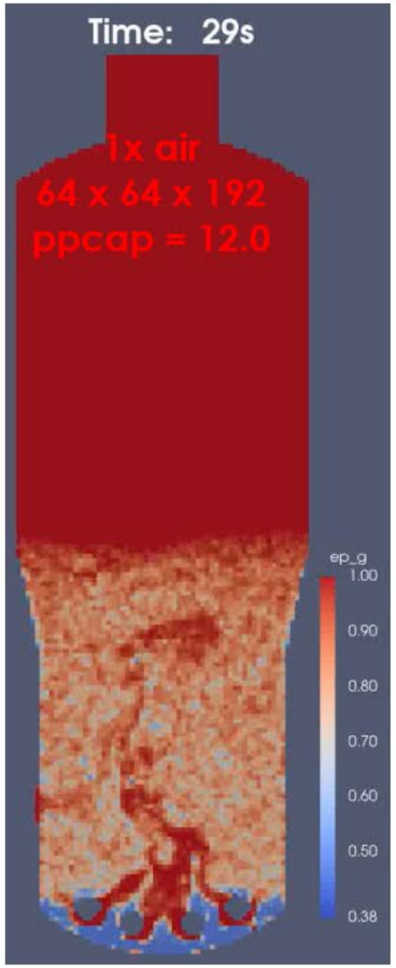
Parcel size study

pic.parcels_per_cell_at_pack (ppcap)

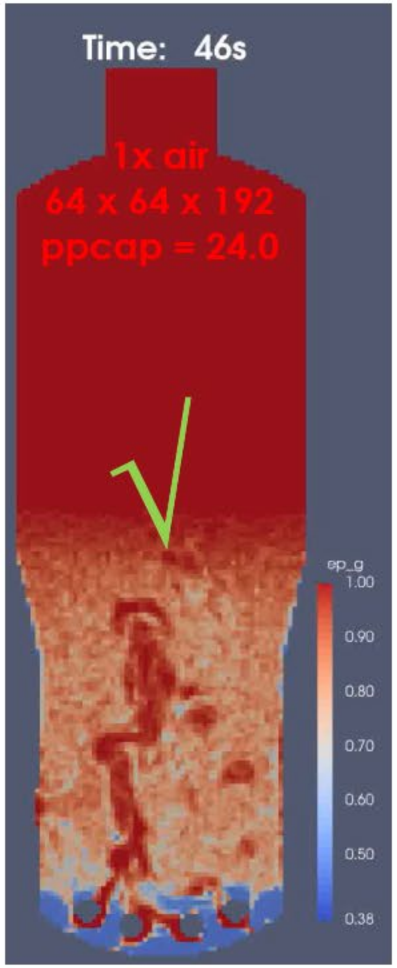
parcels_per_cell_at_pack
= (Vc / Vp) * (ep_cp / statwt)

