Simulation as Various Operating Condition for High Temperature Magnesium Hydride Reactors

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Introduction: Magnesium hydride(MgH_2) reactor has been one of the most promising hydrogen storage methods. But hydrogen adsorption process has a considerable exothermic reaction problem. For stable hydrogen adsorption process, it is very important to understand heat and mass transfer in reactor. In this work, the magnesium hydride reactor is modeled and analyses are performed under various operating conditions.

Modeling: Chemical Reaction Engineering Module of COMSOL Multiphysics® software is used : "Free and Porous Media Flow" and "Heat Transfer in Fluid" interface are used to simulate mass, momentum and energy balance for hydrogen, and "Domain ODEs and DAEs" interface is used to calculate conversion of magnesium with hydride reaction. This model is referred from Bao et al[1].

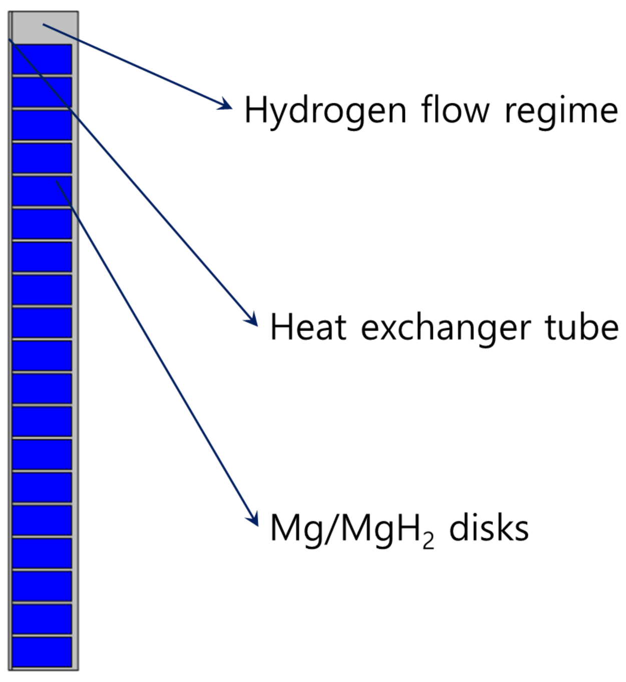

Figure 1. Geometry of magnesium hydride reactor

✓ Reaction kinetics (Chaise et al., 2010 [3])

$$\frac{dX}{dt} = k_0 \frac{p - p_{eq}}{p_{eq}} \exp\left(\frac{-E_a}{RT}\right) \cdot \frac{2}{3} \cdot \frac{(1-X)^{2/3}}{1-(1-X)^{2/3}}$$

