CPFD Simulation of Combustion Process and Investigation of Associated Heat Transfer and Hydrodynamics in Fluidized Bed

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Background:

- Gas-solid Fluidized bed reactor offers several advantages, including high heat and mass transfer rates, and good mixing of solids, making them attractive for several industrial processes.
- The most important application of the FB reactor is fluid catalytic cracking (FCC). FCC unit is to convert high-boiling petroleum fractions called gas oil to high-value fuels (gasoline, jet fuel, and diesel).
- There are over 400 FCC/RFCC units operating worldwide with a total processing capacity of over 20 million barrels per day and generate approximately 40% of the world's gasoline.
- High heat transfer efficiency and good equipment reliability are two main concerns for industrial operators. To achieve the two objectives, a deep understanding of the relationship between hydrodynamic phenomenon and heat transfer properties is needed.
- Most previous literature reported using dimensionless number Nusselt number as a function of Prandtl number and Reynolds number to heat-transfer coefficients predictions in fluidized-bed. Few studies were on surface hydrodynamics, which is directly related to the heat transfer mechanism.
- Computational Fluid Dynamics (CFD) is a powerful tool that allows the study of complex multi-phase systems such as fluidized beds.
- CFD strategies can used when simulating gas-particle systems, Eulerian-Eulerian approach (E–E) such as Two-Fluid Model (TFM), Eulerian-Lagrangian approach (E-L), i.e the Discrete Element or Discrete Particle Method (DEM or DPM) and Multiphase Particle-in-Cell (MPPIC) Model.
- TFM considers both the fluid and the solids as interpenetrating continuous phases. While this method has the advantage of not being computationally expensive, it is not able to account for solid-solid interactions. DEM considers the fluid as a continuous phase while tracking every single particle and its interactions. DEM demands significant computational resources, while its use is limited to a restricted number of particles.
- Barracuda CPFD coop above limitations by introducing Multiphase Particle-in-Cell (MPPIC), which treats the fluid as a continuum and the solids as a group of particles instead of individual particles.
- There are two types of regenerators in FCC operations; one operates in the partial combustion mode and the other in the total combustion mode. In partial combustion mode, no oxygen should be present in the flue gas In the total combustion mode, excess air is provided to the regenerator where coke should be reacted to carbon dioxide, and no carbon monoxide should be present in the flue gas
- The phenomenon of afterburn in the partial combustion regenerator is due to converting carbon monoxide to carbon dioxide in the freeboard. A large amount of heat combustion is released, which can damage the regenerator internals (as cyclones and plenum chamber) and contribute to catalyst thermal deactivation

Motivation:

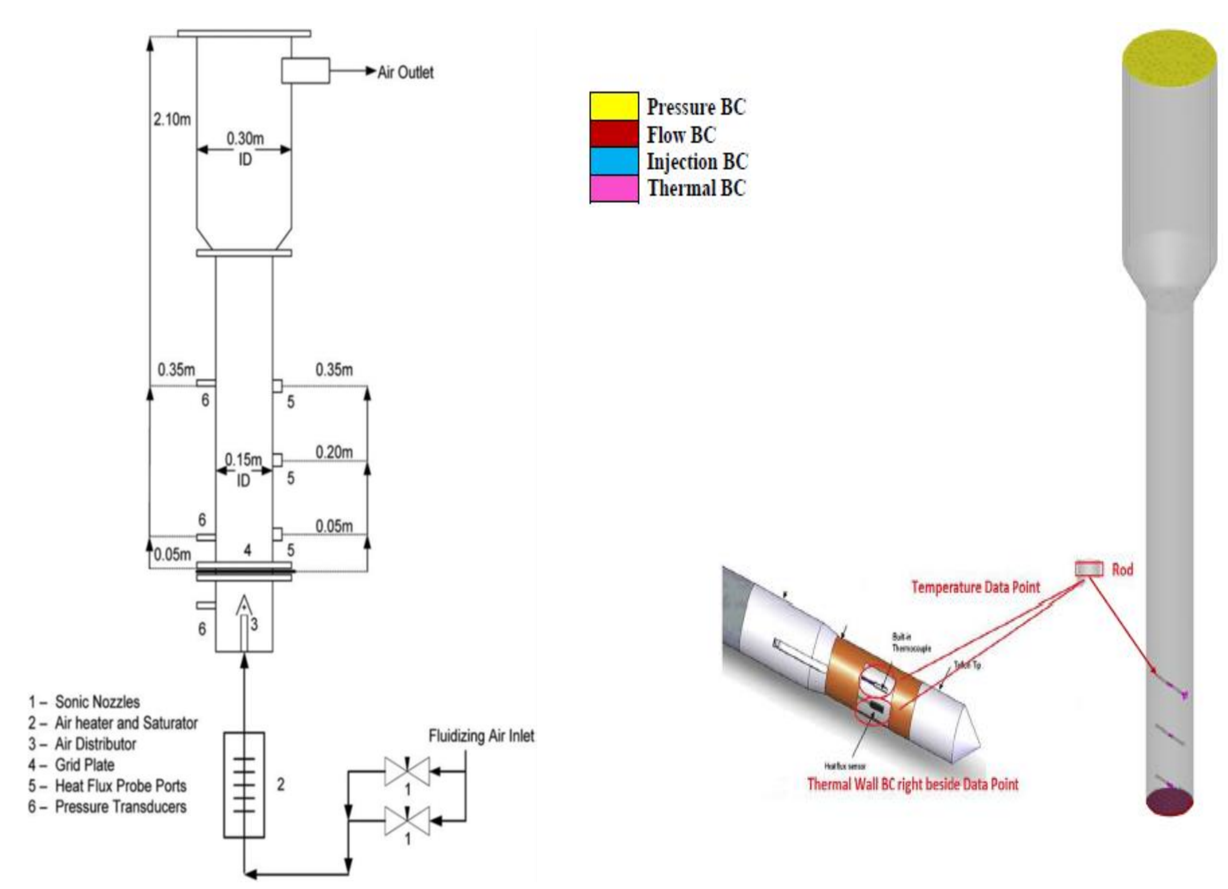
About 90 % of 400 FCC/RFCC units are operating in the partial combustion mode. Thermal management of these processes is always challenging and becomes even more challenging with variations in feedstock compositions affecting the reaction environment. A good understanding of the hydrodynamics, mixing, and heat transfer process is required for better management and control. The exothermic coke combustion process requires careful control and thermal management of the unit to avoid temperature surges in the bed and minimize afterburn in the freeboard region due to incomplete combustion in the bed. Carbon monoxide produced due to incomplete combustion can continue to react in the freeboard region of the regenerator and resulting in high temperature, which impacts the regenerator internals and affects the catalyst activity.

Objectives:

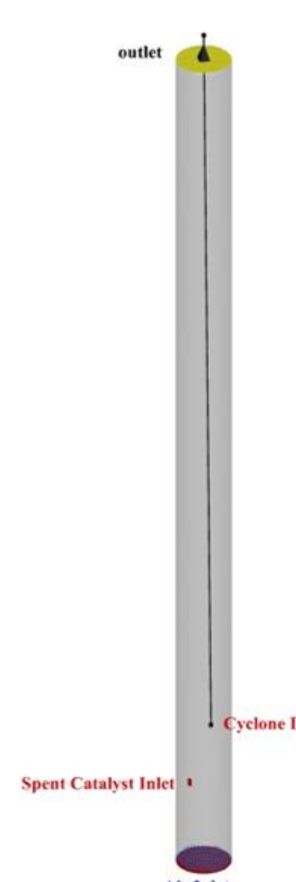
- Investigate heat transfer and mixing processes for better overall thermal management.
- The coke combustion process will be simulated with the help of CPFD-software accounting for kinetics, mass transfer, and mixing effects.
- Heat transfer process in a fluidized bed will be simulated and validated by experimental measurements.
- Particle mixing behavior will be analyzed with appropriate experimental measurements.
- To evaluate design alternatives to improve the operation of a FCC regenerator.
- To develop CFD simulations to better understand the behavior of an industrial FCC regenerator.

Research Methodology (Experimental vs Numerical):

- Measurements have been carried out in a Plexiglas column of inside diameter 0.15 m and height of 2 m. The bed consisted of 150 µm sand particles of static bed height 0.45 m. The gas velocity was varied from 0.1 to 0.4 m/s.
- Radial and axial variations in heat transfer coefficients captured by fast response probe (0.02s)
- Numerical model successfully predicted the heat transfer coefficients and effect of bed hydrodynamics



- CPFD simulated the coke combustion of spent catalyst in FCC regenerator. The obtained results are compared to industrial data.



