Numerical modeling and design optimization of a concentrated solar thermal collector for dry methane reforming

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Introduction

There are tremendous research efforts focused on capturing thermal energy from the sun. Our current application is using this heat to drive a chemical reaction called dry reforming that produces hydrogen from methane and carbon dioxide, 2 potent greenhouse gases. This reaction only occurs at high temperatures (~1000K), requiring concentrated solar power.

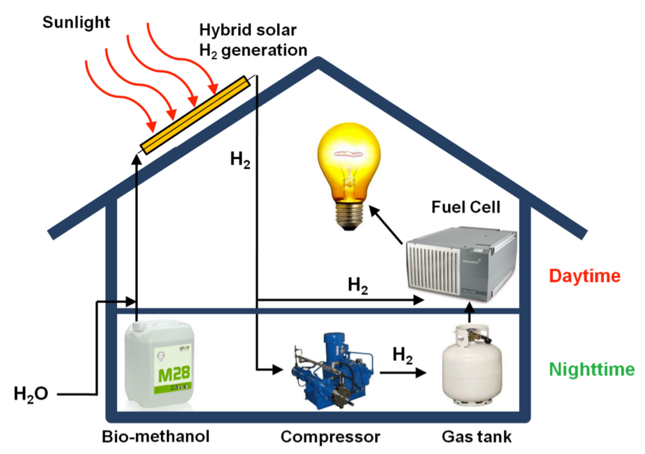


Figure 1. Schematic of overall residential hydrogen production system

Objectives

Modeling the operation of a concentrated solar collector is complex as the physics are highly coupled. Fluid flow of 50% mole fraction CH_4 and CO_2 is introduced at the inlet. The fluid is then heated through contact with a solar absorber, then reacted by flowing through a packed catalyst bed to form H_2 and CO. The following COMSOL Multiphysics model describes the operation of a collector, investigating the influence of various parameters on overall efficiency and H_2 generation.

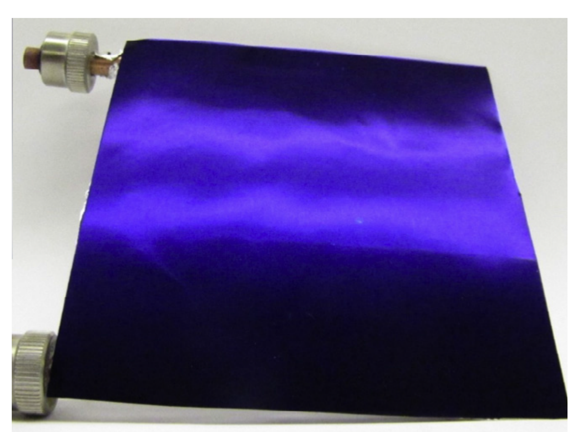


Figure 2. Solar thermal absorber placed inside a vacuum-insulated collector

Modeling

Since the problem includes heat transfer, fluid dynamics, and reaction, the physics interfaces used were Heat Transfer, Laminar Flow, Transport of Concentrated Species, and Chemistry. Non-isothermal and Reacting Flow multiphysics were used to properly couple the various physics.

Within the Heat Transfer physics, surface-to-surface radiation was considered. This was important to define the optical properties of the absorption coating and emissivity of other surfaces. Participating media was initially considered, but it had negligible effects due to the low absorption coefficient of the gases.

The equations used are listed below:

Heat Transfer

$$\rho c_p \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = Q \qquad \mathbf{q} = -k \nabla T$$

Laminar Flow

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot \left[-p\mathbf{I} + \mu \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right] + \mathbf{F}$$

$$\nabla \cdot (\rho \mathbf{u}) = 0$$

Reacting Flow

$$\nabla \cdot \mathbf{j}_i + \rho(\mathbf{u} \cdot \nabla)\omega_i = R_i \qquad \mathbf{N}_i = \mathbf{j}_i + \rho \mathbf{u} \omega_i$$

$$R_i = \nu_i \left[A^f \exp\left(\frac{-E^f}{R_0 T} \right) \right] \prod_{i=1}^{Q_r} c_i^{\nu_i}$$

