Heat and Mass Transfer Modelling of Fuel Reactor for Chemical Looping Combustion: Concept and Review

Presented By

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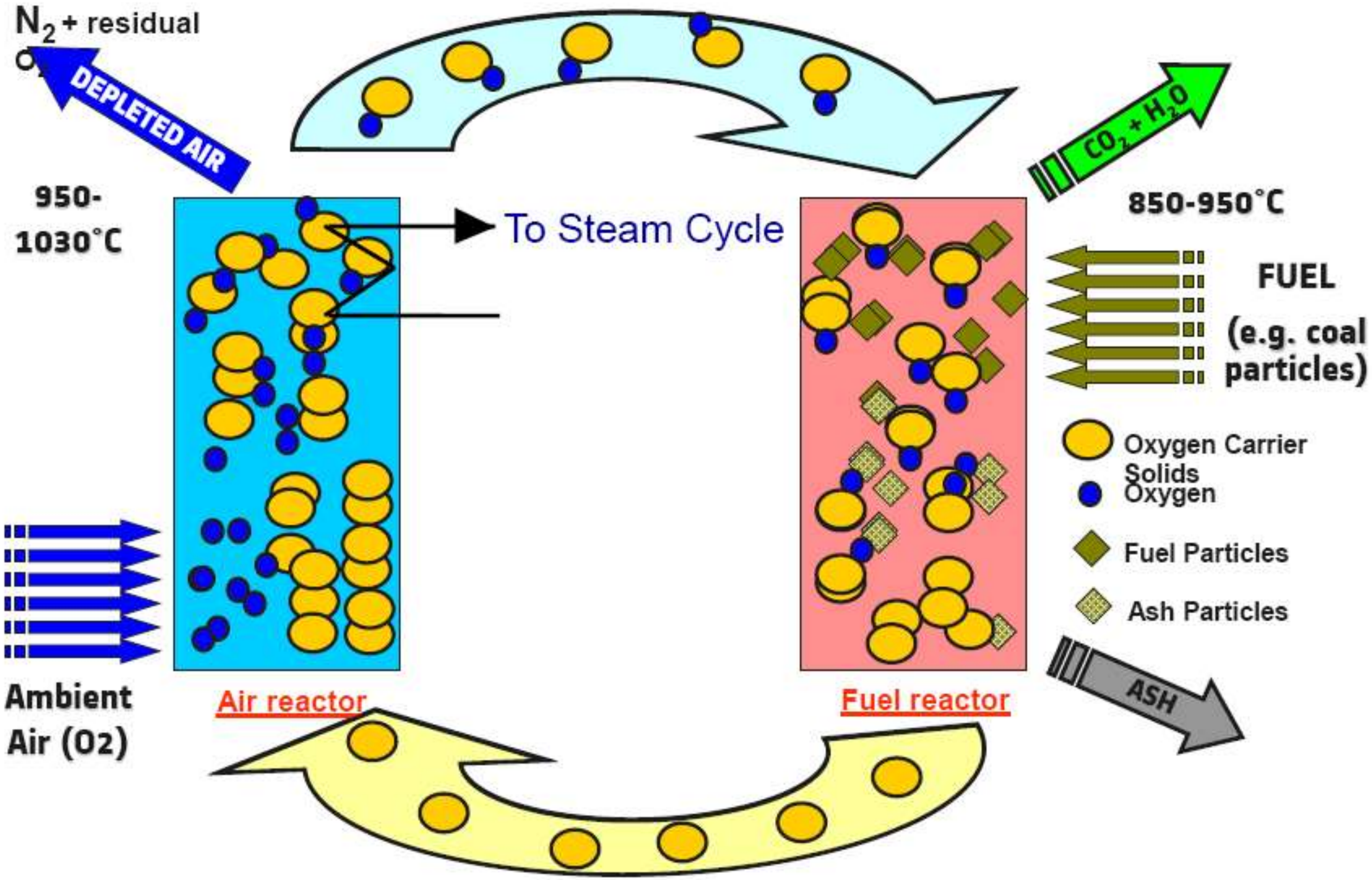
Outline for the Presentation