Continuity equation of gas phase:

$$\frac{\partial(\varepsilon_f \rho_f)}{\partial t} + \nabla\cdot(\varepsilon_f \rho_f u_f) = \delta \dot{m}_p \qquad (1)$$

Momentum equation of gas phase:

$$\frac{\partial(\varepsilon_f \rho_f u_f)}{\partial t} + \nabla\cdot(\varepsilon_f \rho_f u_f u_f) = \begin{cases} \text{Model A} \\ -\nabla p + F + \varepsilon_f \rho_f g + \nabla\cdot(\varepsilon_f \tau_f) \\ \text{Model B} \\ -\varepsilon_f \nabla p + F + \varepsilon_f \rho_f g + \nabla\cdot(\varepsilon_f \tau_f) \end{cases} \qquad (2)$$

Enthalpy:

$$\frac{\partial(\varepsilon_f \rho_f h_f)}{\partial t} + \nabla\cdot(\varepsilon_f \rho_f h_f u_f) = \varepsilon_f\left(\frac{\partial p}{\partial t} + u_f\cdot\nabla p\right) + \phi - \nabla\cdot(\varepsilon_f q) + \dot{Q} + S_h + q_D \qquad (3)$$

Species Transport Equation:

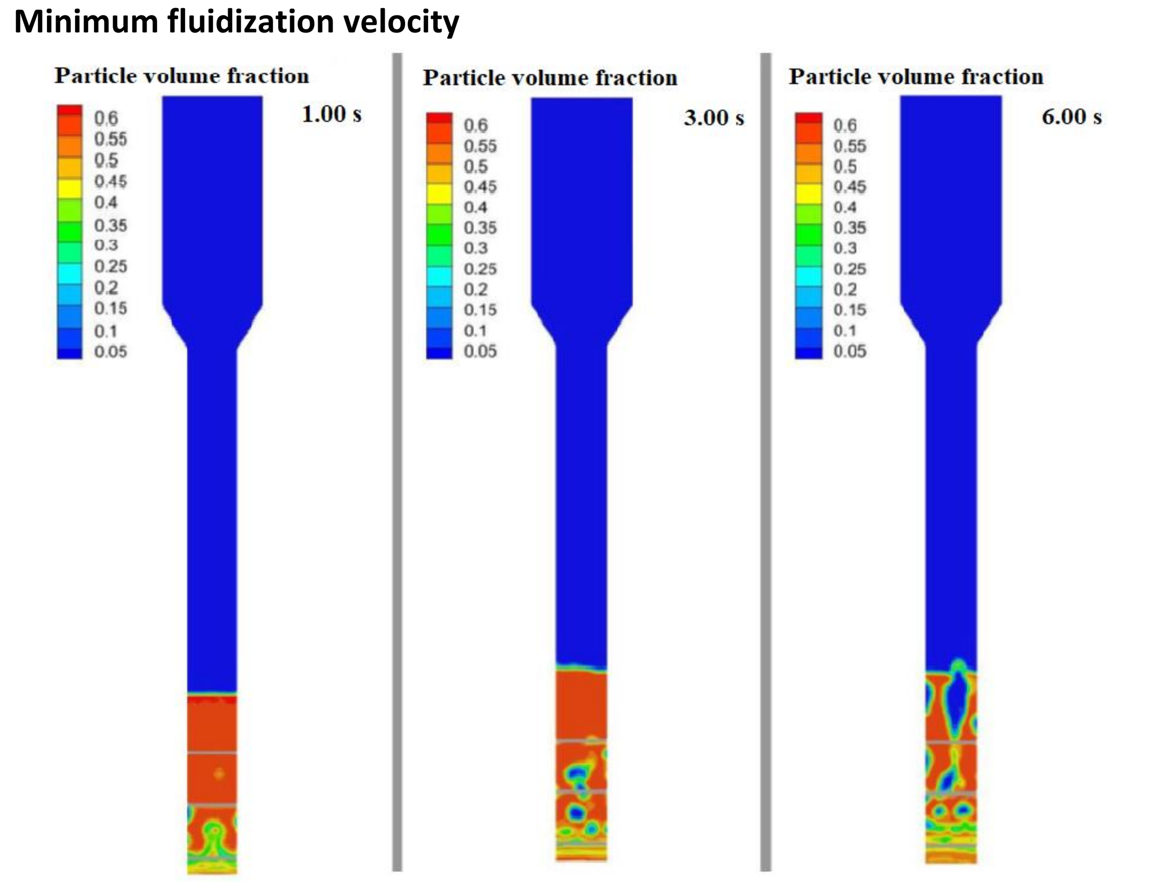
$$\frac{\partial(\varepsilon_f \rho_f Y_{f,i})}{\partial t} + \nabla\cdot(\varepsilon_f \rho_f Y_{f,i} u_f) = \nabla\cdot(\rho_f D \varepsilon_f \nabla Y_{f,i}) + \delta \dot{m}_{i,chem} \qquad (4)$$

