Thermal Energy Storage: Advances & Challenges in Physics-Based Modeling

Rohini Bala Chandran
Assistant Professor, Department of Mechanical Engineering
University of Michigan, Ann Arbor

February 4th, 2020
University Panel Discussion
TMCES Workshop, Pittsburgh

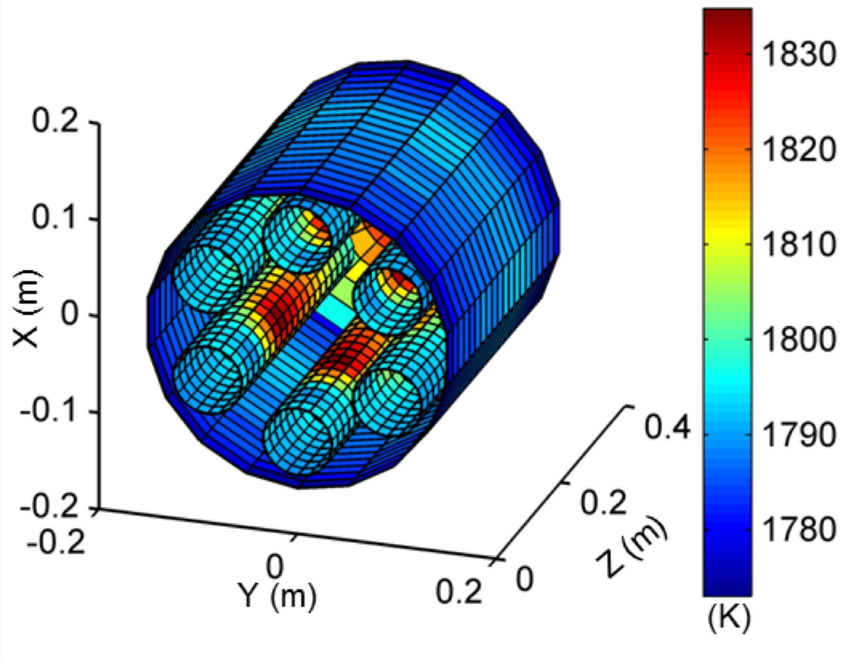
rbchan@umich.edu

www.rohinibc.com

Transport and Reaction Engineering for Sustainable Energy
TREE Lab, PI Bala Chandran

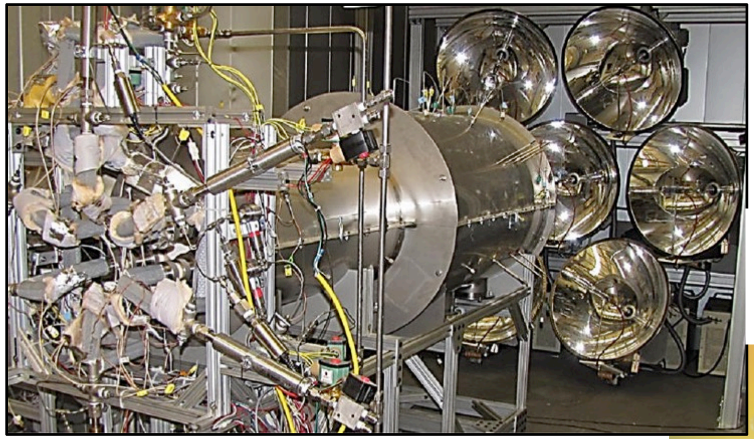
Transport + chemical phenomena

Radiative transport + heat- and mass-transfer + cyclic reactions in a solar thermochemical reactor

