Thermodynamic Simulation of Hydrogen Chemisorption in Hydride Beds using External-Internal Cooling

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Presentation Outline

- Introduction
- Background
- Mathematical Model
- COMSOL Model Setup
- Model Validation
- Results
- References
- Acknowledgments

Introduction

- Hydrogen is a clean and renewable fuel source.
- Using metal hydride forming alloys as carriers safe storage is possible.
- Metal hydrides have a equilibrium chemisorption reaction with hydrogen.

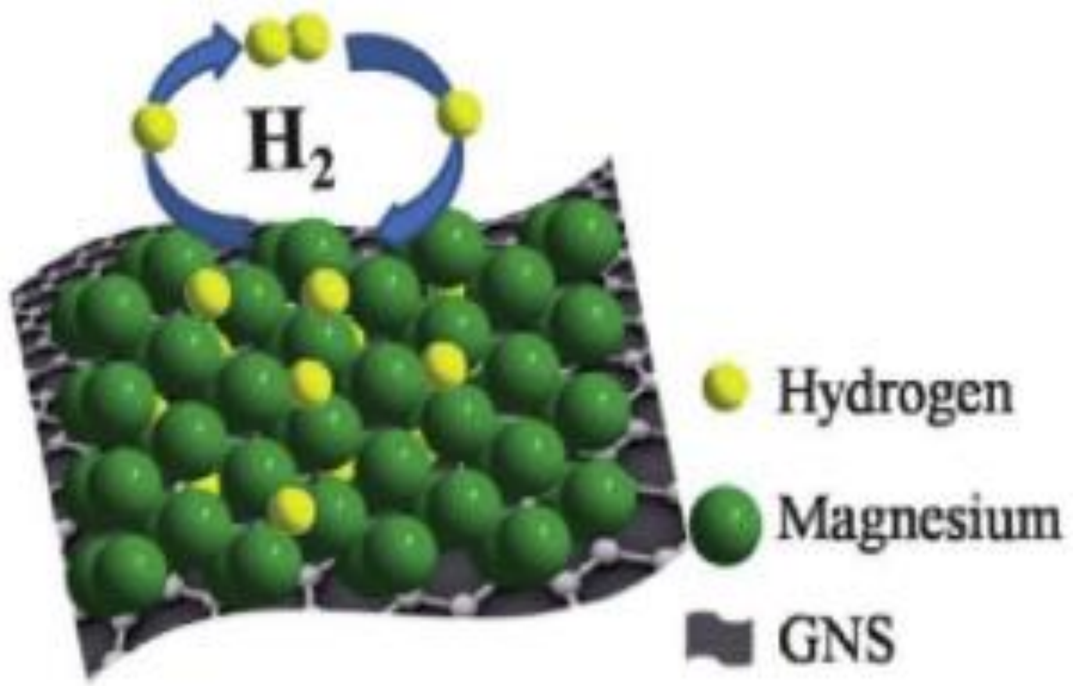

Figure 1: Schematic diagram showing hydrogen chemisorption from and to a grapheme nano-sheet (GNS) supported magnesium compound (Yartys et al. 2019)

Introduction Continued

- $M(s) + \frac{x}{2} H_2(g) \rightleftharpoons MH_x(s) + Heat$

- Storage tanks require effective heat management for fast charging.