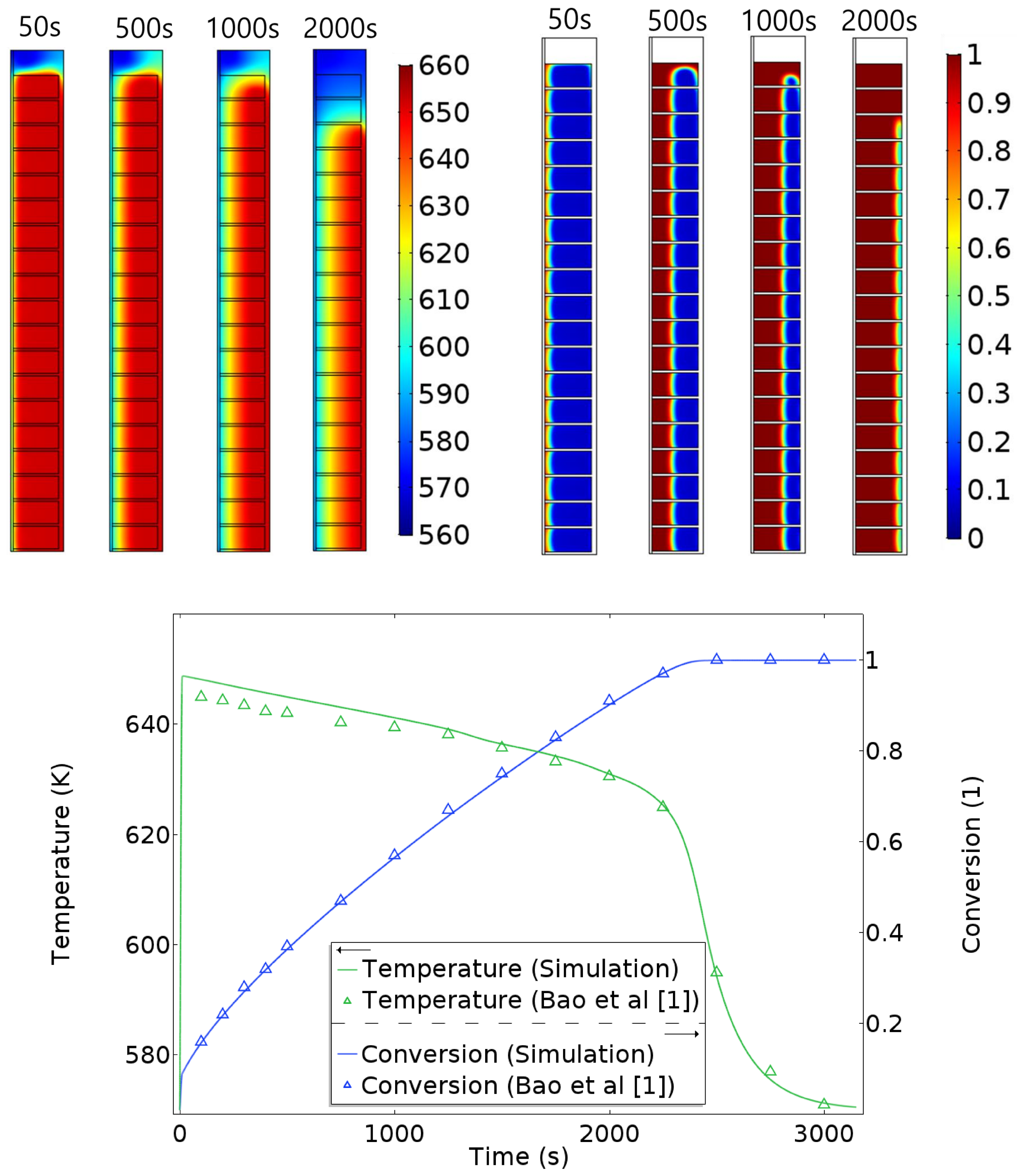

Figure 2. Simulation Results for reference conditions : Temperature profile (Upper left), Conversion profile (Upper right), and comparison results with respect to Ref[1]

Results: Using this magnesium hydride reactor model, we have studied simulations under various operating conditions.