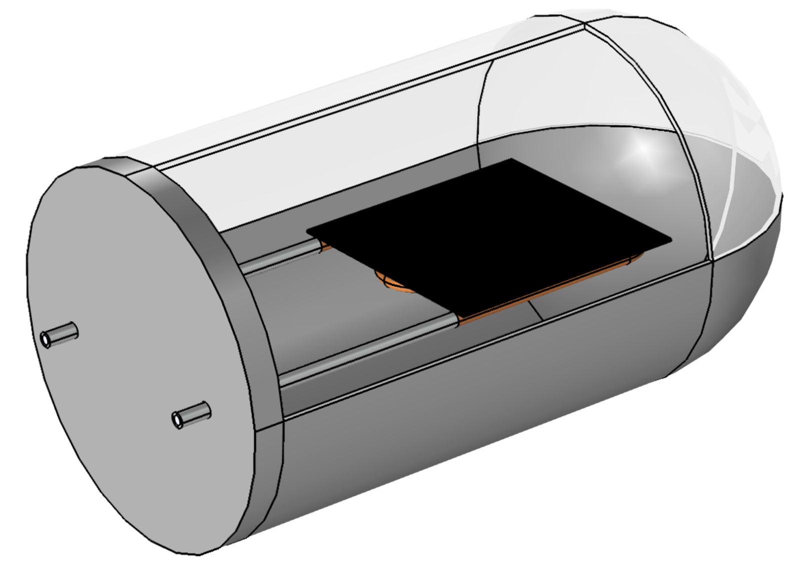


Figure 3. Geometry of overall 3D model including glass cover and steel bulkhead

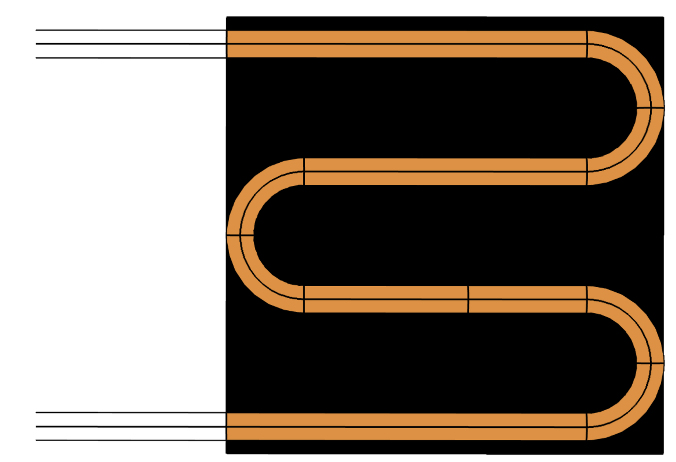
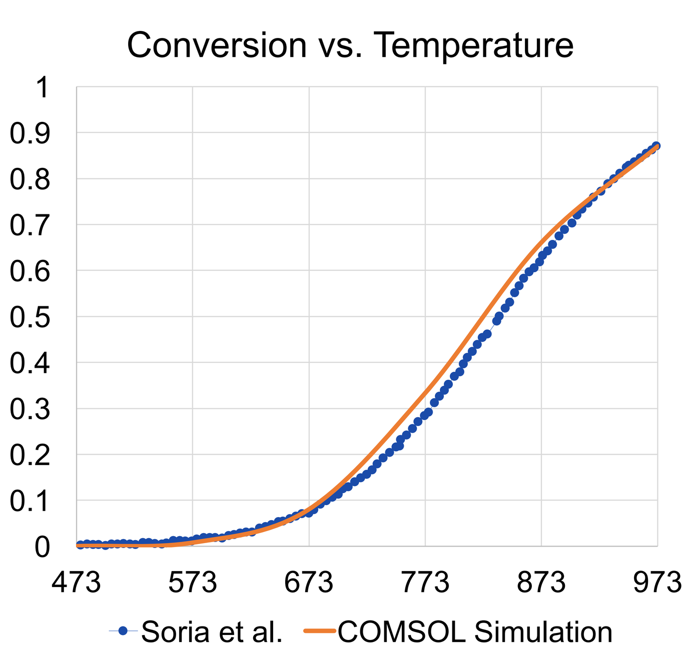
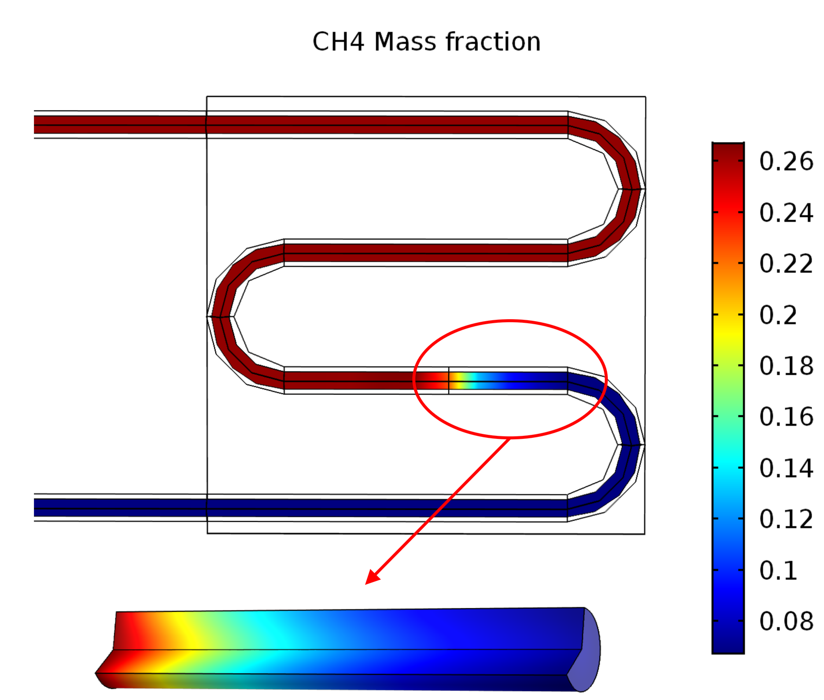


