Chemical Looping Combustion: Hydrodynamic and Internal Diffusion Effects

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Motivation for Research

- CO_2 from coal combustion systems is a major contributor to global warming
- Annually, 2.15 billion tons of CO_2 are produced from coal fired power plants worldwide*
- CO_2 content in a typical flue gas in a coal plant is 12-15%
- Technologies producing enriched CO_2 are needed for CO_2 recovery or sequestration.

*Annual Energy Outlook 2010 with Projections to 2035. US-DOE, Report #:DOE/EIA-0383(2010). Downloaded (www.eia.doe.gov/oiaf/aeo/emission.html)

Sequestration Friendly Technologies

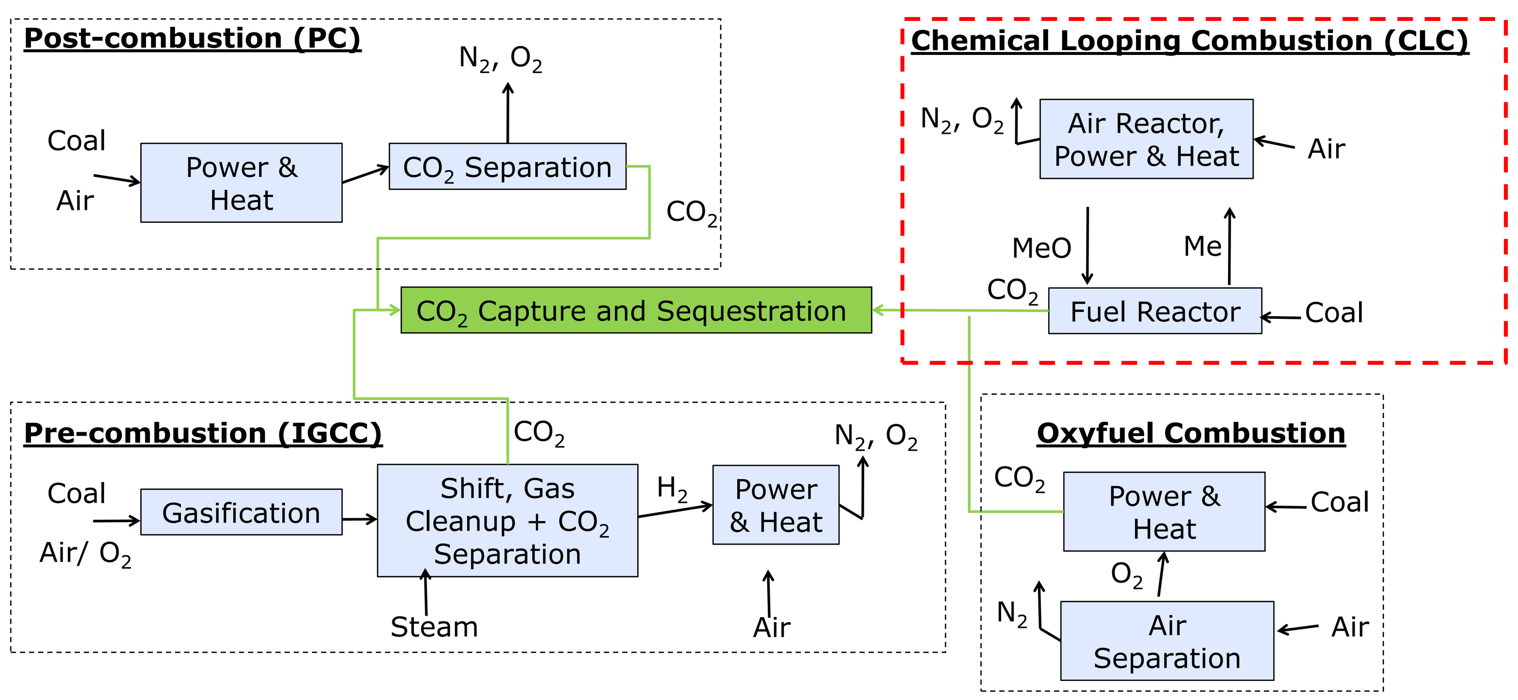


Figure 1: Various technologies for separating and capturing CO_2 for sequestration