- What is Chemical Looping Combustion and its importance in Carbon Capture and Utilization
- Importance of Oxygen Carrier in CLC
- CFD modelling of fuel reactor in CLC
- Review of some research work in CFD modelling of fuel Reactors
- Research opportunities in this field

Chemical looping combustion

Chemical looping combustion (CLC) has emerged as one of the most promising technologies for low-cost CO_2 capture technologies for solid fuels. CLC provides the possibility of CO_2 capture without the requirement of an air separation unit or an absorption process.

What is Chemical Looping and does it work?



Chemical Looping features

- Up to 100% CO_2 capture efficiency,
- Highly concentrated stream of CO_2 ready for sequestration,
- No NO_x emissions,
- No costs or energy penalties for gas separation

Classification of CLC

- Syngas CLC
- In-situ CLC
- Chemical Looping with Oxygen Uncoupling (CLOU)

Oxygen Carriers

- The oxygen carrier is generally composed of a metal oxide (active phase) and support (inert phase).

- The inert phase acts as a porous support providing a higher surface area for the reaction and increased mechanical strength of the particles.

- In regular CLC, the oxygen carrier should be able to convert the fuel completely to CO_2 and H_2O in the fuel reactor.

Desired Properties of Oxygen Carrier

- High reactivity during reduction by fuel gas and oxidation by air.
- The particles should be resistant towards carbon formation.
- The particles should have enough mechanical strength to bear the stress resulting from circulation of the particles between the two reactors.
- The particles should be resistant towards agglomeration.
- The particles should be cheap to produce and in an environmentally sound way.
- The cost of production should be low.

CFD Analysis and Modelling

- Computational fluid dynamics (CFD) provides an efficient means to analyze the performance of a CLC system and characterize the fluid mechanics and chemical kinetics in the system.
- Although laboratory-scale studies of CLC with various experimental setups are widespread in the literature, numerical studies using CFD have been limited.
- Numerical modeling of multiphase flows involving a granular solid and a gas of the kind seen inside a CLC fuel reactor can be achieved with different levels of accuracy with very differing computational costs depending on the modeling approach, which can be broadly categorized as either Eulerian or Lagrangian.

Results From Literature Review based on Indian Coal

- Kavitha G Menon et al has done CFD Simulation of in-situ gasification chemical looping combustion of Indian coal.
- The geometry of fuel reactor considered was cylindrical in shape with conical bottom. The reactor was having provisions for single inlet, through which gasifying agent enters in to the reactor and an outlet through which the product gases leave the reactor.
- Multiphase Eulerian approach has been used to model both solid and gaseous phases. Here, three phases were considered in the calculations: one gas phase and two solid phases. k-Ɛ model has been used to characterize the turbulent flow behavior of components.
- Heat transfer between the phases was defined using Gunn correlation available in fluent database but heat transfer between solid phases is considered to be small and negligible.
- Three oxygen carriers are considered for the CLC of Indian coal are compared and examined to find out the oxygen carrier which can be most promising for the process. Comparison is made based on the maximum concentration of CO_2 attained by each carrier for a particular circulation rate.