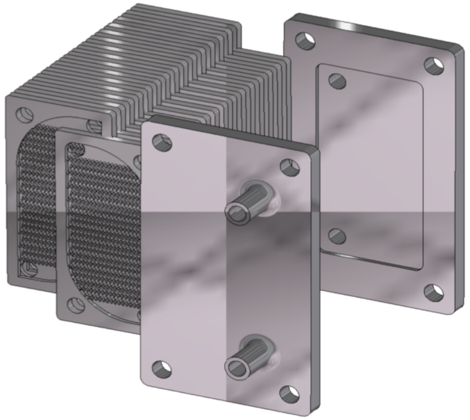


Solar-Fuel Reactors & Advanced Heat Exchangers

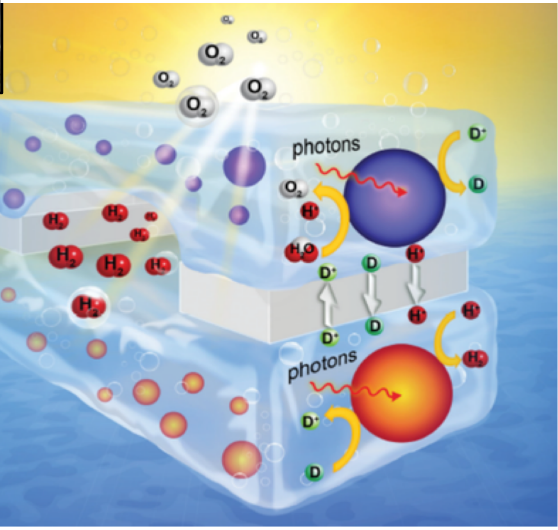
“On-sun” testing of a 4 kW reactor



Additive manufacturing for high-temperature HX

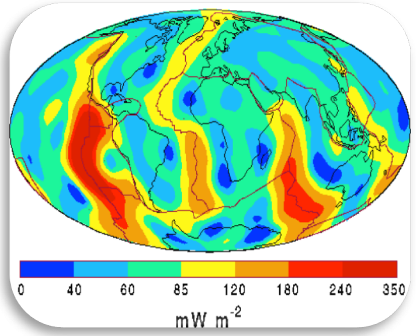


Particle-suspension Z-scheme water splitting

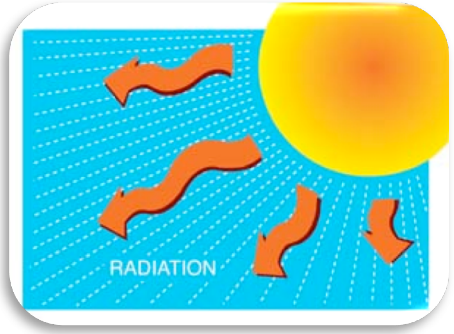


1. Bala Chandran, R. & Davidson, J. H., *Chem. Eng. Sci.* **146,** 302–315 (2016)
2. Hathaway, B.J., Bala Chandran, R., et al., Energy & Fuels, 2016
3. Bala Chandran, R., De Smith, R. M. & Davidson, J. H., *Int. J. Heat Mass Transf.* **81,** 404–414 (2015)
4. Banerjee, A., Bala Chandran, R. & Davidson, J. H., *Appl. Therm. Eng.* **75,** 889–895 (2015)
5. R. Bala Chandran, S. Breen, Y. Shao, S. Ardo and A. Z. Weber, *Energy Environ. Sci.*, 2018