Figure 4. Geometry of copper tube layout underneath absorption coating

Catalytic Reaction Tuning

Instead of modeling a porous media for the packed catalyst bed, a simple control volume reactor was used. To tune the reaction, the activation energy and pre-exponential constant were varied to accurately match experimental data, obtained both in a laboratory setting and by Soria et al. [2]. The results of the simulation are shown below.





The final values for the properties of the catalyst were:

$$E_f = 77 \frac{\text{kJ}}{\text{mol}}, \; A_f = 1.3\text{e}5 \frac{\text{m}^3}{\text{mol s}}$$

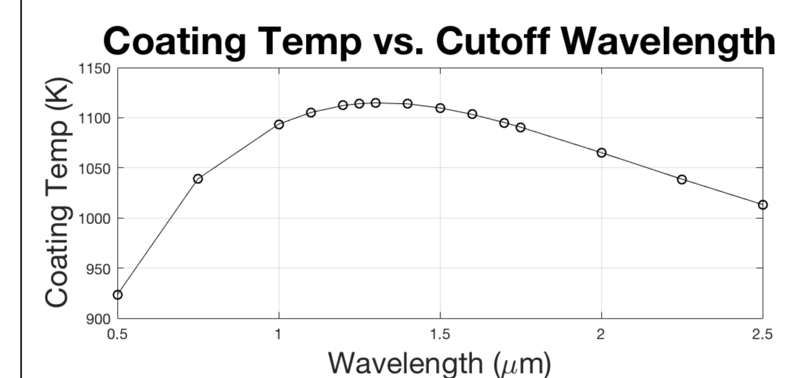
Materials Analysis

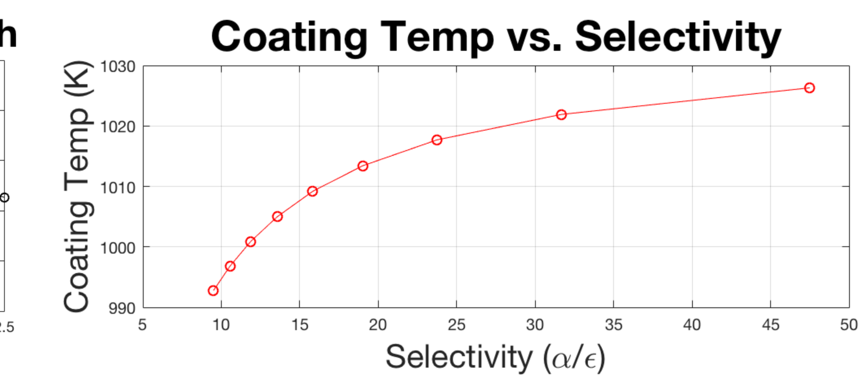
Copper tubes have been used in the past due to their high thermal conductivity. However, this results in high losses, especially considering the thermal short circuit created by the looped entry-exit. Therefore, various other better-insulating materials were modeled.