Using Fe2O3 as an oxygen carrier

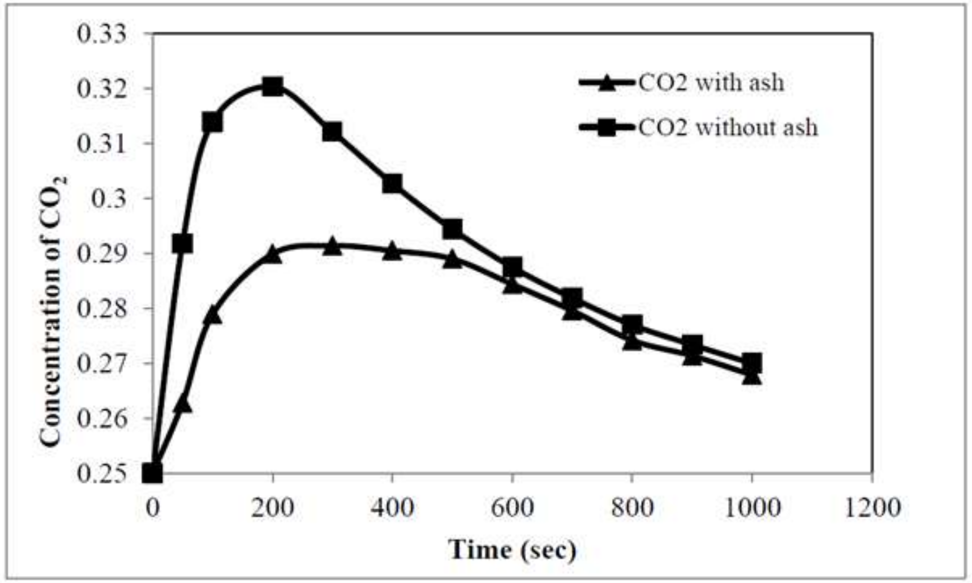


Fig. Variation in concentration of CO_2 in fuel reactor with time at a height of 0.1m and 1223K using Fe_2O_3 as oxygen carrier with and without including ash effects

Using Fe2O3 as an oxygen carrier

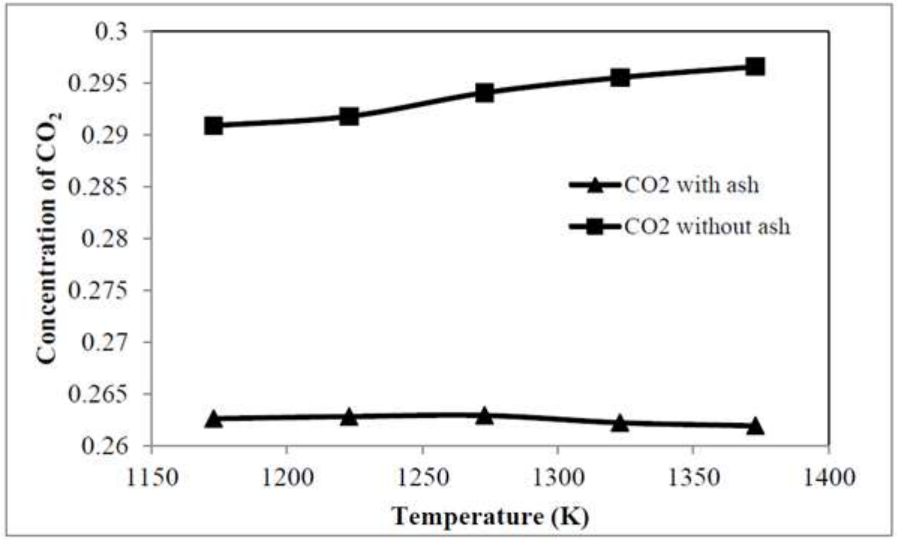


Fig. Variation in concentration of CO_2 with temperature at 50sec and 0.1m using Fe_2O_3 as oxygen carrier with and without including ash

