Experimental and Modeling Studies for Capturing and Converting CO_2 in Chemical Looping Technology

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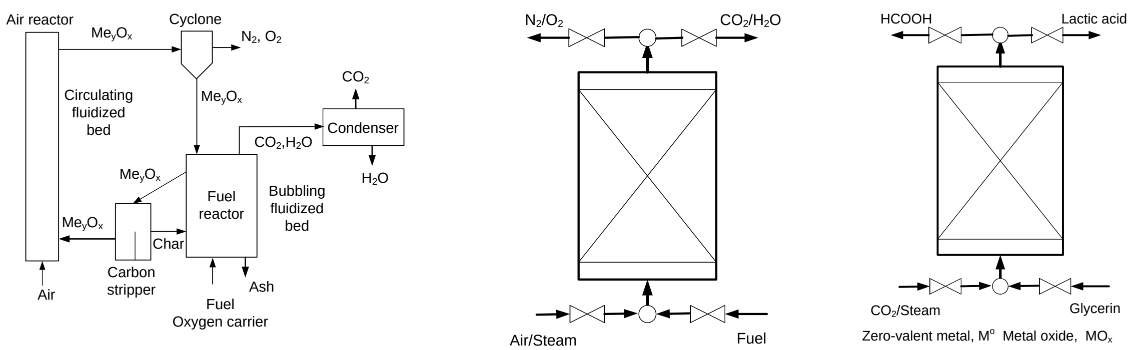
This research is for experimental and modeling studies of A) chemical looping (CL) combustion of solid and gaseous fuels for capturing CO_2 and B) converting CO_2 to high value added chemicals. In CLT, as seen in Fig 1 a, a metal oxide as an oxygen carrier (OC) oxidizes the fuel to mainly CO_2 and H_2O in the fuel reactor. The reduced OC is oxidized in the air reactor; hence the direct contact between air and the fuel is avoided. After condensing the H_2O, a flow of almost pure CO_2 becomes ready for sequestration.

A) One of the main drawbacks of the CLT is the transport of the OC between the two reactors and separate the OC from the hot air stream, ash, and char at high operating temperatures (Fig. 1a).



(a) (b) (c)

Figure 1. Reactor configurations for CLT: (a) Schematic of the CLC system, (b) Periodically operated CLT in packed bed system; (c) CO_2 conversion to formic acid in periodically operated CLT in packed bed system.

In a new reactor concept, the oxygen carrier is not transported but kept inside a packed bed reactor and is alternately exposed to oxidizing and reducing conditions by periodic switching of the feed streams (Fig. 1b) [1-4]. The main advantages of this reactor concept are:

- Avoiding cyclone operation and better utilization of the oxygen carrier,
- Controlling the air temperature with the amount of active material in the bed,
- High thermal energy efficiencies can be realized,
- The oxidation may be modeled similarly to an adsorption problem [5],

For solid fuel like coal and biomass, *in situ* or separate gasification will be required [6].

B) Fig. 1c shows the reduction of CO_2 to produce formic acid using the oxidation of a zero-valent metal (Zn, Al, Fe, Mn, Ni) under hydrothermal conditions in periodically operated CLT in packed bed system [7] with the following main reactions

$$M^0+CO_2+H_2O \rightarrow MO_x+HCOOH$$

The oxidized metal can be regenerated by a chemical such as glycerin, which is converted to lactic acid

$$MO_x+C_aH_bO_c \rightarrow M^0+C_aH_{b-2c}O_c+xH_2O.$$

The overall reaction with glycerin is exothermic

$$CO_2 + C_3H_8O_3 \rightarrow HCOOH + C_3H_6O_3.$$

Experimental analysis- Experiments on oxidation and reduction cycles *with a regenerating chemical*, operating conditions, oxygen carrier stability, CO_2 capture and conversion rates will be performed.
Computational- Continuity equation, gas and solid component balance equations, energy balance, and reaction rate equations will be solved with the initial and boundary conditions to analyze mass and heat fronts as a consequence of the reaction kinetics.
Simulation- Aspen Plus modeling with sensitivity analyses and feasibility studies will be performed.
Deliverables- a) Optimum oxygen carrier and zero-valent metal, b) regenerating chemical, c) mass and energy balances, d) validation of theoretical analysis, e) Aspen Plus modeling, f) economic analysis.

References

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