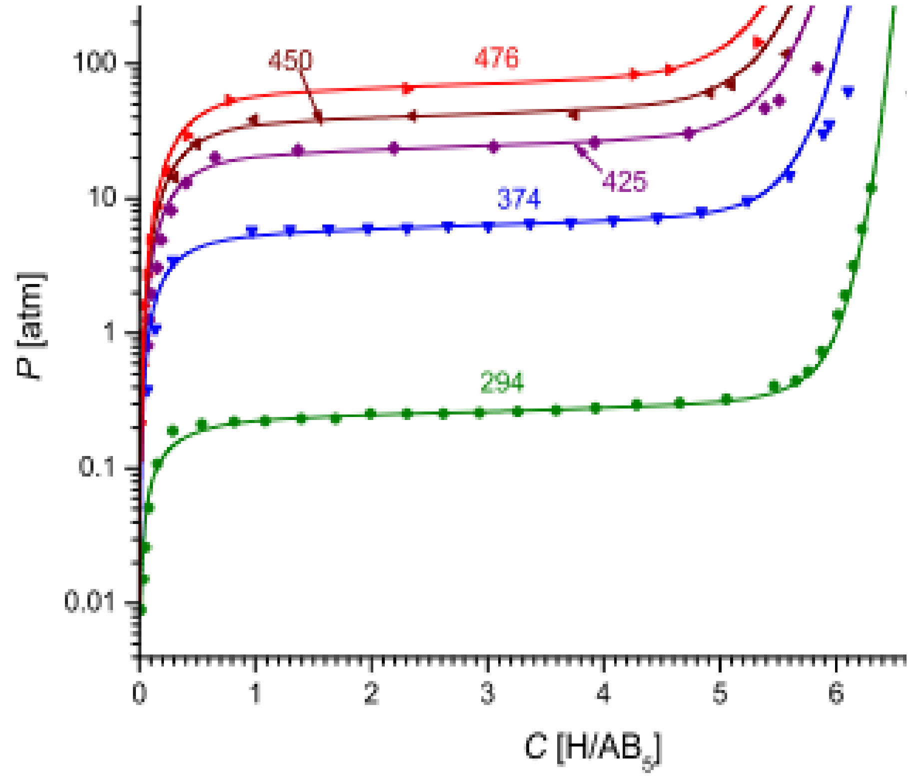

Figure 2: $LaNi_{4.8}Sn_{0.2}$ isotherms (Lototskyy 2016)

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Background

Usually hydride based storage takes one of two forms:

- External cooling
- Internal Cooling

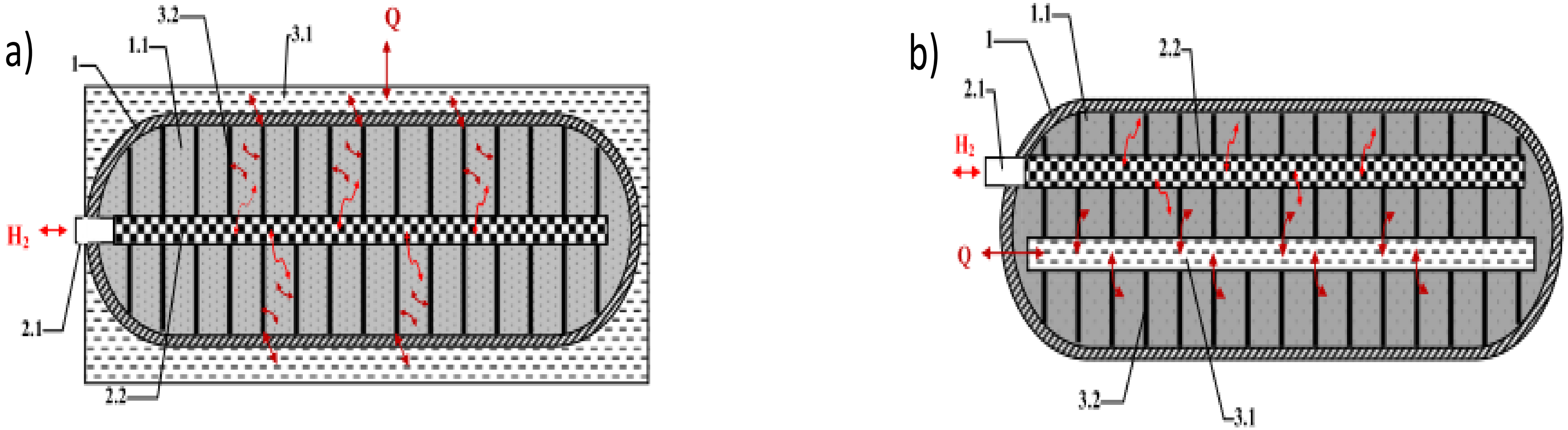

Figure 3: Typical designs of metal hydride tanks with (a) utilizing external heating or cooling and (b) utilizing internal heating or cooling (Lototskyy et al. 2017)