Using CuO as oxygen carrier

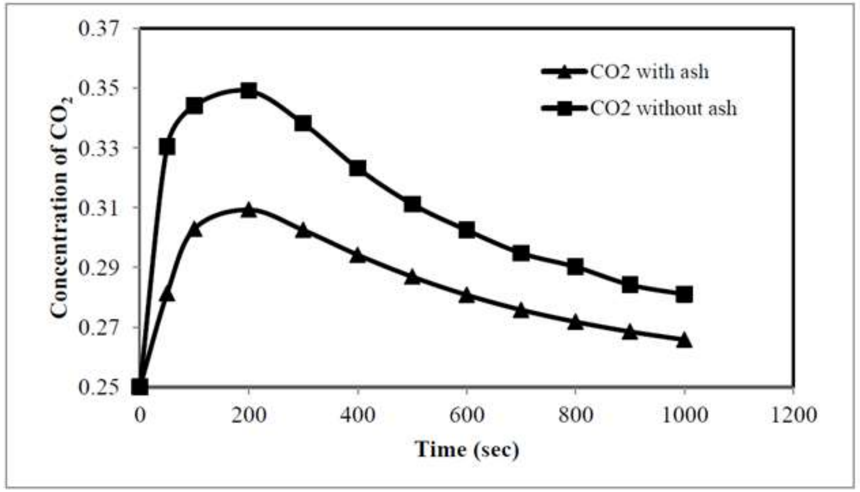


Fig. Variation in concentration of CO2 with time at a height of 0.1m using CuO as oxygen carrier with and without including ash

Using CuO as oxygen carrier

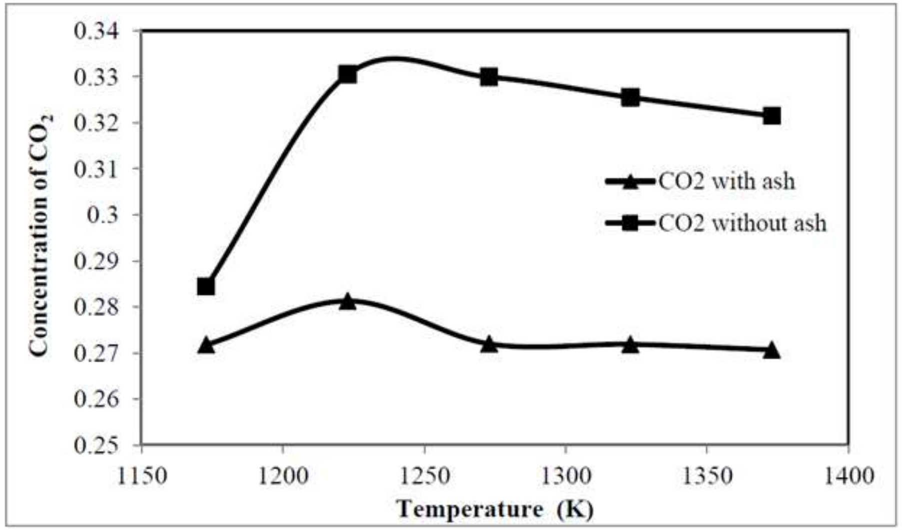


Fig. Variation in concentration of CO2 with temperature at 50sec and 0.1m using CuO as oxygen carrier with and without including ash

Using Fe2O3 & CuO as carrier

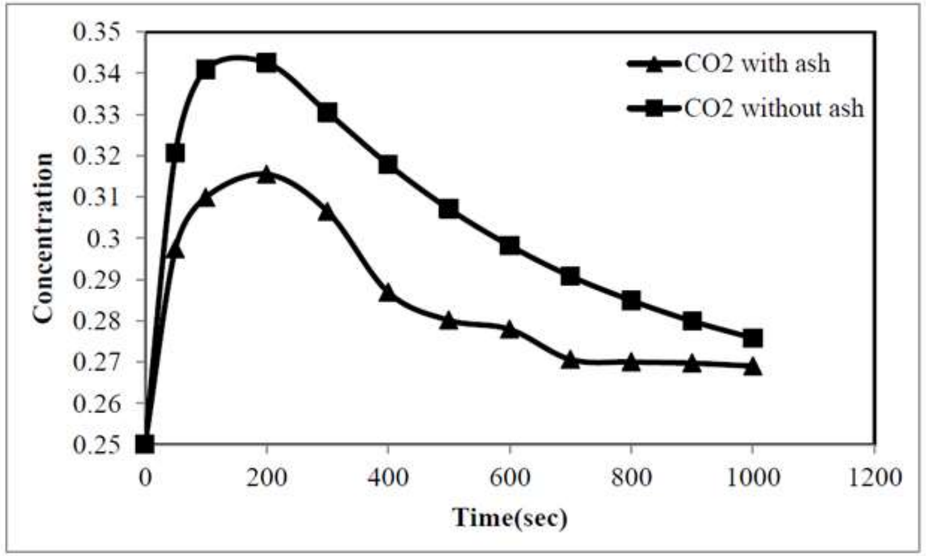


Fig. Variation in concentration of CO_2 with time at 1223K and 0.1m using Fe_2O_3 & CuO as oxygen carrier with and without ash effects

