A multi-scale, multi-disciplinary approach to solar thermochemical metal oxide looping

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Solar thermochemical looping of metal oxides is investigated for the applications of carbon dioxide capture and thermochemical energy storage. Metal oxide looping is a two-step process consisting of carbonation and calcination reactions. Current areas of research on this topic are: sorbent material synthesis and characterisation; thermodynamic analysis; thermal transport modelling; and prototype reactor design, fabrication, and evaluation.

Background

Goal: Maximize solar-to-chemical energy conversion in a metal oxide looping system for carbon dioxide (CO_2) capture or thermal energy storage.

Thermal transport modelling

Numerical models of thermal transport phenomena have been developed for a single sorbent particle (Figs 2a and 2b) and a packed bed of sorbent particles (Fig 2c) undergoing metal oxide looping. The numerical models have been used to investigate **physical and operational parameters** on the particle level and physical dimensions and temperature and reaction gradients on the packed bed level. gas flow out

How: Iterative process between (1) understanding thermal transport phenomena and chemical kinetic interactions at relevant length scales and (2) appropriate reactor and system design that matches chemical kinetics to heat and mass transfer processes.

Model system, calcium oxide

Due to its low cost, well understood kinetics, and suitability for use with concentrated solar irradiation, calcium oxide (CaO) looping has been selected as the model system. In the carbonation step of CaO looping, CaO particles are exposed to gas containing CO₂. CO₂ concentration of the gas is adjusted according to the application: flue gas like composition for CO₂ capture or high-purity CO₂ for energy storage. CO₂ reacts with the particles to form solid calcium carbonate (CaCO₃). In the high-temperature calcination step, CaCO₃ particles are exposed to concentrated solar radiation. CaCO₃ decomposes into regenerated CaO particles and CO₂. Highpurity CO₂ is used as a sweep gas during calcination for both CO₂ capture and energy storage applications to ensure high-purity CO₂ at the outlet.





Figure 2: Thermal transport modelling of heat and mass transfer coupled to reversible chemical kinetics. (a) Single particle system schematic, (b) selected particle level thermal cycling numerical results, and (c) packed bed system schematic.

Prototype reactor

A 1 kW_{th} solar reactor prototype for metal oxide looping CO₂ capture or energy storage has been designed (Fig 4a). It features a cavity receiver with a windowless aperture at the bottom. The receiver cavity is surrounded by an annular region of reacting sorbent particles. Gases enter the reaction zone via a gas manifold and radial inlet ports at the bottom of the reactor and exit similarly at the top.

The reactor is currently being fabricated at the ANU (Fig 3). The reactor's thermochemical performance will be experimentally investigated in the ANU's 45 kW high-flux solar simulator (Fig 4b).

Material development

Naturally occurring CaCO₃ is known to lose reactivity quickly, so new materials are being investigated for CO₂ capture and energy storage. New materials based on calcium and other metal oxides are synthesised and characterised with the goal of creating a sorbent with improved kinetics, maximized energy storage density/CO₂ capture capacity, and/or improved long term reactivity.

Thermodynamics

Thermodynamic models for CO₂ capture and energy storage systems have been developed. For the energy storage system (Fig 1a), the model includes a power cycle for generating electricity. The model is used to assess the system's storage efficiency and capacity. For the CO₂ capture system (Fig **1b**), the model is used to examine the effects of **CO**₂ concentration, heat recovery, and reaction temperatures on energy required.





Temperatures, product gas flow rates and composition, pressure drop, and extent of the calcination and carbonation reactions will be measured and used to obtain performance maps of the reactor. Experimental data will also be used to validate the numerical heat and mass transfer model developed previously to guide the reactor design and predict its performance.



Figure 3: Selected reactor components fabricated at the ANU in early 2016.



Figure 1: Schematics for thermodynamic analysis of (a) energy storage and electricity generation system and (b) CO₂ capture system

Figure 4: Thermochemical and thermomechanical performance of (a) the solar thermochemical reactor prototype will be evaluated using (b) the ANU's high-flux solar simulator.

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