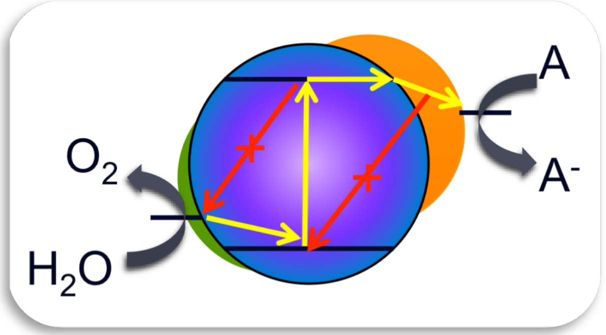
TREE Lab: Research Expertise & Team



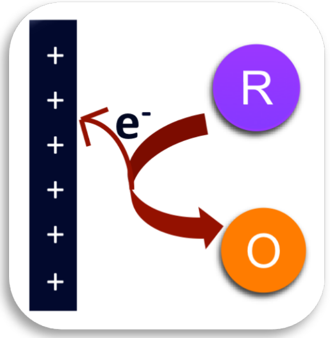
Computational Multiphysics Modeling



Radiative Heat Transfer



Semiconductor Materials

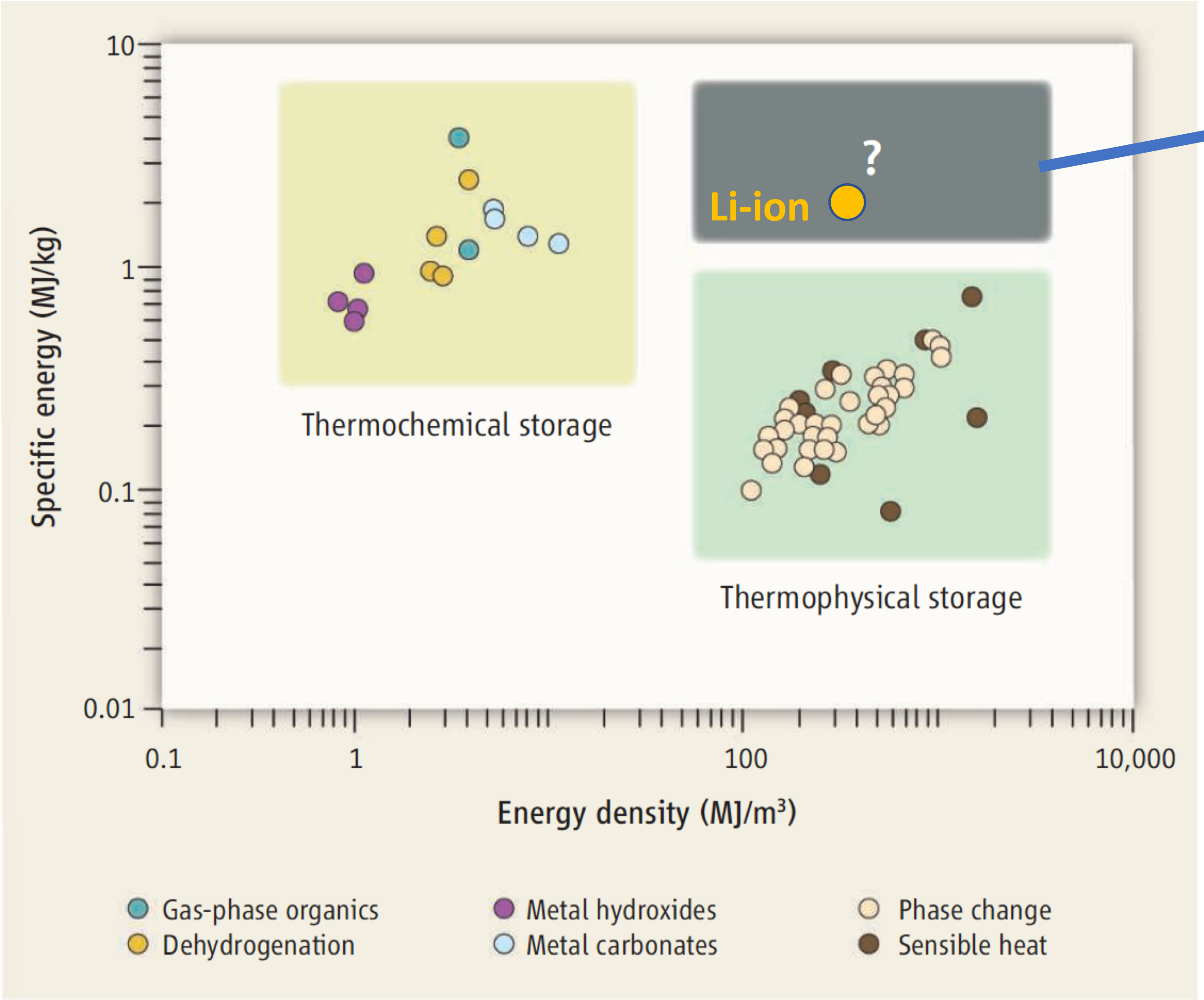


Electrochemistry

UM Research Team, Fall 2019

TREE LAB
UNIVERSITY OF MICHIGAN

Next-Gen Innovations for Thermal Energy Storage Technologies



Gur, I., Sawyer, K. & Prasher, R. Searching for a Better Thermal Battery. *Science* **335,** 1454–1455 (2012)

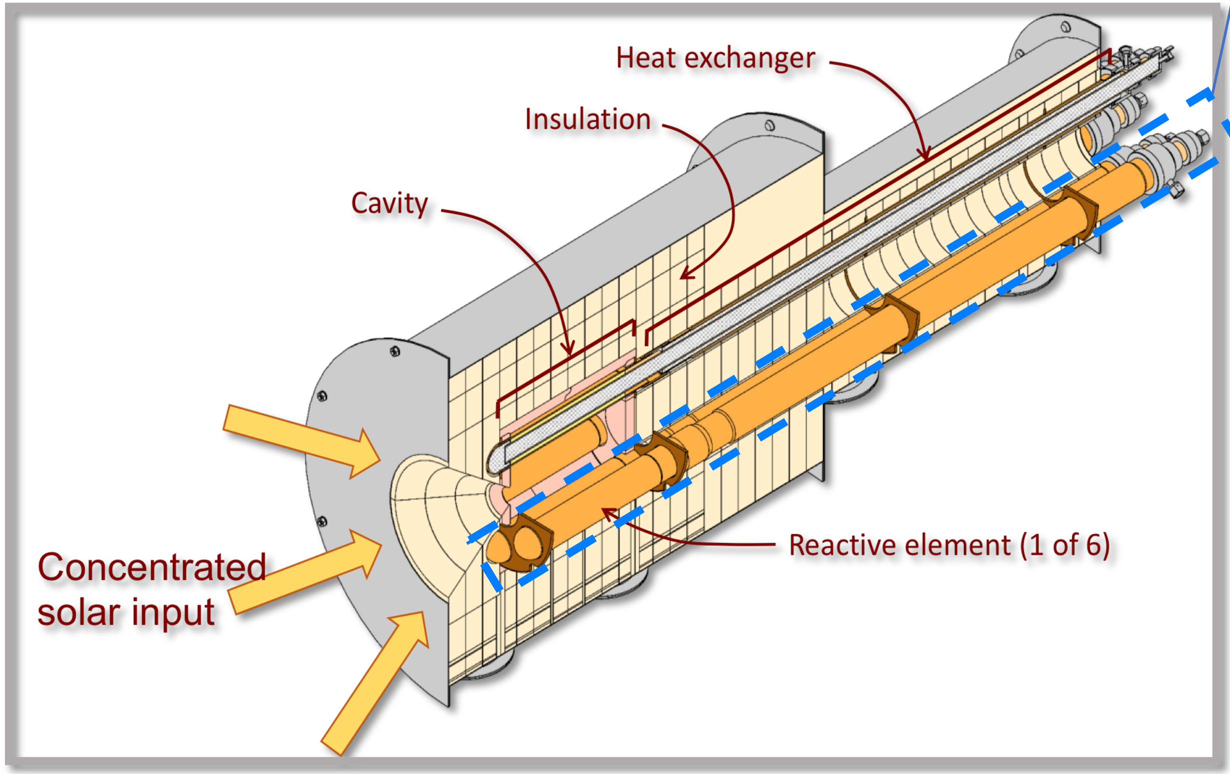
Ripe for new materials discovery and engineering breakthroughs

- Water is still the most abundantly used thermal energy storage medium
- Next-gen features:
  1. high energy density
  2. stability and good heat-transfer performance
  3. tunability to increase utilization
  4. sufficient power, cycle life and efficiency

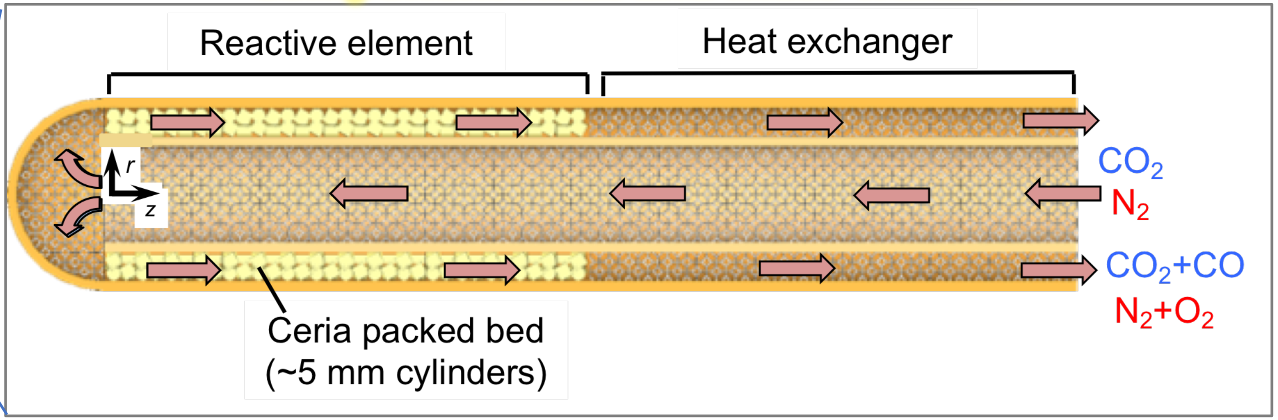
We have to consider multiscale heat and mass transfer in Thermal Energy Storage Systems