Using Fe2O3 & CuO as carrier

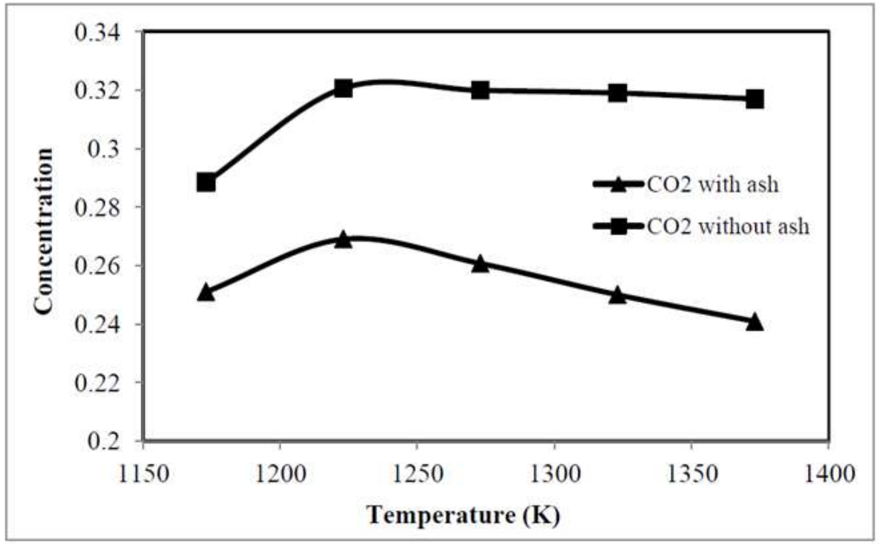


Fig. Variation in concentration of CO_2 with temperature at 50sec and 0.1m using Fe_2O_3 & CuO as oxygen carrier with and without including ash affects

Concluding Observation

- Although lots of research work has been done on CLC using high grade coal but for low grade coal like Indian coal , it is limited.
- Numerical design and analysis may also be considered before actually performing experiment
- Oxygen carriers are important in the development of chemical-looping processes. It is important to develop oxygen carriers using low cost materials which are adequate for different types of coal and chemical-looping processes

Research Opportunities

- Extend the CFD modeling to 3-dimensional CLC fuel reactor.
- Extend the CFD model to include the agglomeration and slagging of ash effects

References

- J. Jung and I. Gamwo, “Multiphase CFD-based models for chemical looping combustion process: Fuel reactor modeling,” Powder Technol., vol. 183, pp. 401-409, 2008.
- K. Mahalatkar, J. Kuhlman, E. D. Huckaby and T. O’Brien, “Computational fluid dynamic simulations of chemical looping fuel reactors utilizing gaseous fuels,” Chem. Eng. Sci., vol.66, no. 3, pp. 469-479, 2011.
- H. Kruggel-Emden, F. Stepanek and A. Munjiza, “A study on the role of reaction modelling in multi-phase CFD-based simulations of chemical looping combustion,” Oil & Gas Sci. Tech., vol. 66, no. 2, pp. 313-331, 2011.
- D. J. Patil, M. V. Annaland and J. A. M. Kuipers, “Critical comparison of hydro-dynamic models for gas–solid fluidized beds—Part II: Freely bubbling gas–solid fluidized beds,” Chem. Eng. Sci., vol. 60, no. 1, pp. 73-84, 2004.
- K.G. Menon, V. S Patnaikuni, ‘’ CFD simulation of fuel reactor for chemical looping combustion of Indian coal,’’ Fuel, vol. 203, 90–101, 2017

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