Solar powered two-step thermochemical water-splitting cycle to produce H_2 (STCH)

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$$MO_x \rightarrow MO_{x-\delta} + \frac{\delta}{2} O_2 \quad \text{(1) Reduction}$$

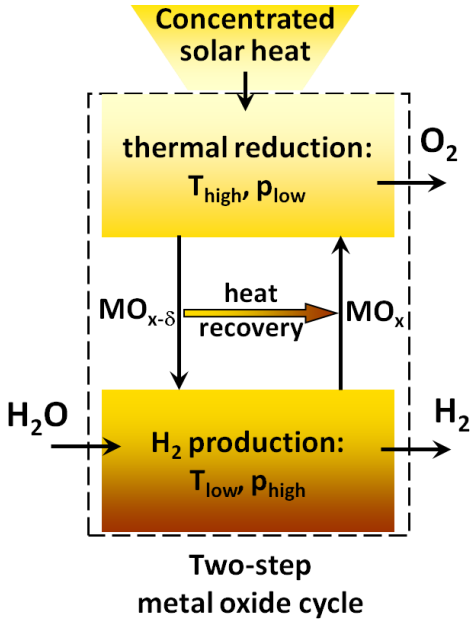
$$MO_{x-\delta} + \delta \cdot H_2O \rightarrow MO_x + \delta \cdot H_2 \quad \text{(2) Oxidation}$$

$$\delta \cdot H_2O \rightarrow \frac{\delta}{2} O_2 + \delta \cdot H_2 \quad \text{(3) Thermolysis}$$

MW scale concentrating solar power facilities provide heat

Cycle conditions and system metrics:

Reduction Temperature (T_{high})	<2000°C
O_2 fugacity in reduction (p_{low})	f_{gas}<<solid
Oxidation Temperature (T_{low})	debated
O_2 fugacity in oxidation (p_{high})	f_{gas}>>solid
H_2 production rate	50-100mt/day
Solar-to-H_2 conversion efficiency	>25%
H_2 production cost	$3/gge at plant gate



Two-step metal oxide cycle

- What and how to benchmark materials?
  - composition, thermodynamics, kinetics, mechanical properties, compatibility, etc...

Benchmarking STCH materials at Sandia

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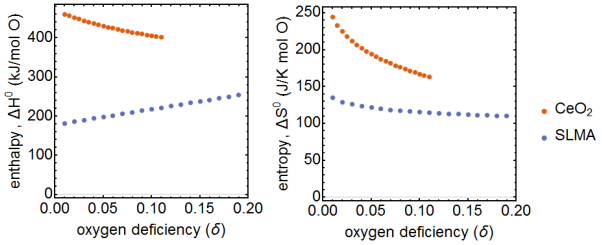
derive P_{O2}-T-δ relation from experimental data (i.e., TGA, other)



apply material thermodynamic model to reactor efficiency model

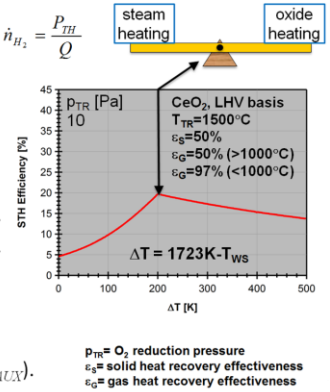
$$\eta = \left(\frac{P_{TH}}{P_S}\right)\left(\frac{LHV_{H_2}}{Q}\right) = \frac{\dot{n}_{H_2} LHV_{H_2}}{P_S} \rightarrow \dot{n}_{H_2} = \frac{P_{TH}}{Q}$$