Background Continued

- I: a single tube heat exchanger.
- II: a spiral heat exchanger.
- III: only external cooling.
- IV: heat sinks with external cooling implementation.

- Heat sinks with external cooling proved more effective (Satya Sekhar et al. 2015)

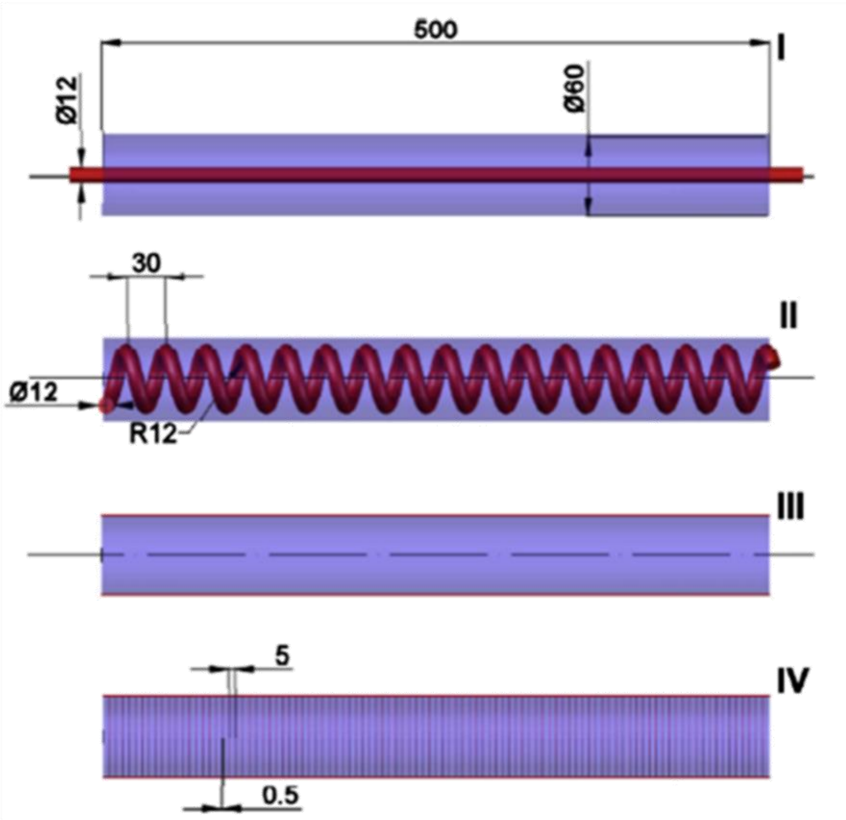

Figure 4: Experimental simulation setup of Satya Sekhar et al.

Mathematical Model

$$(1-\varepsilon)\frac{\partial \rho}{\partial t} = m \qquad (1)$$

$$m = C_A exp\left(-\frac{E_A}{RT}\right) ln\left(\frac{P_g}{P_{eq}}\right)\left(\frac{\rho_s M_g}{M_s}\right)(\,C_{ss} - C_s) \qquad (2)$$

Mathematical Model Continued

To determine equilibrium pressure and final saturated concentration Lototskyy's model was used.

- Lototskyy's model developed as a function in MATLAB
- MATLAB function was used to populate tables with 3360 data points.
- These tables were imported and interpolated using COMSOL.