Consider a thermochemical solar reactor to store energy in chemical bonds as an example

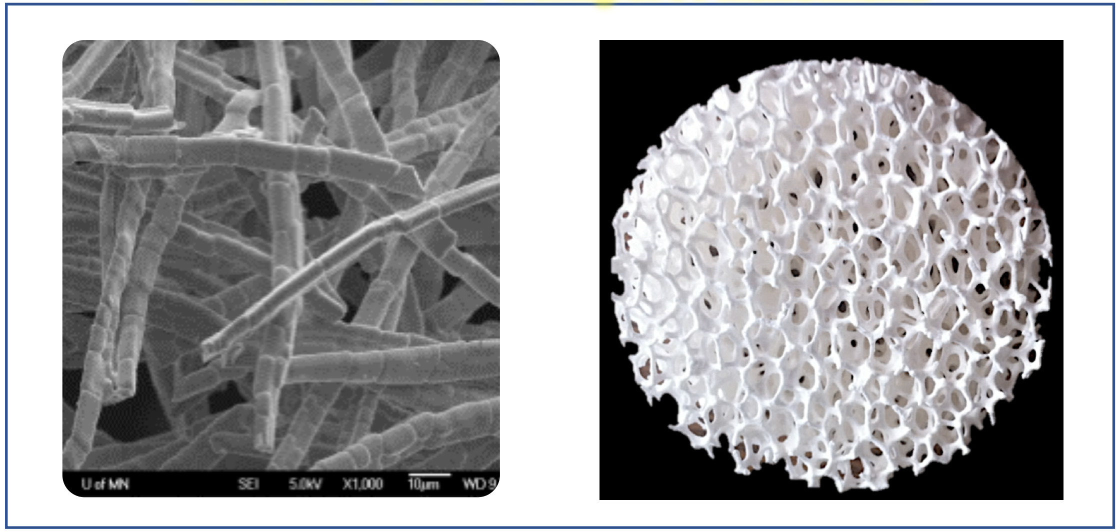
Overall Reactor/System Performance



Component Heat and Mass Transfer

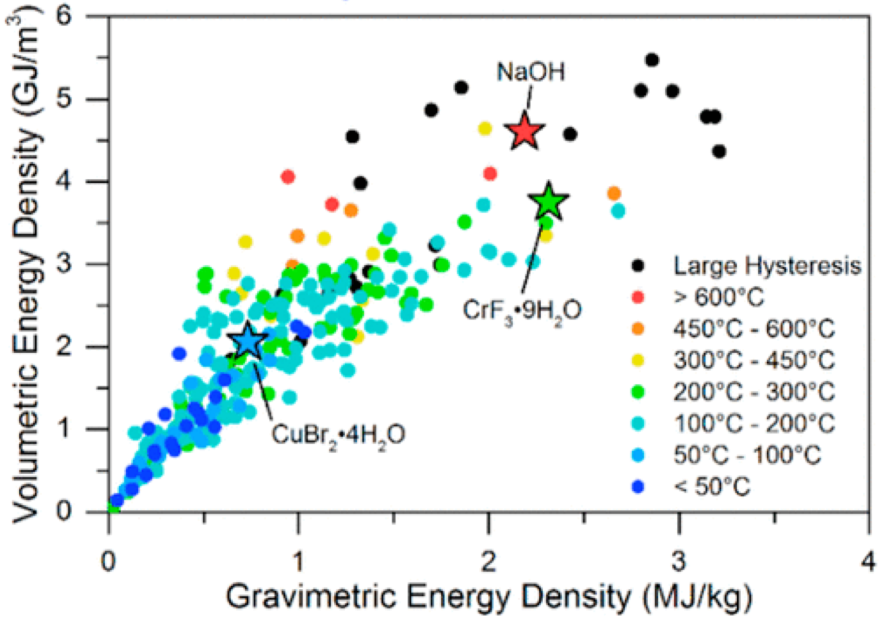


Materials-scale Transport Phenomena



Challenge #1: Materials Discovery for Thermochemical Storage

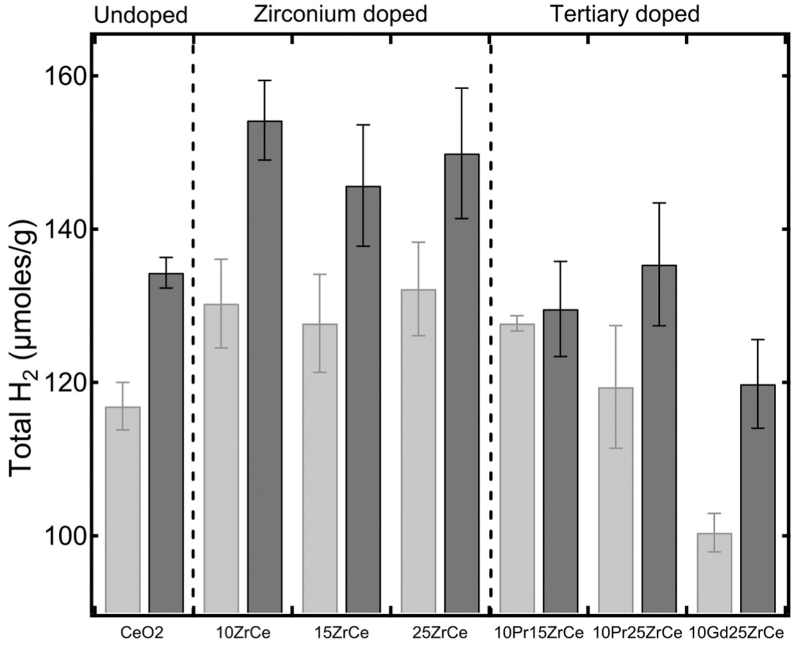
T < 700 C



S. Kiyabu et al., Chem. Mater. 2018, 30, 2006–2017

- 265 hydration reactions were characterized by high throughput DFT calculations.
- Several new high-energy density reactions