$$P_{TH} = r_{12} * r_d * t_W * A * P_S - P_{rad}$$

$$Q = Q_{TR} + Q_{SH} + Q_{AUX}$$

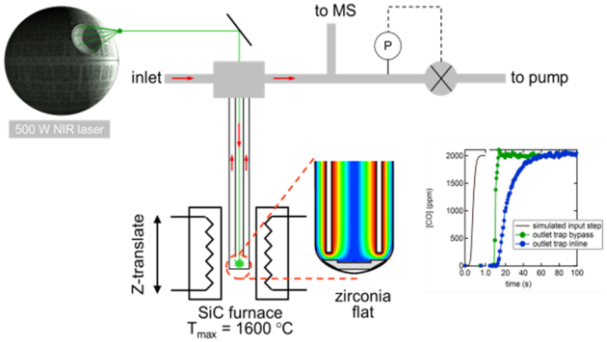
All inclusive efficiency metric

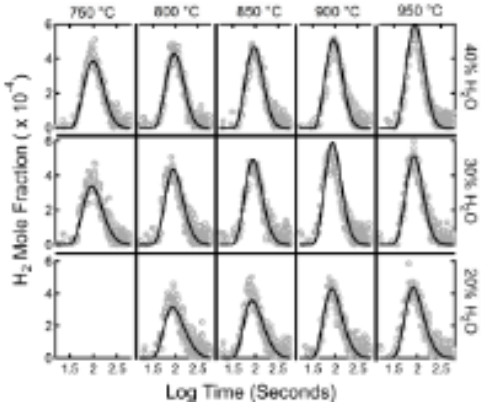
- Collection losses (P_{TH}).
- Concentrator and re-radiation.
- Oxide thermal reduction (Q_{TR}).
- Oxide heating (Q_{SH}).
- Steam heating (Q_{AUX}).
- Pump work (Q_{AUX}).
- Electrical/mechanical work (Q_{AUX}).



- Requires high-quality experimental data over large P_{O2}-T-δ range.

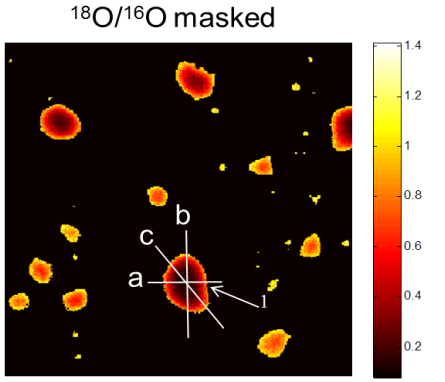
derive kinetic information at technology-specific conditions using idealized flow reactor

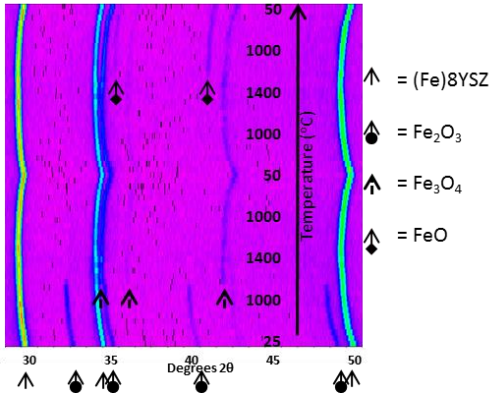




- Many cycles under high radiative flux.
- Technology-specific operation.

derive structural and mechanistic information using advanced diagnostics (i.e., HTXRD, ToF-SIMS)





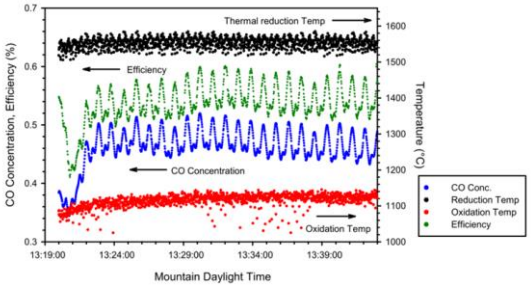
- Great potential for operando synchrotron X-ray scattering!

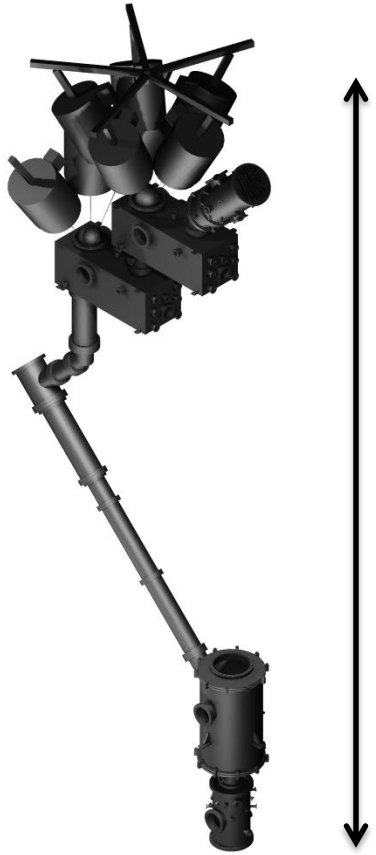
Benchmarking STCH materials at Sandia

National Solar Thermal Test Facility

Cascading Pressure Receiver/Reactor (CPR2)

PATHWAY FOR ADVANCING TRL...





25 ft tall

- 16kWth solar furnace.
- 6MW$_{th}$ power tower.
- Technology-specific operation at scale.

- ~5kW$_{th}$ system capable of producing 0.5slpm H_2.
- Derive engineering test data necessary for model validation and scale-up.