Unlocking Solar Thermochemical Potential: Leveraging CSP Experience for Solar Thermochemistry

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SETO CSP Virtual Workshop
19 Nov 2020
Solar Flux as a Thermal Energy Input

- **Motivation**
  - Decarbonizing industrial processes such as steel, ore refining, cement, fuel or chemical production, and food products
  - Can provide both heat and electricity for processing
  - Ability to achieve high temperatures

- **Key Considerations**
  - Intermittency
  - Integration into existing technology?
  - On-site production vs. transportation costs
    - Point of production does not always equal point of use
  - Location
  - Scale
  - Cost

I will address some of these considerations in the context of solar thermal production of ammonia.
Deep decarbonization

Example: Ammonia Production

- Ammonia (NH₃) is an energy-dense chemical and a vital component of fertilizer, hydrogen carrier, and energy supplier.
- NH₃ synthesized via the Haber-Bosch process:
  - Requires high pressures (15-25 MPa) and temperatures (400-500 °C)
  - Consumes > 1% of global energy use
  - Heat, power, and hydrogen are all sourced from hydrocarbons
- Process including H₂ production generates about 2.3 t of fossil-derived CO₂ per t of NH₃, and is responsible for ~1.4% of global CO₂ emissions
- Steam reforming of natural gas for H₂ generation accounts for 84% of req’d energy

Can NH₃ be synthesized via a renewable, carbon-neutral technology powered by concentrating solar?
Solar Thermal Ammonia Production (STAP)

An advanced solar thermochemical looping technology to produce and store nitrogen (N₂) from air for the subsequent production of ammonia (NH₃) via an advanced two-stage process

- Inputs are sunlight, air, and hydrogen; the output is ammonia
- Significantly lower pressures than Haber-Bosch
- Greatly decreases or eliminates carbon footprint
- The process consumes neither the oxide nor the nitride particles, which actively participate cyclically
- The project consists of four thrusts:
  - N₂ production via air separation
  - NH₃ production via a cyclic nitride reaction
  - Reactor modeling and design
  - Systems analysis
- Low TRL
Materials

Materials choice influences every aspect of system design

- Materials must be carefully and comprehensively characterized
  - Reactivity
  - Durability: is structural integrity maintained
  - Thermodynamics: enthalpy, reactivity, reaction temperature
  - Kinetics: does the reaction proceed quickly (determines time on-sun)
  - Cyclability: can they be cycled repeatedly with no loss of performance
  - Particle size: affects kinetics, heat and mass transfer
  - Chemical stability: no undesired phase changes, deactivation

- Economic considerations
  - Synthesis: an they be easily synthesized and scaled up?
  - Cost/Availability: avoid critical elements

Metal oxide for air separation

TGA showing redox capacity and cyclability
Intermittency

To maximize productivity, a plant must be able to operate 24/7

- A feature of CSP is the ability to store heat for off-sun operation or electricity generation
  - Storage can be sensible (molten salt, particles), latent (phase change), or thermochemical (sensible + reaction enthalpy)
  - Solids are generally easier to store— they are dense, do not require compression, noncorrosive, stable at T > 1100 °C, and are amenable to multiple scales
    - Thermochemical materials have added benefit of storing energy in the form of chemical bonds, irrespective of storage temperature
- H₂ generated on-site via solar thermochemical water splitting can also act as a chemical storage material, in addition to as a feedstock for chemical processes, e.g., ammonia production
Intermittency (cont’d)

To maximize productivity, a plant must be able to operate 24/7

- Process can be decoupled:
  - High temperature cycle, e.g., air separation, can be performed on-sun
  - Resulting N₂ can be stored as compressed gas or chemically, as the nitride (MNₓ)
  - Ammonolysis can be run off-sun or evening utilizing recuperated or stored heat
- Similar decoupling can apply to other chemical processes
New vs. Existing Plants

- Co-locate CSP plant with existing Haber-Bosch infrastructure
  - Hybrid model: CSP replaces methane reforming to synthesize H₂ for H-B process via thermochemical water splitting
  - Retains H-B infrastructure; no need to build new plant or transportation lines
  - Not completely green
  - Can be a bridge to fully green process
  - Also an option (or necessity) for processes such as steel production, ore refining, food processing

- Construct new plant for renewable NH₃ synthesis utilizing alternative process, e.g. STAP
  - Large up-front CapEx
  - Complete decarbonization of process – both environmentally sound and fiscally beneficial in case of carbon tax
  - Potential savings in long run due to less expensive, cyclable materials, lower temperatures and pressures
  - Consider smaller, distributed plants
Receiver/Reactors

Design and scale of receiver/reactor must be assessed early in the process

- Many considerations:
  - Direct or indirect irradiation?
  - Temperature requirements?
  - Size?
  - Window or windowless receiver?
  - Particle or monolith working material?
  - Batch or moving particle reactor?
  - Sweep gas or pumping?

- Requires combination of experiment and modeling
  - Decisions will be informed by properties of reactive material
    - In the case of STAP, oxide and nitride particles
  - Heat and mass transfer modeling, supported by experimental data, will inform scale and design
From material implications and system modeling, best estimate for receiver conditions is a temperature rise of 200-500 °C and scale <100 MW.
Techno-economics and Systems Analyses

- To attract industry and investment, it’s essential to model systems and techno-economics from the beginning of a project
- Continuously refine model as data is collected
- Techno-economic considerations:
  - CAPEX (infrastructure, construction costs, raw materials, labor...)
  - Capacity
  - Energy inputs/outputs
  - O&M
  - Lifecycle
  - Return on investment
- Systems analysis:
  - Solar input
  - Balance of plant
  - Scale
  - Operating conditions
  - Efficiency
  - Are there any show-stoppers?

System description of air separation cycle

System description of ammonia synthesis cycle
Acknowledgements

Kevin Albrecht, H. Evan Bush, Matthew W. Kury
Ellen B. Stechel, James E. Miller, Ivan Ermanoski, Xiang Michael Gao, Alberto de la Calle
Peter Loutzenhisier, Nhu “Ty” Nguyen, Tyler Farr
Dr. Levi Irwin (DOE Project Manager)

This work is supported by the U.S. Department of Energy’s Office of Energy Efficiency and Renewable Energy (EERE) under the Solar Energy Technologies Office (SETO) Award Number DE-EE0034250.
THANK YOU FOR YOUR ATTENTION