Chemical-Looping Combustion (CLC)

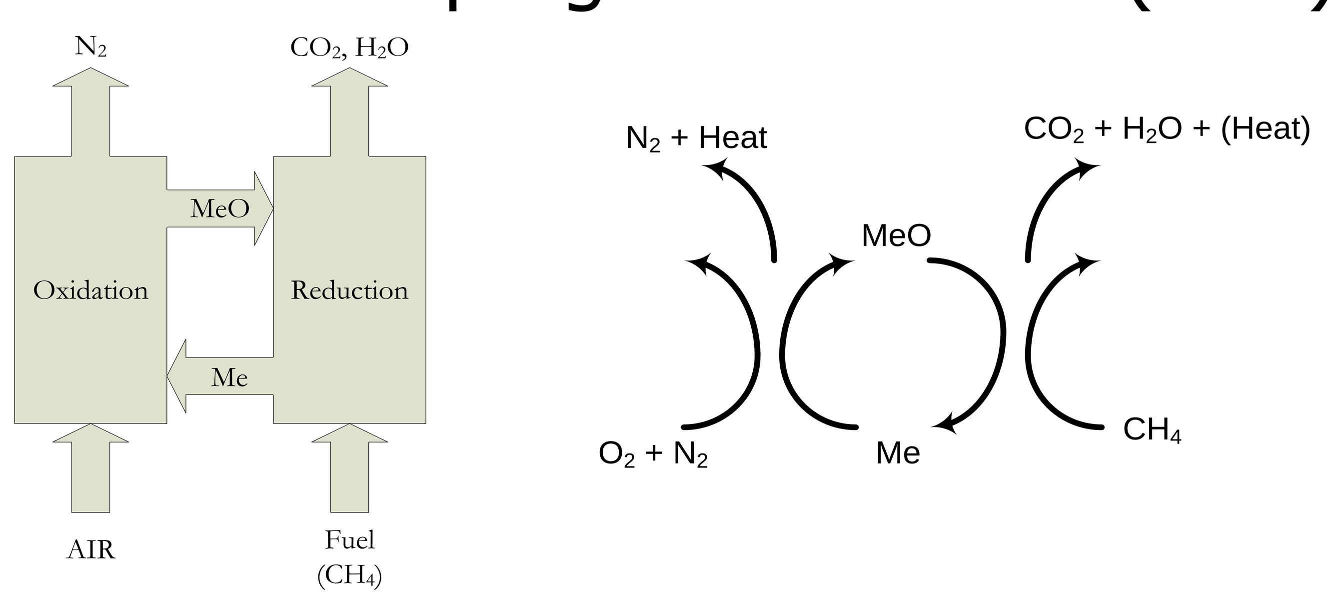


Figure 2: Schematic of 2 bed CLC unit (left) and representative chemistry and heat evolution involved in CLC process (right)

Main Points of Process

- Utilizes two separate fluidized beds of metal oxide particles to carry oxygen for combustion.
- Offers inherent CO_2 separation for use in sequestration process.
- Since CLC is a relatively new technology, much research needs to be done in modeling, metal oxide particle design, reactor design (continuous or transient)