(Lototskyy 2016)

COMSOL Model Setup General

Assumptions:

- Hydrogen acts as an ideal gas.
- Bed and gas are at thermal equilibrium.
- Radiative heat transfer is negligible.
- Cooling fluid temperature remains constant.
- Thermo-chemical properties remain constant.
- Exclusive heat transfer between fluid and system.
- No heat loss to the ambient environment.
- $LaNi_{4.8}Sn_{0.2}$ hydride forming metal was selected.

COMSOL Model Setup Geometry

External-Internal cooled:

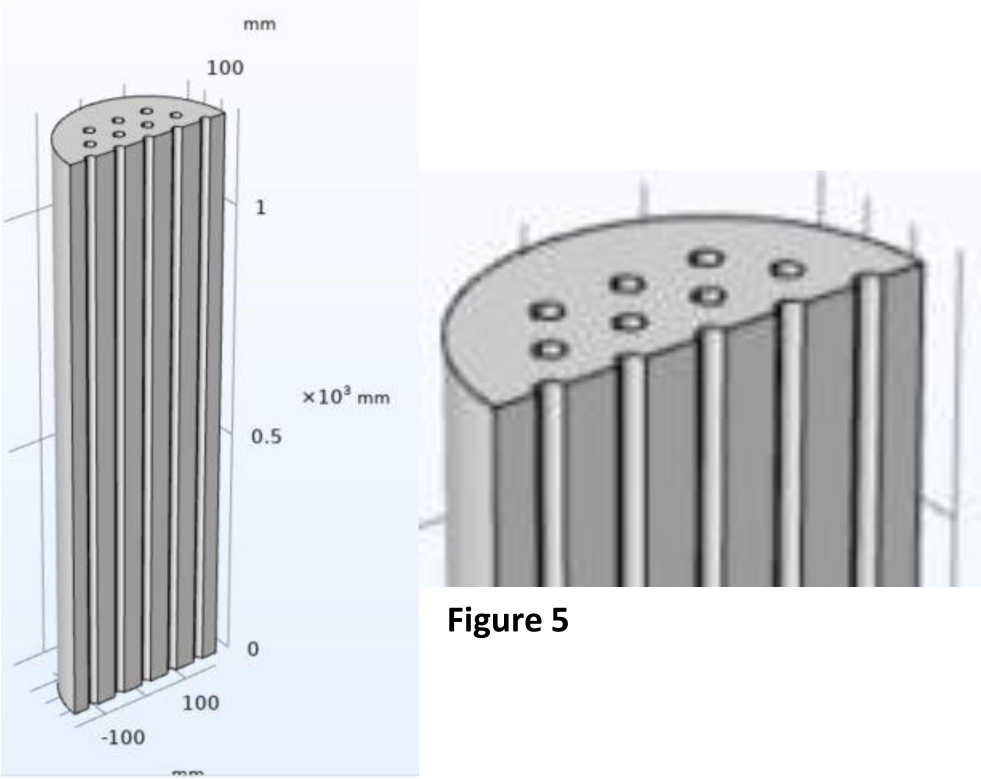

Figure 5

External cooled with fins:

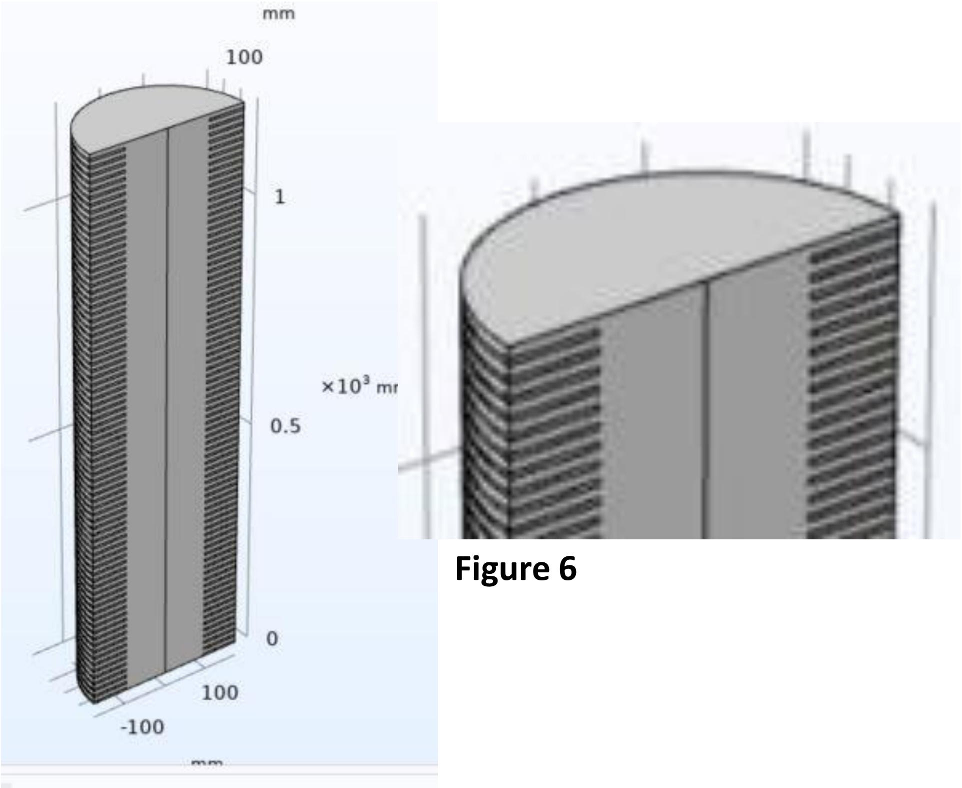

Figure 6

COMSOL Model Setup Physics

- For mass balance two domain ODE physics was used:
  - First to calculate the change in density of the bed using equations 1 & 2.
  - Second to calculate the change of hydrogen concentration in the bed.
- This was accompanied heat transfer porous media for energy balance.
  - Heat source was set as the bed domain and calculated based on mass balance.
  - Heat flux set to surfaces where fluid contact occurs.

COMSOL Model Setup Mesh

Physics-controlled normal element size mesh was used for both.

External-Internal cooled:

- 23851 elements
- 0.1874 minimum quality
- 0.6343 average quality

External cooled with fins:

- 134420 elements
- 0.0854 minimum quality
- 0.3732 average quality

Model Validation

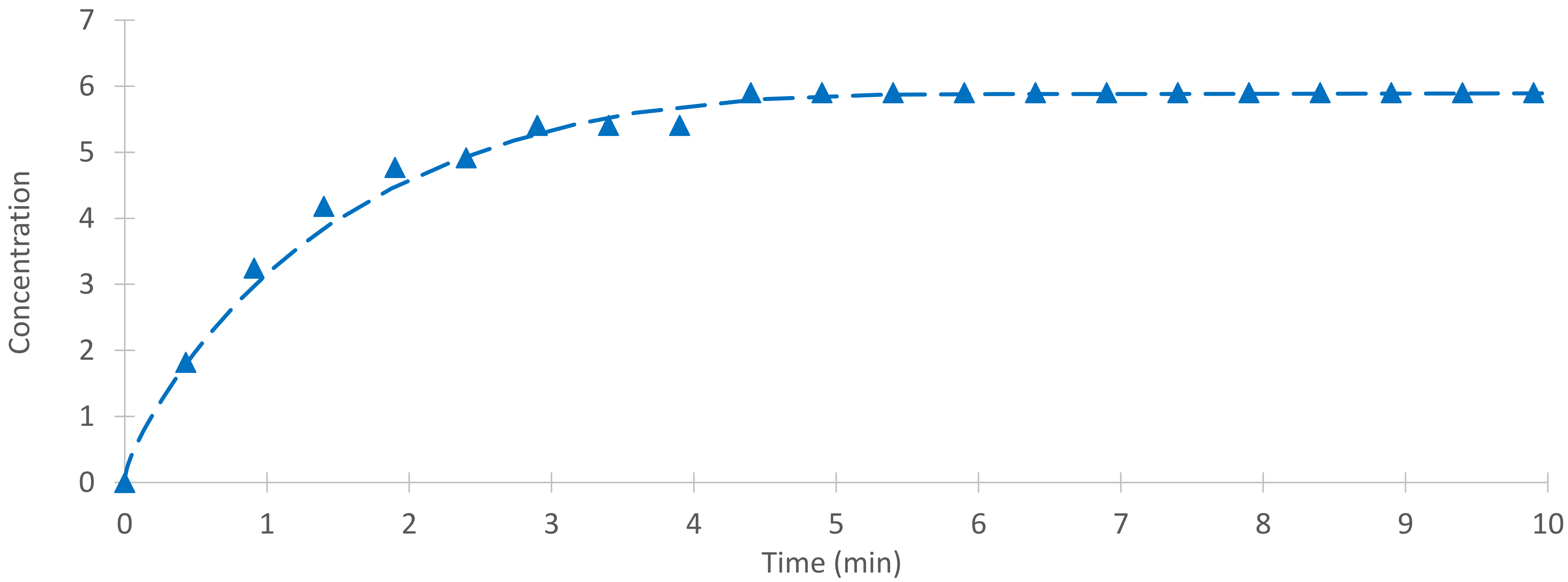

Figure 7: Model validation

Results

External-Internal cooled:

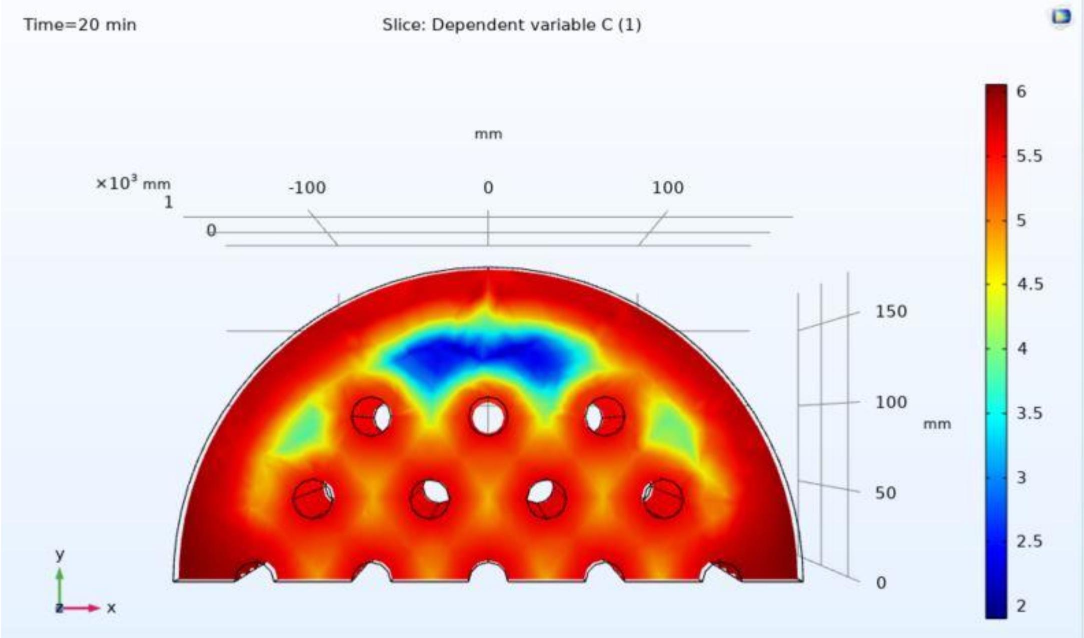

Figure 8

External cooled with fins:

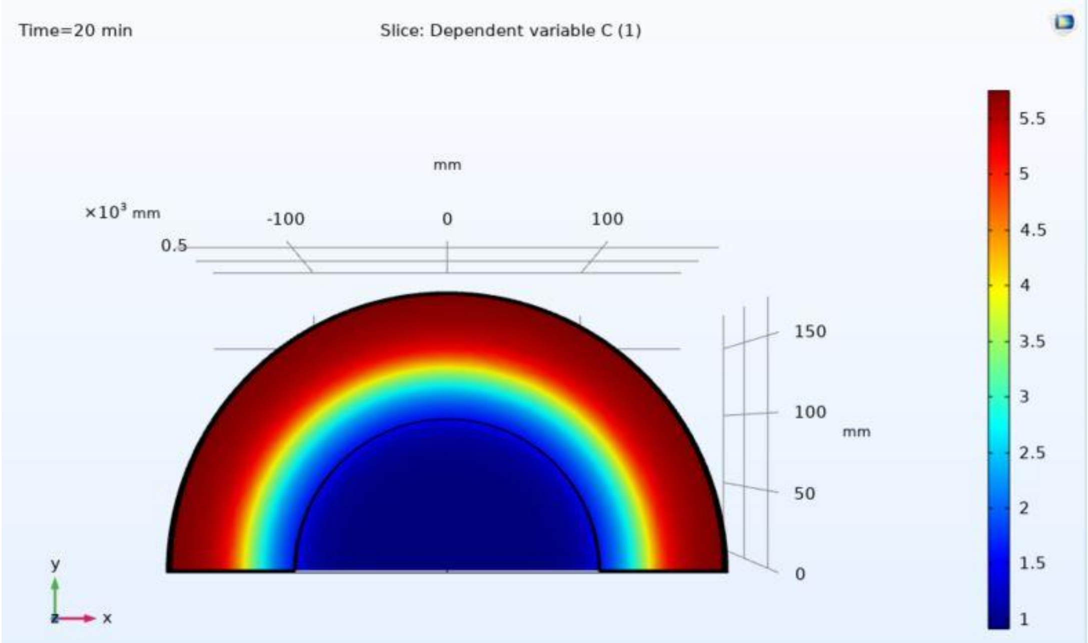

Figure 9

Results Continued

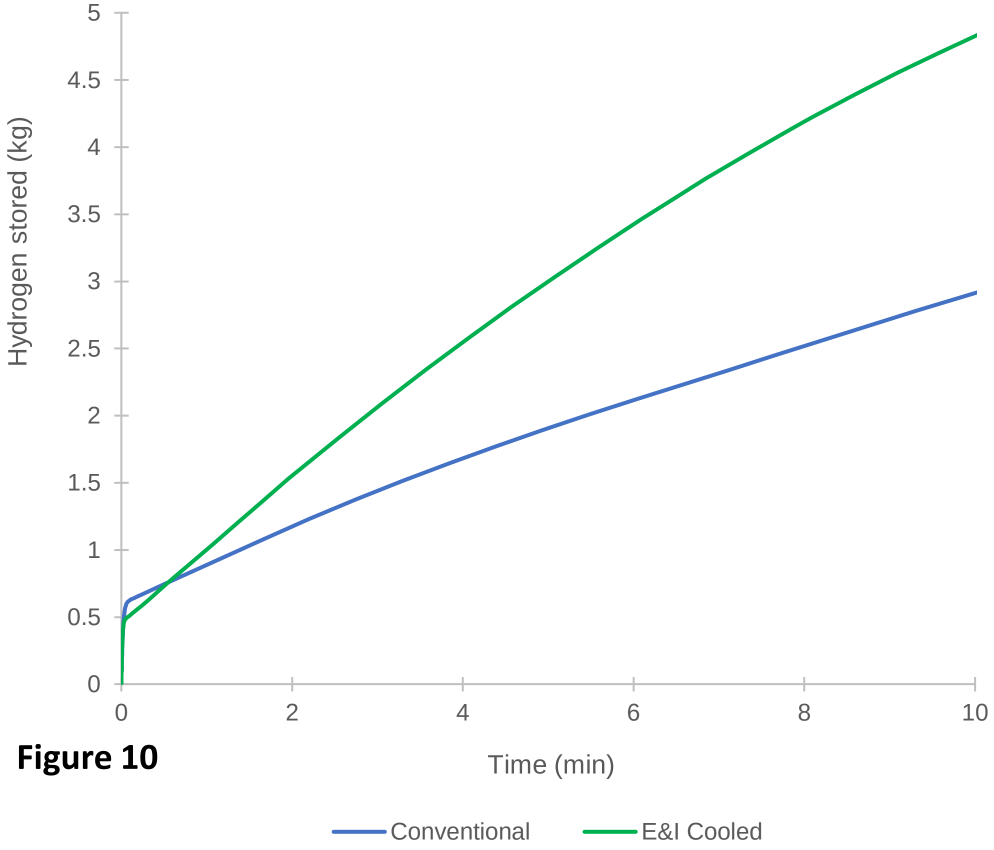

Figure 10

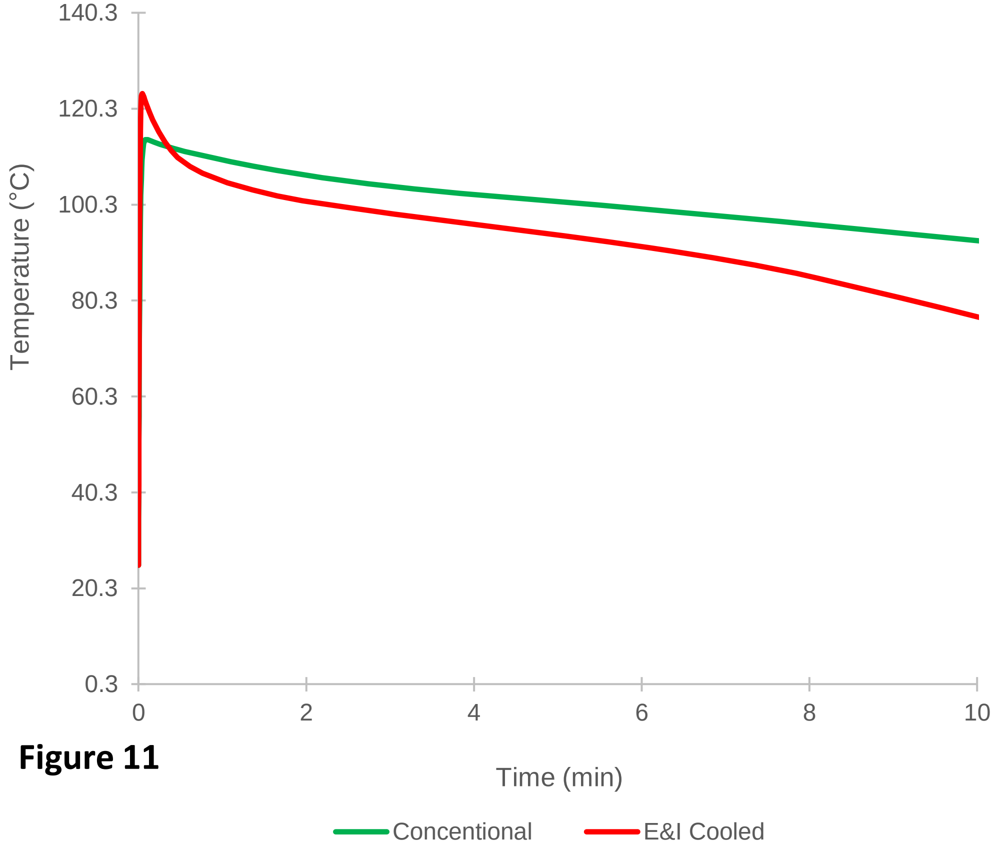

Figure 11

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Acknowledgements

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