2 air distributor rings
of different heights

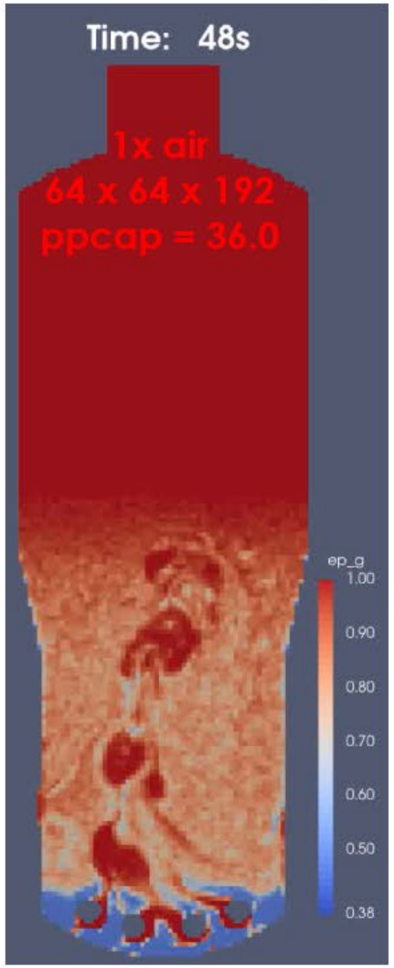




Parcel size x0.5



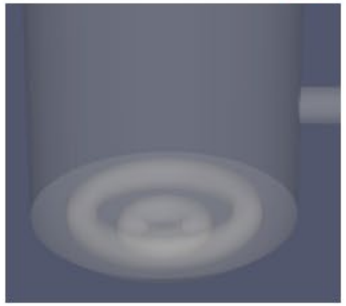
Parcel size x1/3

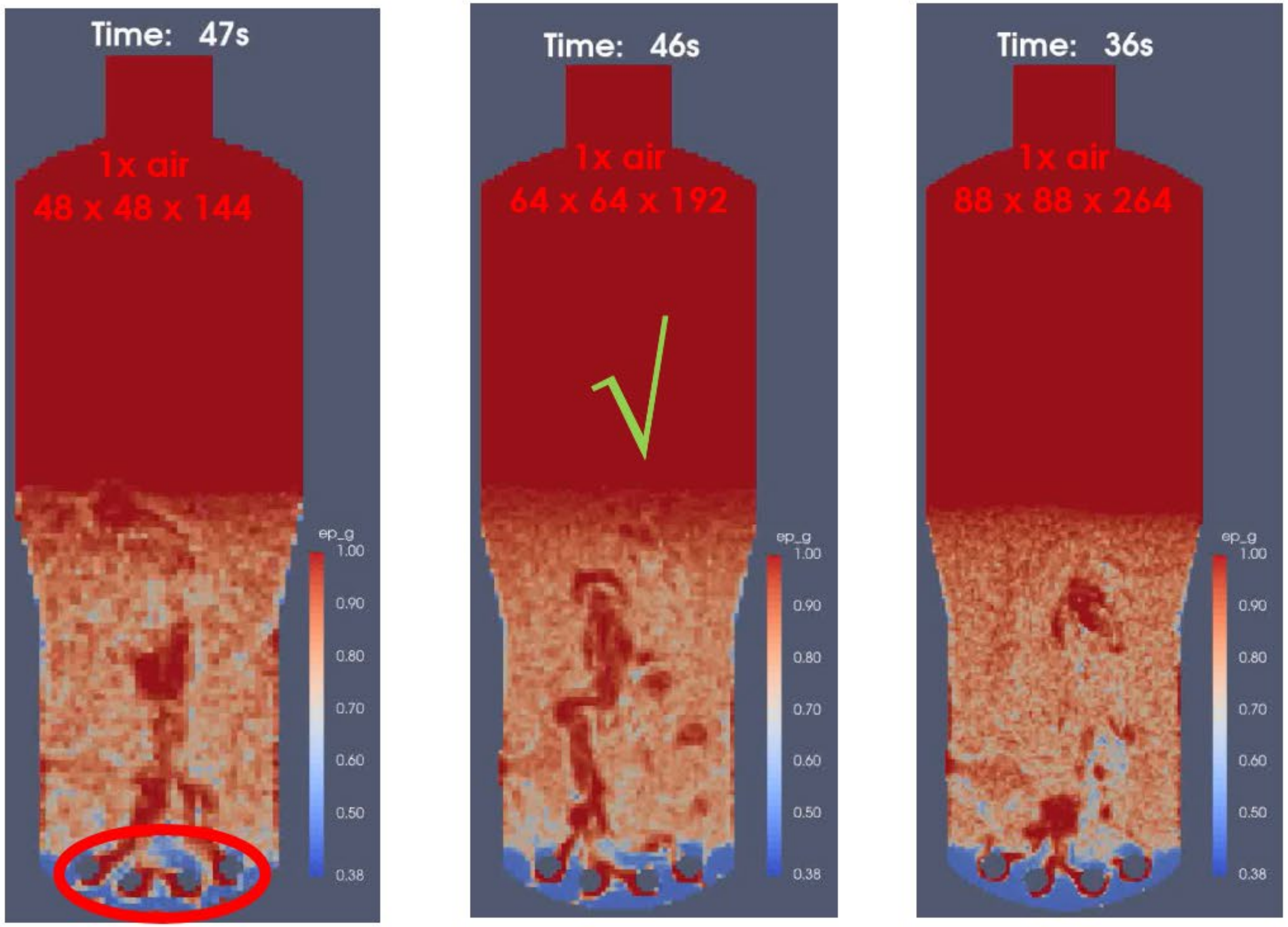


Grid convergence study

pic.parcels_per_cell_at_pack = 24.0

2 air distributor rings of different heights





Summary and Future work

Summary

- A new kinetic model for BFCC catalyst regeneration derived from TPO and COMSOL DNS dataset were developed and implemented both in MFiX and Exa.
- A new E-cat PSD was incorporated in the new simulations.
- A demo 5 ton-per-day BFCC regenerator was simulated.
- An industrial 2,500 mTPD BFCC regenerator was simulated.
- Key parameters regarding the reactor performance were investigated.
- Air distributor configuration and other simulation parameters were determined.

Next Steps

- Reacting case study of the 2,500 mTPD reactor.
- Reactor optimization and improvement.

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