Multiscale Nature of CLC

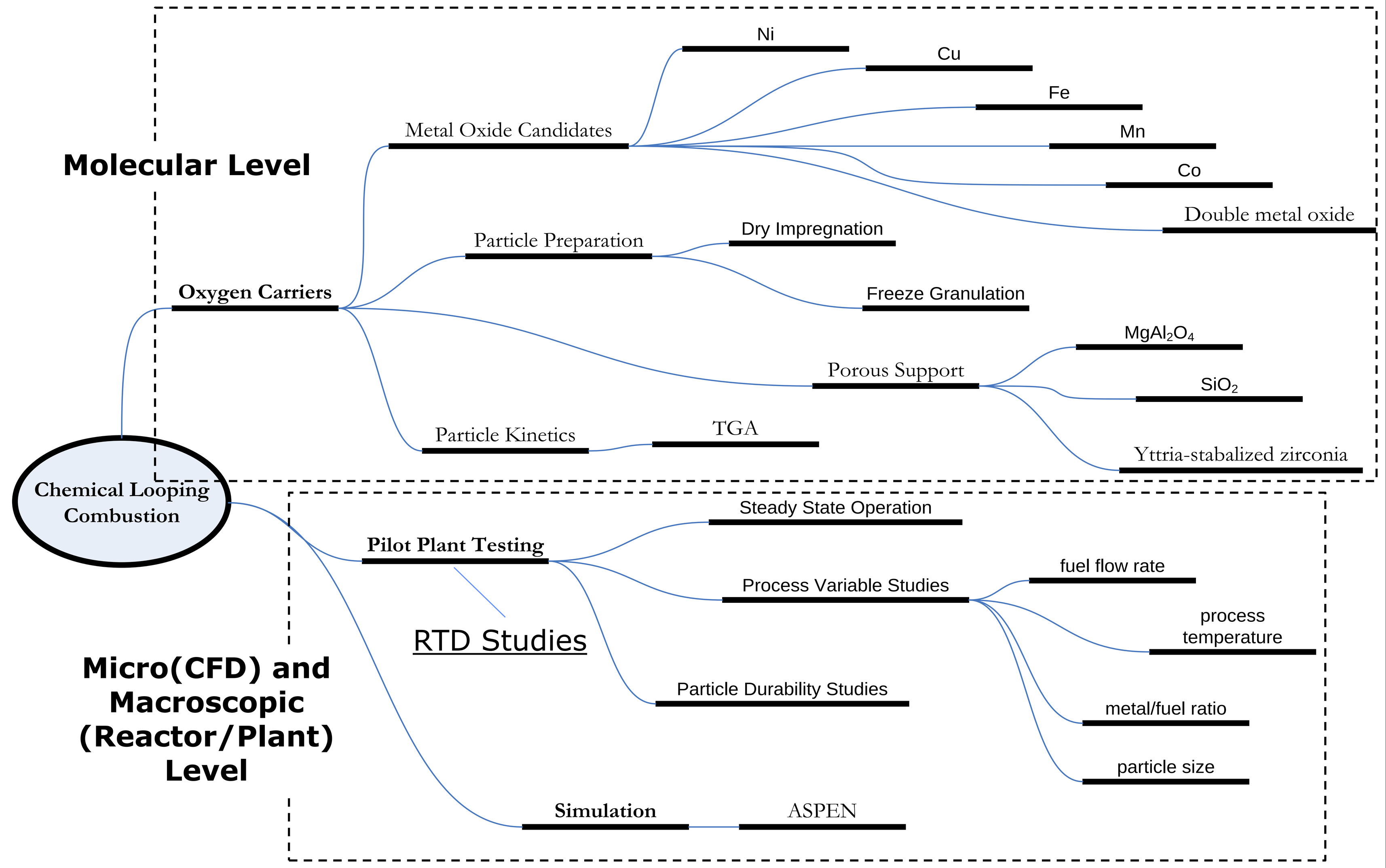


Figure 3: A brief outline of the different length scales that must be taken into account to develop an optimized industrial process for chemical looping combustion

Chemical Looping For Coal

Scheme 1:

- System where pre-gasification of coal is first performed and the syn-gas produced is used in the reduction step (i.e., fuel reactor) of the CLC process.

Scheme 2:

- System where the reduction step (fuel reactor) involves simultaneous gasification of coal and reduction of OC thus eliminating the need for the pre-gasification unit.