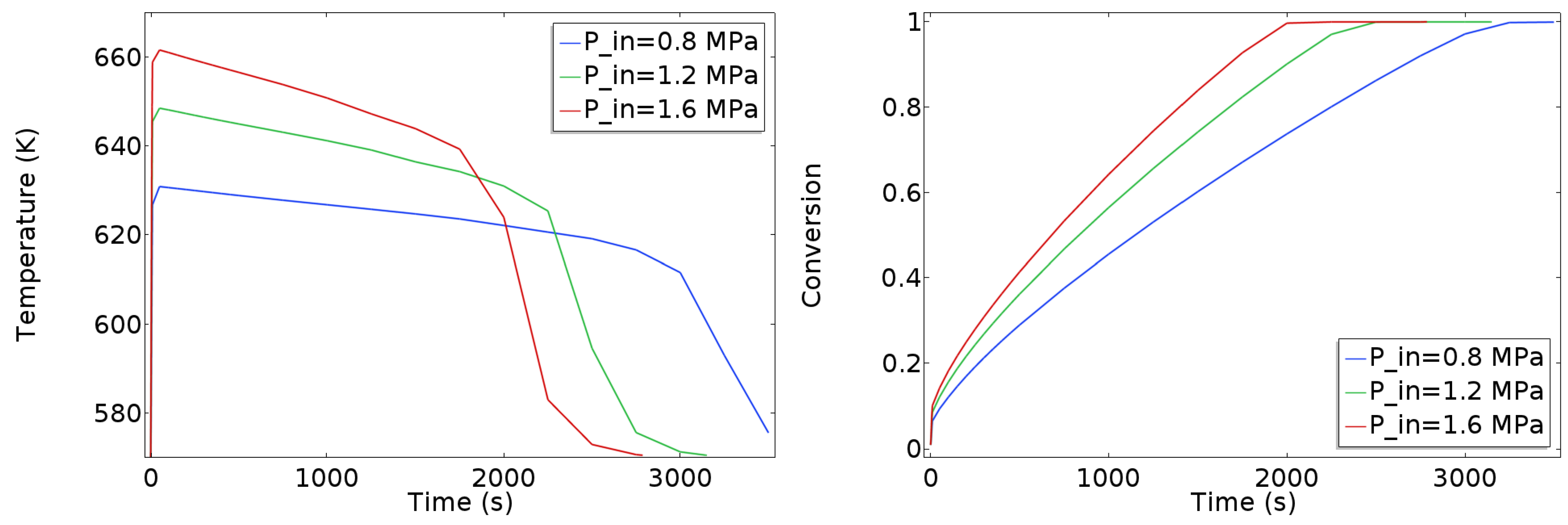

Figure 3. Results of average temperature and conversion as pressure

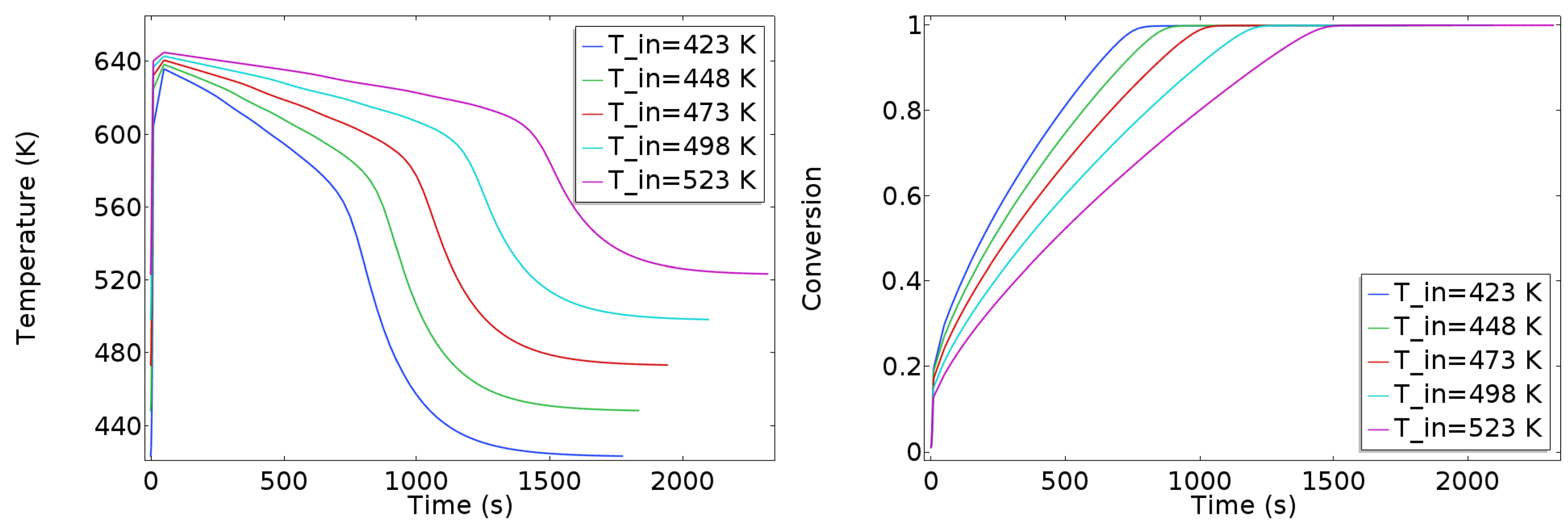

Figure 4. Results of average temperature and conversion as temperature

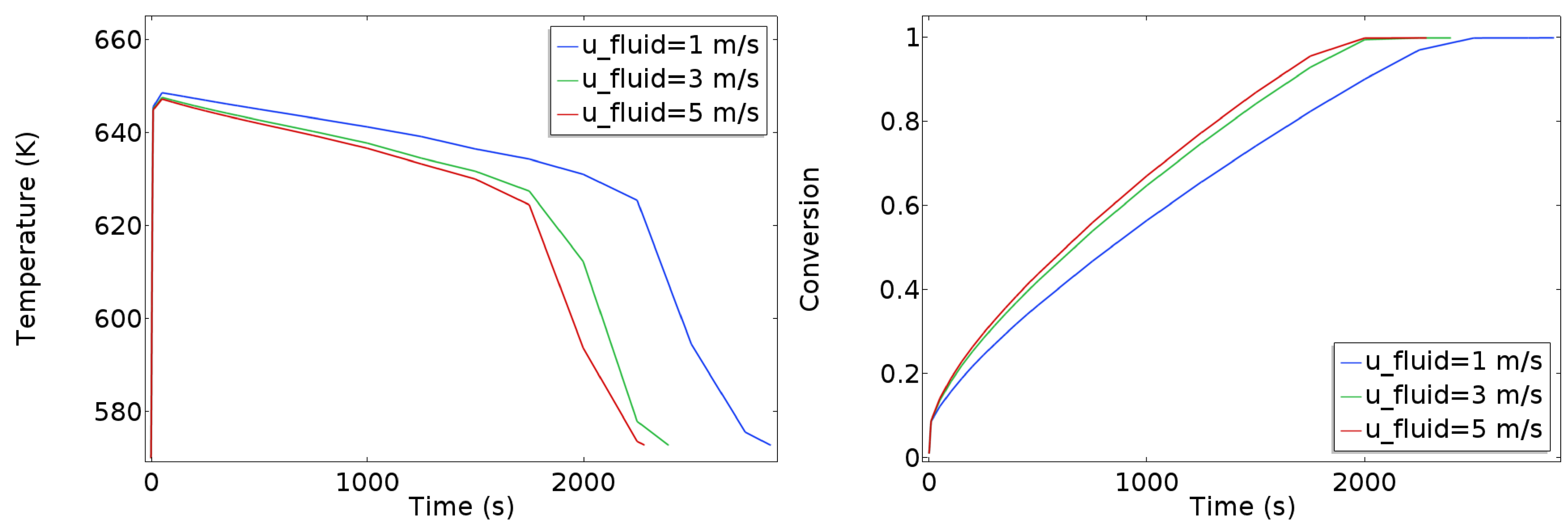

Figure 5. Results of average temperature and conversion as flow rate in heat exchanger tube

Conclusions: Simulation results are matched comparing with the reference results. Also, results as various conditions are properly expected with respect to previous studies in references. Being based on this basic simulation model, we will investigate adsorption/desorption cycling process for future works.

References:

1. Bao et al., Simulation studies on heat and mass transfer in high-temperature magnesium hydride reactors, Applied Energy, Vol 112, p. 1181 (2013)
2. Chaise et al., A simple criterion for estimating the effect of pressure gradients during hydrogen absorption in a hydride reactor, International Journal of Heat and Mass Transfer, Vol 52, p. 4564 (2009)
3. Chaise et al., Experimental and numerical study of a magnesium hydride tank, International Journal of Hydrogen Energy, Vol 35, p. 6311 (2010)