T > 700 C



Arifin, D. *et al.* , *Int. J. Hydrogen Energy* **45**, 160–174 (2020)

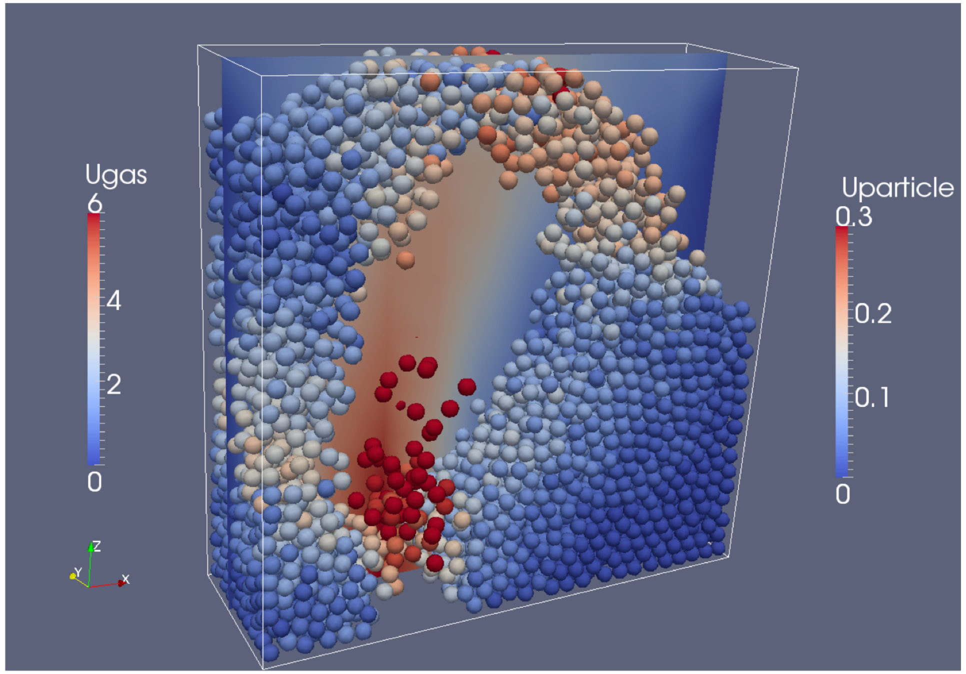
- DFT calculations to determine dopants to improve
  - CeO2 thermodynamic capacity
  - Lower reduction temperatures

- ○ Accelerated materials discovery could be a game-changer for TES
- ○ Potential to be combined with in-situ high throughput materials characterization
- ○ Challenges:
  - reaction kinetics
  - stability assessments
  - rates of heat and mass transfer
  - corrosivity and toxicity effects

TREE LAB
UNIVERSITY OF MICHIGAN

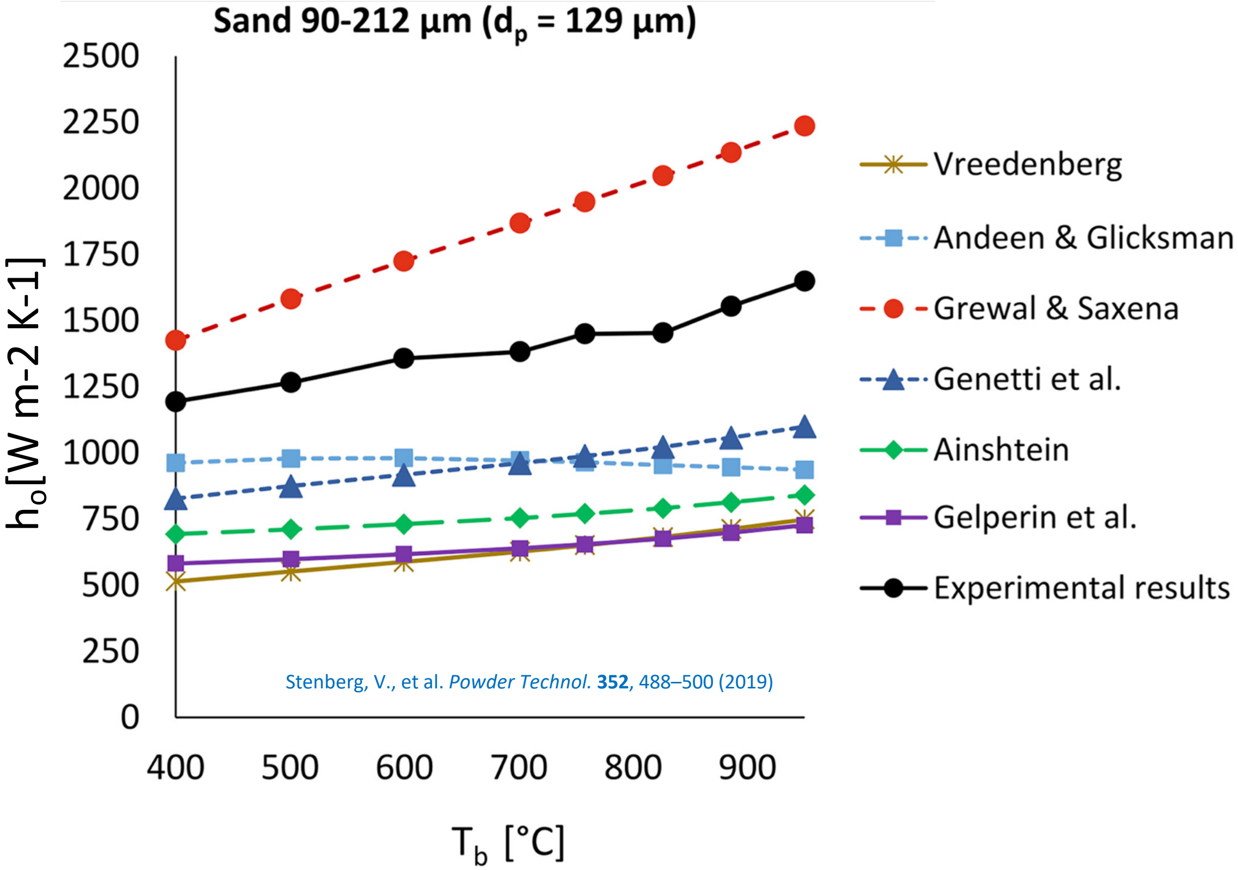
Challenge 2a: Predicting Heat- and Mass-Transfer Behavior