Heterogeneous reactions:
$C + O_2 \longrightarrow CO_2$ R1
$C + 0.5O_2 \longrightarrow CO$ R2
$2H + 0.5O_2 \longrightarrow H_2O$ R3
$CO + 0.5O_2 \overset{het}{\longrightarrow} CO_2$ R4

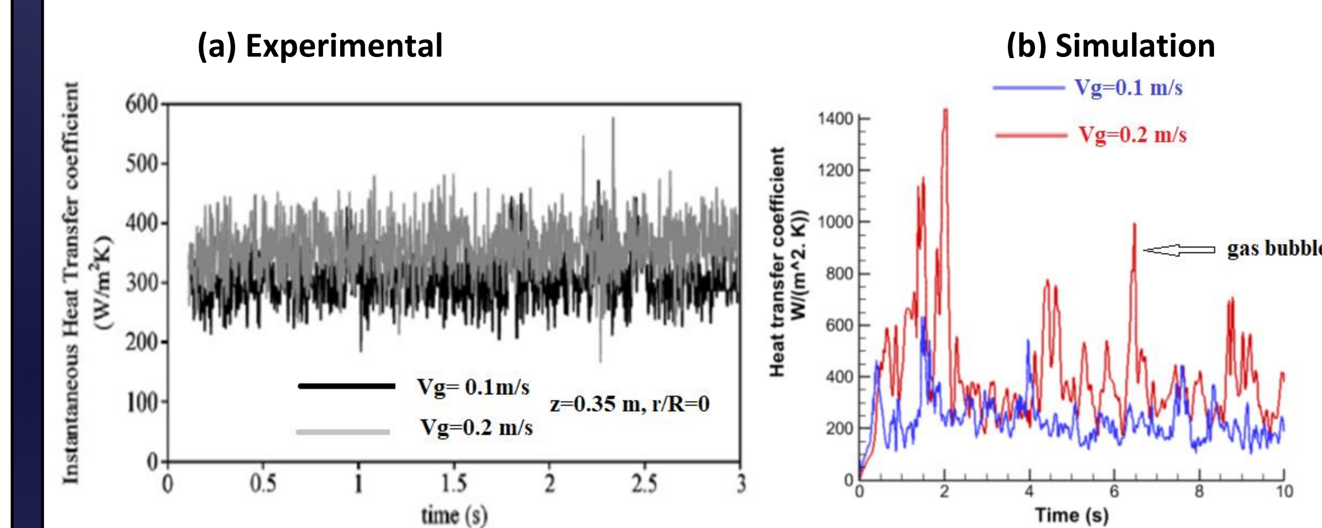
Homogeneous Reaction: $CO + 0.5O_2 \overset{hom}{\longrightarrow} CO_2$ R4