Note:
In both Scheme 1 and Scheme 2, heat is generated in the oxidation step (air reactor) without CO_2 production; in the reduction step, a concentrated CO_2 stream is obtained which can be easily captured and sequestered.

Long Term Research Goals

Reactor Modeling Study

- Develop mathematical models for a fluid bed reactor used in oxidation and reduction step of the CLC process. These models will span the spectrum from a phenomenological model to a comprehensive CFD based model that accounts for the flow pattern and all the transport phenomena effects. In particular **the impact of residence time distribution on the combined system performance** and operability of the process will be evaluated.

Reactor CFD Study

- Reactor modeling studies using CFD will characterize flow pattern by using virtual tracer simulations and will predict RTDs for various flow arrangement of the reactor.

Cold Flow Hydrodynamics

- Design and build a pilot scale cold flow model reactor to evaluate the residence time distribution in a reactor-regenerator arrangement. This part of the work will be done at CSIRO since they already have relatively large scale fluid beds. (Lim et al., 2001). The data obtained will provide validation of the CFD models. Once validated these models can be used for scale-up.

Oxygen Carrier Study

- Design and build a well mixed continuously stirred reactor (MCSR) to investigate reaction rates, catalyst deactivation and carbon deposition for different oxygen carriers. Additional funding will be sought for this effort.

Current Work

Year 1

- Develop and complete detailed phenomenological model for inter-connected reactors.
- Prepare companion proposal and initiate a collaborative team for further research.

Year 2

- Develop detailed multiscale CFD and model reduction techniques with a goal of predicting RTD of solids for various reactor arrangements.
- Simulate virtual RTD using the CFD models for various configurations.
- Compare with experimental results on the pressure loop reactor from CSIRO.