Fluidized beds of solid particles provide the benefit of “fluid-like” behavior to enhance heat- and mass-transfer



Simulation results from Bala Chandran’s group

Large variations in predicted heat-transfer coefficients (and correlations) especially at higher temperatures



Stenberg, V., et al. *Powder Technol.* **352**, 488–500 (2019)

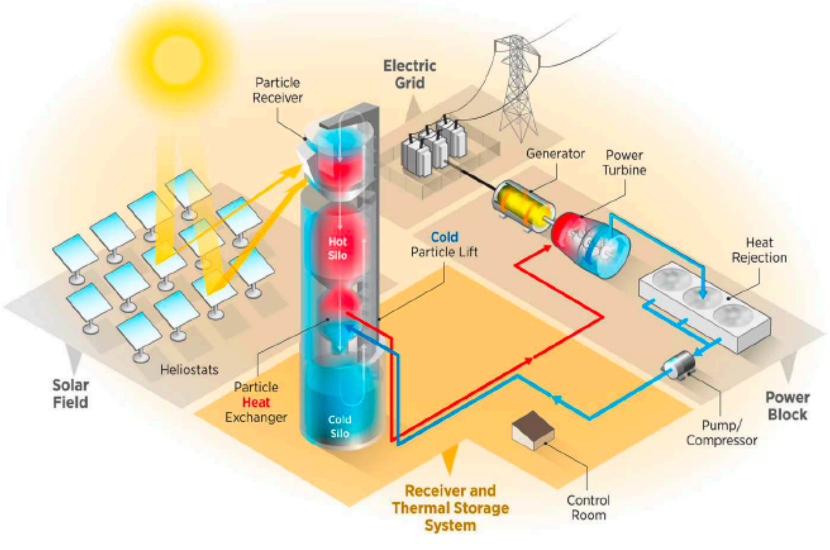
TREE LAB
UNIVERSITY OF MICHIGAN

We need high-fidelity modeling approaches + experimental validation

$$Nu = f(Re, Pr, d_p, \phi_s, \epsilon, ...)$$

Challenge 2b: Taking into Account Radiative Heat Transfer

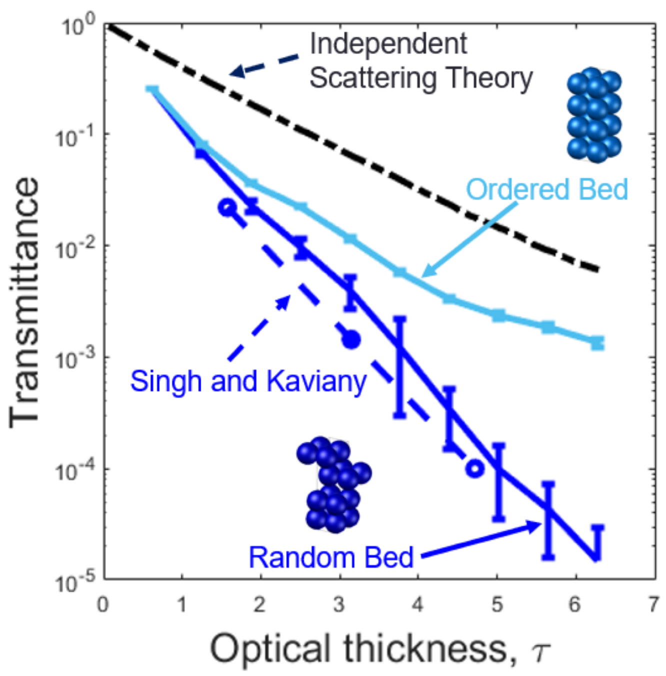
Gen3 CSP Technologies: T > 700 C



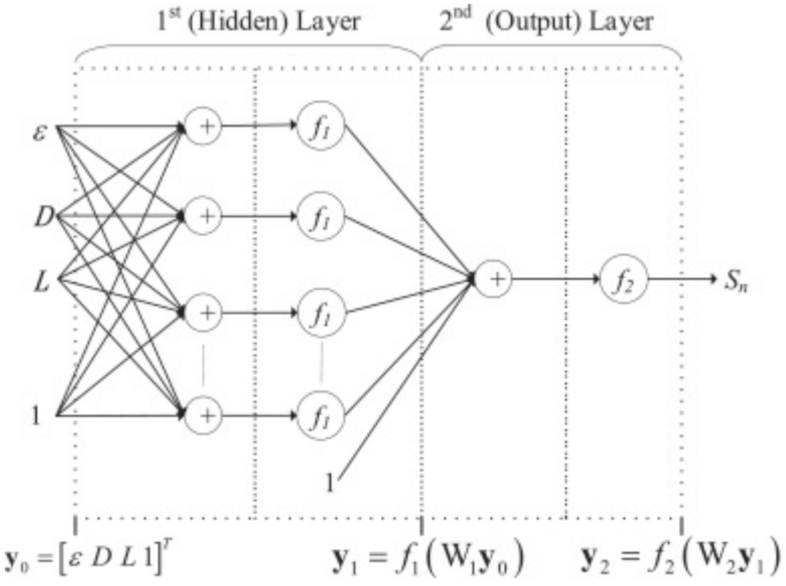
Mehos, M. *et al. Concentrating Solar Power Gen3 Demonstration Roadmap*. (2017)

Ray-tracing simulations in particulate media

Solid volume fraction: 0.52%



Neural network models for metallic packed beds



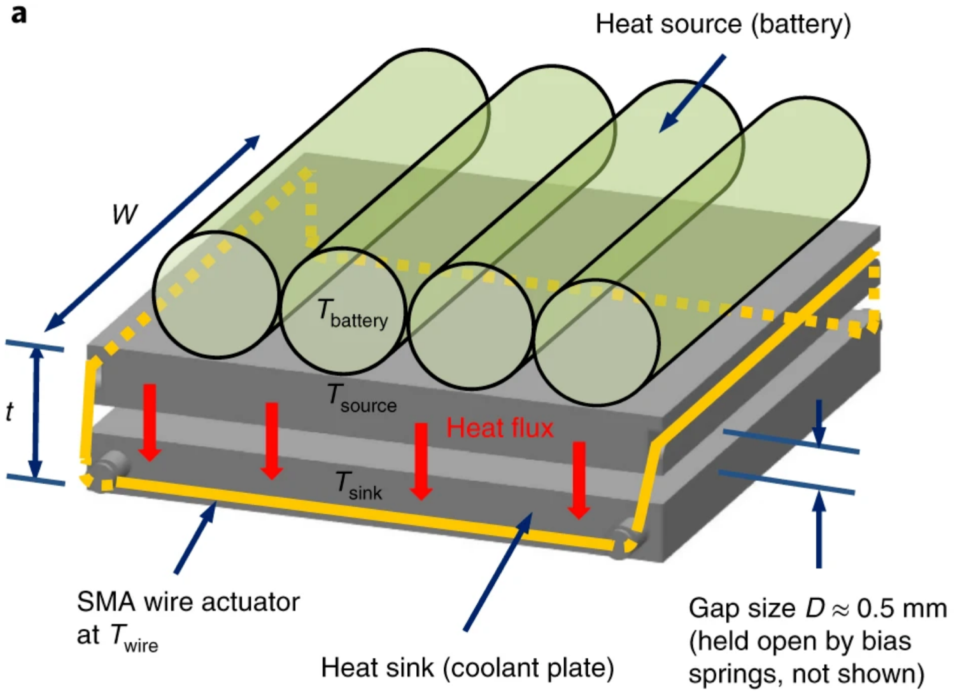
Kang, H. H., Kaya, M. & Hajimirza, S. *J. Quant. Spectrosc. Radiat. Transf.* **226**, 66–72 (2019)

- Radiative heat-transfer -> intrinsically 3-D, spectral and highly non-linear T-dependence, hard to obtain material properties