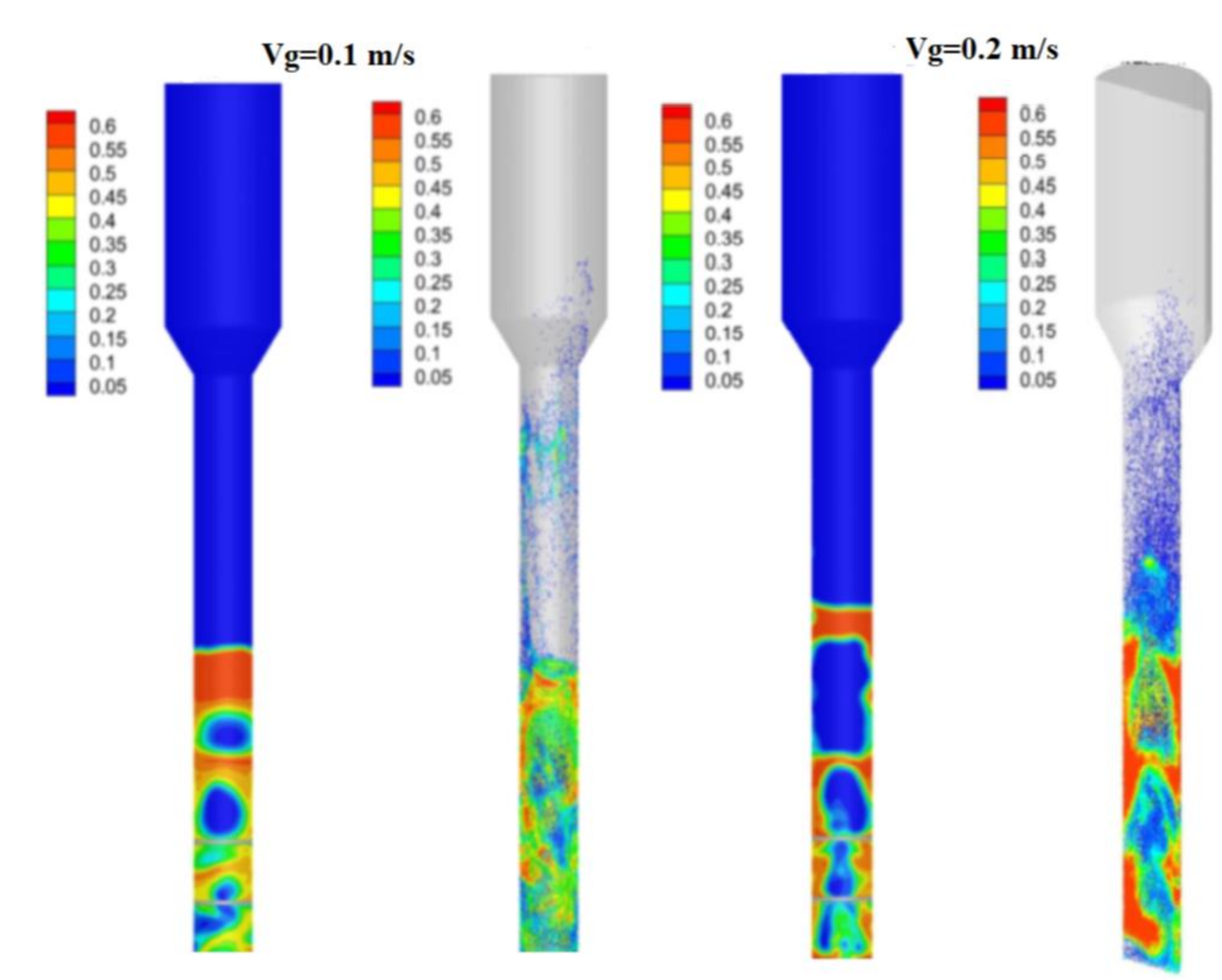
Results:

- Minimum fluidization velocity

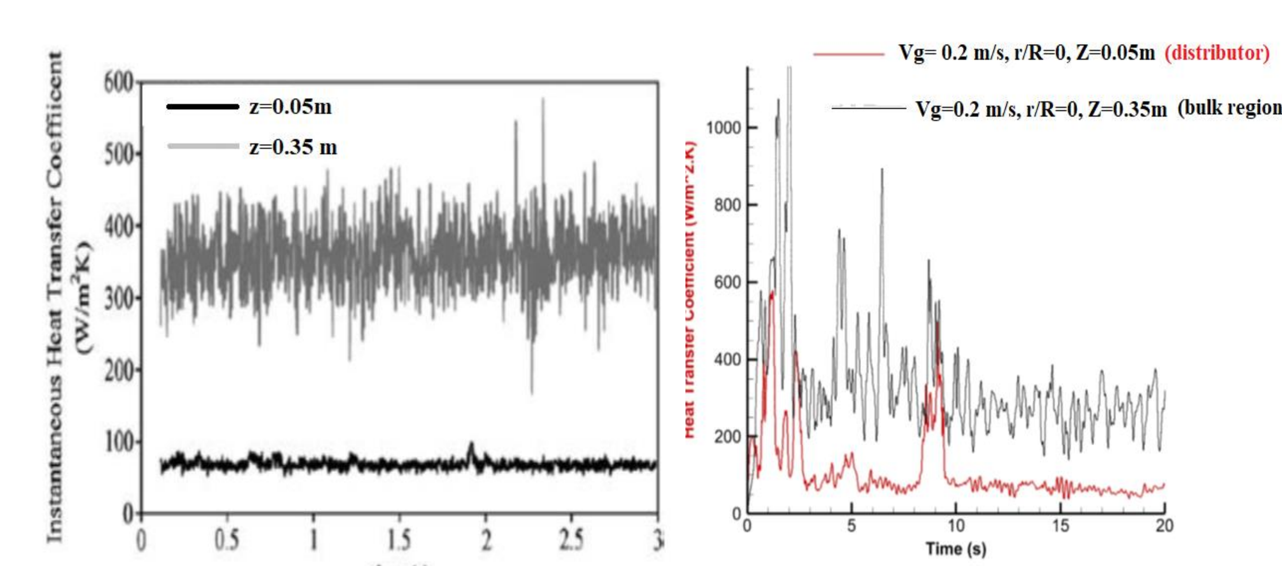


- Effect of superficial gas velocity

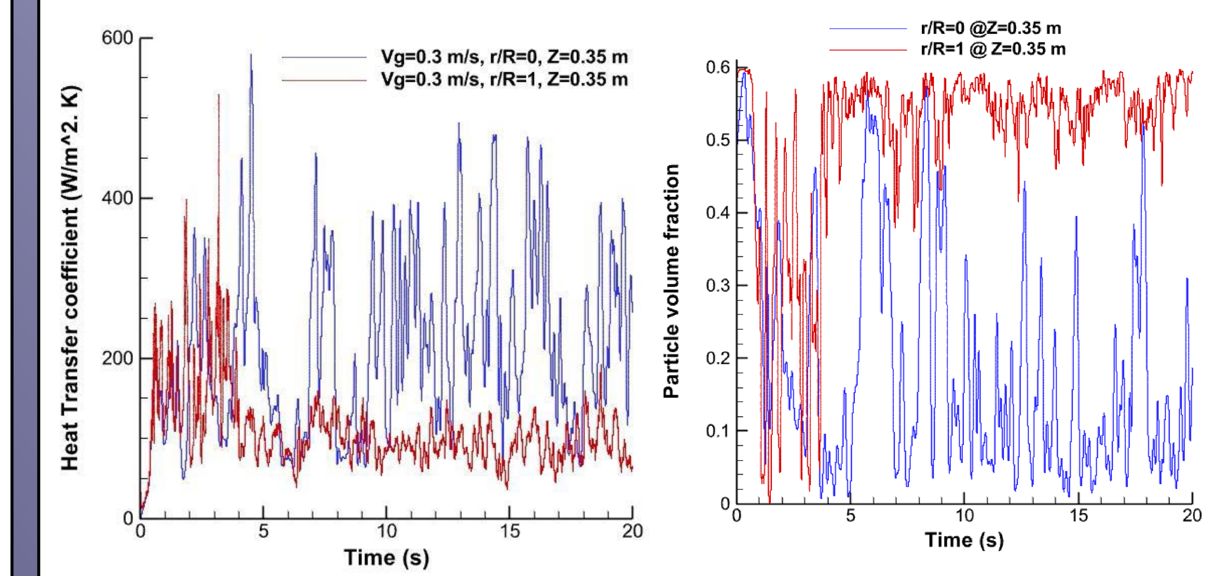




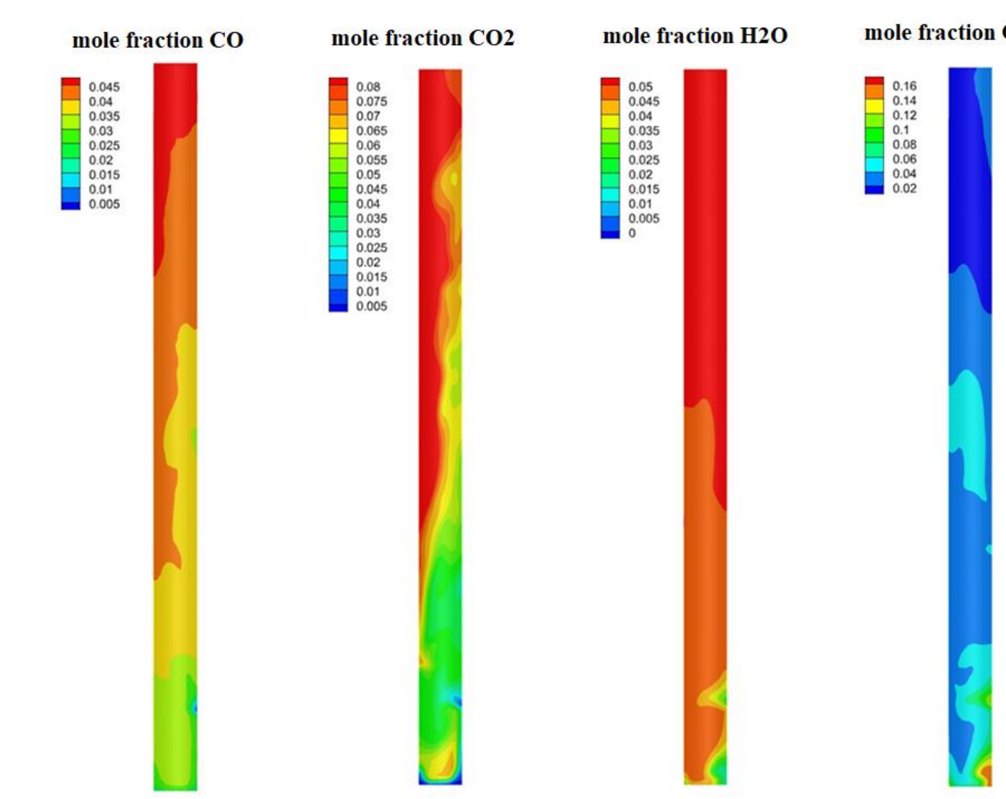
- Axial variations of heat transfer coefficient (distributor and bulk regions)

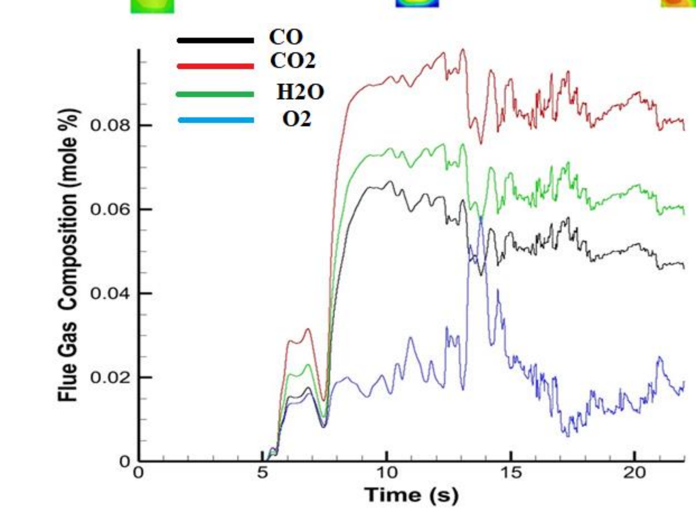


- Radial variations of heat transfer coefficient (core and wall regions) core(r/R=0), wall (r/R=1)



- FCC regenerator flue gas composition





Conclusions:

- The heat transfer in the distributor regime is lower than in the bulk regime, where large bubbles wake region is well developed.
- Heat transfer in the center region is higher than near the wall due to more frequent packet renewal on the tube surface at the bed's center.
- The time series data obtained from simulations compare well with the heat transfer process captured with a fast response probe.
- Coke combustion was successfully simulated using the kinetic model, and the results were well-matched with industrial data.

Acknowledgment of Sponsors:

The authors would like to thank The Libyan-North American Scholarship Program (LNASP) and Natural Resources and Engineering Research Council (NSERC) for their financial support during this project. CPFD Software LLC for technical support.

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