Illustrative Sketch of Simulated RTD

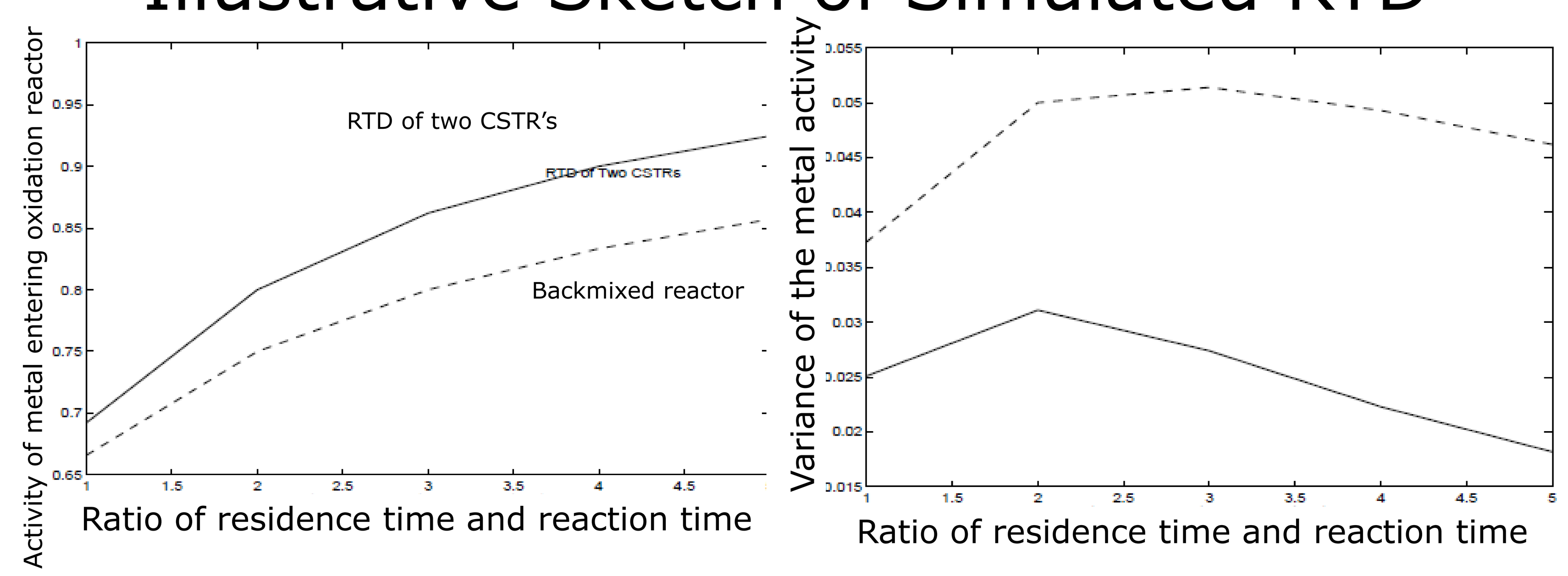
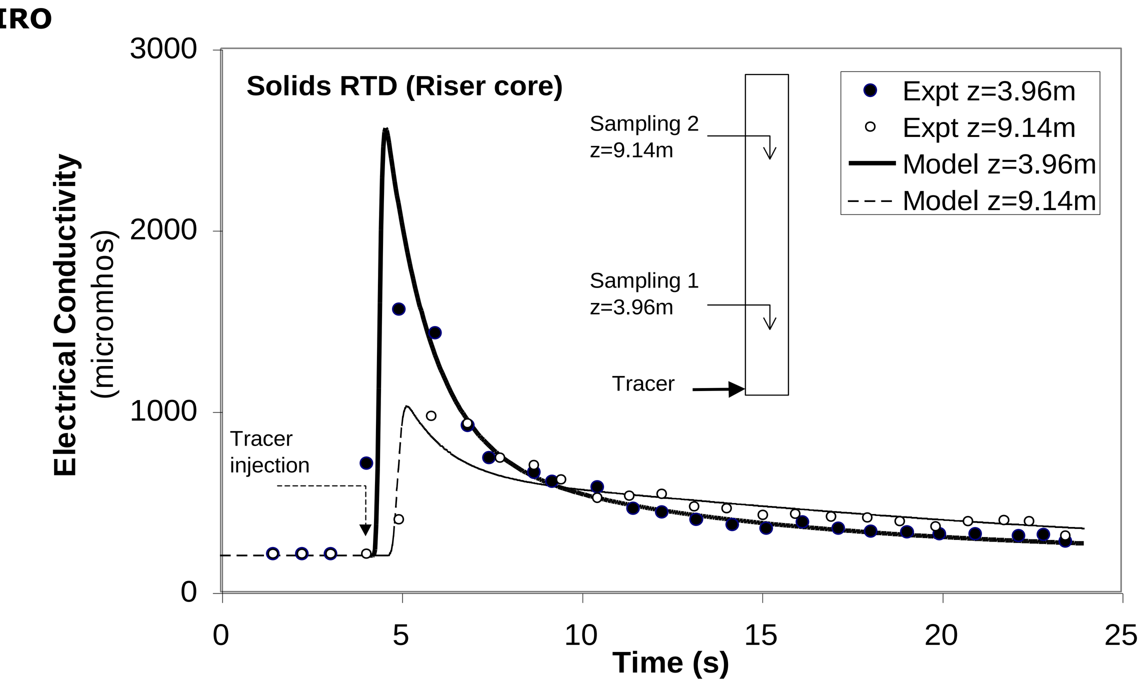


Figure 4: Effect of solid RTD on the dimensionless concentration entering the oxidation Reactor (left). Effect of solid RTD on the variance of the concentration of the feed entering the oxidation reactor (right).

RTD Model Validation in Circulating fluidized bed (CFB)

Cold model of CLR at CSIRO



Take Home Messages

- Since CLC is a potential novel technology, the reactor scale RTD effects are important for operability and success of the project
- The work is expected to highlight some of these effects.