- System-scale reduced order models are needed to account for radiative transport
- Methodologies to marry physics-based models with data-driven approaches

TREE LAB
UNIVERSITY OF MICHIGAN

Challenge 3: Achieving tunability with thermal switches

Recent work from Dames et al., at UC Berkeley to use shape memory alloys for passive thermal management for Li-ion batteries



Hao, M., Li, J., Park, S., Moura, S. & Dames, C.. *Nat. Energy* 3, 899–906 (2018)

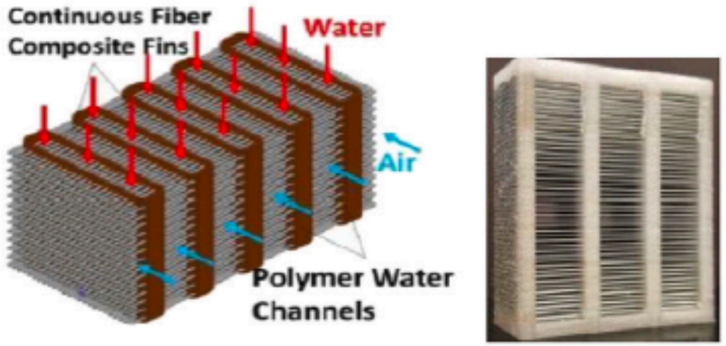
- Can the thermal energy storage systems self-regulate, based on temperature for how quickly they charge and discharge?
- Tunable thermal energy storage could improve utilization efficiency
  - PCMs in buildings are inactive for more than 50% of the time
- Concepts have existed for decades but for niche applications – spaceships and cryogenic systems
- Issues: Low switching ratio, large footprint, high cost and poor cyclability

TREE LAB
UNIVERSITY OF MICHIGAN

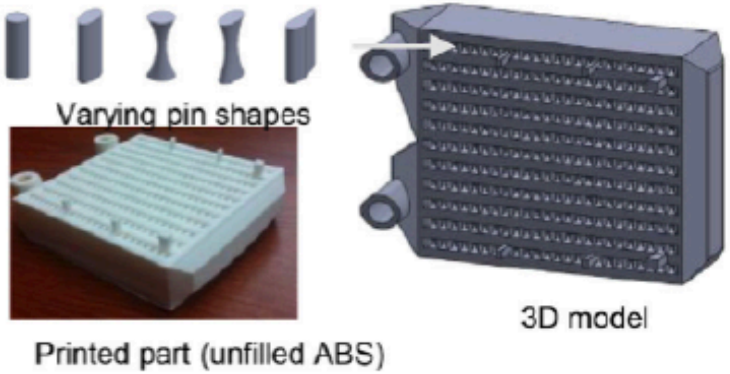
Challenge 4: Heat Exchanger Design and Modeling

3-D printed HX could allow for geometries precluded by conventional manufacturing

Cross-media metal fiber fin heat exchangers via multi-media 3D printing approach.