Material	Thermal Cond (W/mK)	Coating Temp (K)
Copper	400	971.9
Aluminum	238	988.9
Steel	44.5	1011.2
Alumina	27.0	1013.4
Silica Glass	1.38	1017.1

Absorption Coating Properties

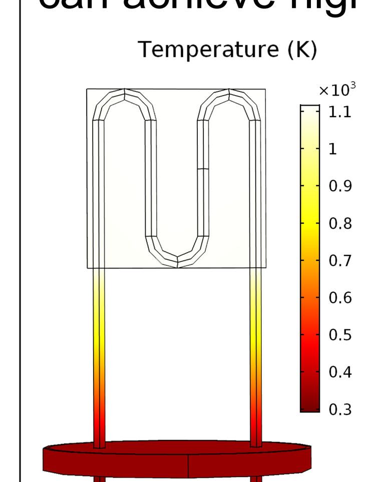
The optical properties of the absorption coating are critical to operation. High-temperature selective absorbers are difficult to make, so their properties should be determined before fabrication. The model was run for various cutoff wavelengths and selectivities to maximize temperature.

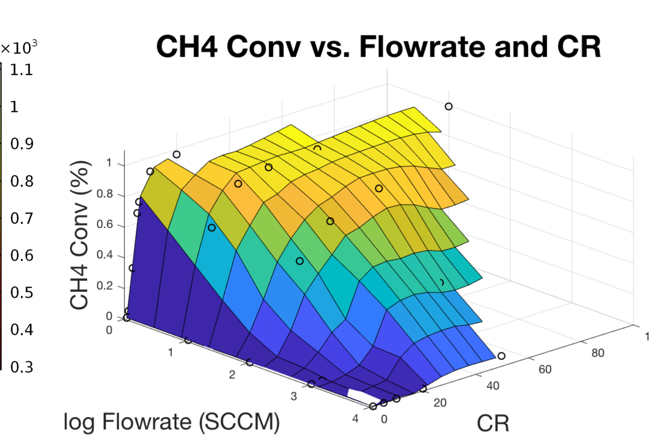


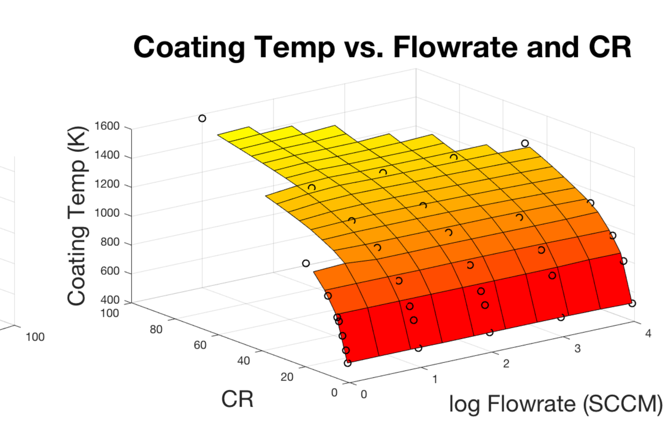


Steady State Results

Once the model was created, validated against experimental data, and optimized for high-temperature operation, steady-state results were obtained. For various concentration ratios and flowrates, the coating temperature and conversion were calculated, giving the final results below. As seen, the collector can achieve high conversion with low concentration.







Conclusions and Next Steps

- A numerical model was successfully created to determine conversion and efficiency for various flowrates and concentration ratios
- Results show concentrated solar thermal power is effective in producing hydrogen from methane
- Optical properties of the absorption must be tuned properly to optimize efficiency and create the ideal collector
- Future work:
  - Fabricating a high-temperature coating
  - Modeling phase change through steam methane reforming.

References

1. Real et al. "Novel non-concentrating solar collector for intermediate-temperature energy capture" Solar Energy 108 (2014). Duke University.
2. Soria et al. "Thermodynamic and experimental study of combined dry and steam reforming of methane on Ru/ ZrO_2-La_2O_3 catalyst at low temperature." International Journal of Hydrogen Energy 36 (2011). CSIC-UNED, Spain.