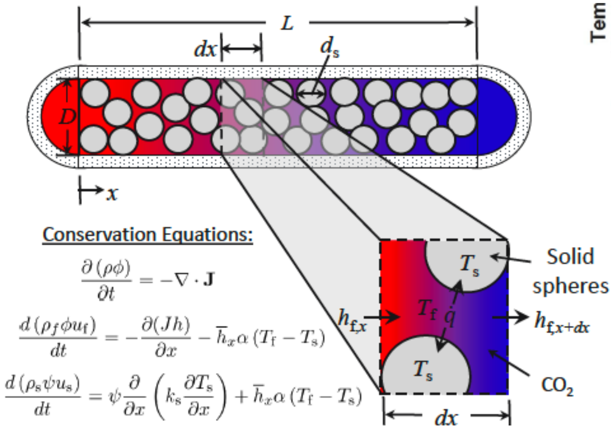


Optimized 3D heat transfer surfaces in printed composite (polymer + metal filler) heat exchangers.



Stark & Klausner, Joule, 2017

Beyond steady-state heat-transfer models

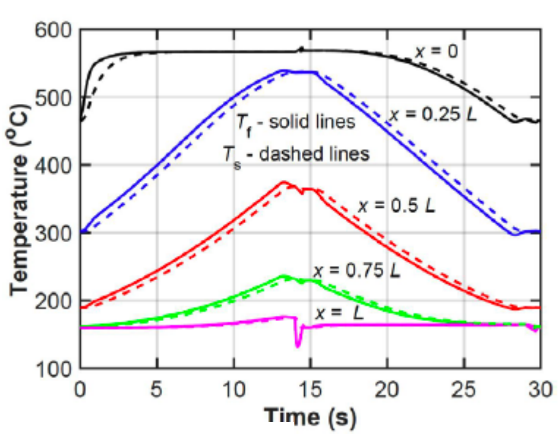


Conservation Equations:

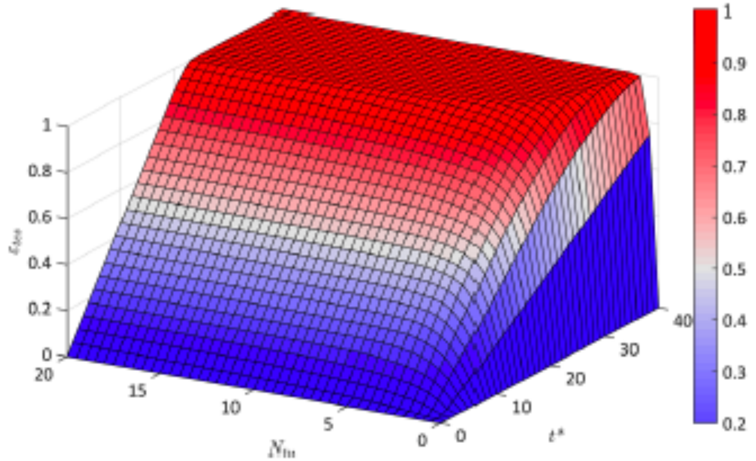
$$\frac{\partial(\rho\phi)}{\partial t} = -\nabla\cdot\mathbf{J}$$

$$\frac{d(\rho_f\phi u_f)}{dt} = -\frac{\partial(Jh)}{\partial x} - \bar{h}_x\alpha(T_f - T_s)$$

$$\frac{d(\rho_s\psi u_s)}{dt} = \psi\frac{\partial}{\partial x}\left(k_s\frac{\partial T_s}{\partial x}\right) + \bar{h}_x\alpha(T_f - T_s)$$



Anderson et al., sCO2 Regenerators, DOE Presentation Slides



Helmns, A. & Carey, V. P. *J. Therm. Sci. Eng. Appl.* **10**, (2018)

Summary of Research Questions & Needs

1. **Accelerated Materials Discovery, Development and Stability Testing**
   - Strategies to incorporate reaction kinetics
   - Corrosivity, toxicity and stability issues

2. **Predictions for Heat and Mass Transfer Performance**
   - Complex challenges for multiphase flows
   - High-fidelity computational heat and mass transfer predictions
   - Experimental validation for predicted data
   - Reduced-order models for device-scale performance predictions

3. **Tunability in thermal energy storage systems**
   - Lack of practically viable spatio-temporal control for TES
   - Quantification of where and when to deliver heat
   - Achieving improvements in switching ratio
   - Low-cost compact designs
   - Improved stability and cyclability

4. **Advanced heat exchanger design and model development**
   - Reimagine heat exchanger design with computational tools for topology optimization
   - Dynamic models for HX performance prediction

TREE LAB
UNIVERSITY OF MICHIGAN

Thankyou

Rohini Bala Chandran
Assistant Professor, Department of Mechanical Engineering
University of Michigan, Ann Arbor

February 4th, 2020
University Panel Discussion
TMCES Workshop, Pittsburgh

rbchan@umich.edu

www.rohinibc.com