## Simulation As Various Operating Condition for High Temperature Magnesium Hydride Reactors

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## **Abstract**

Magnesium hydride (MgH2) has been one of the most promising hydrogen storage methods that can be applied to commercial hydrogen energy systems due to magnesium's safety, low cost, and excellent storage capacity for hydrogen, compared to other reversible metal hydrides. But hydrogen adsorption/desorption process has a considerable exothermic/endothermic reaction problem. For stable hydrogen adsorption process, it is very important to control heat from reactor. Therefore, it is essential to understand heat and mass transfer in reactor on operating process, and simulations would be needed under various conditions

In this work, the magnesium hydride reactor is modeled and analyses are performed under various operating conditions. The modeling for magnesium hydride reactor is performed with reference to Bao's paper [1]. The effects of various operating conditions are evaluated for conversion for magnesium and temperature profile. For this work, 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.

## Reference

- [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] Wu et al, Magnesium based metal hydride reactor incorporating helical coil heat exchanger: Simulation study and optimal design, Applied Energy, Vol 2014, p. 712 (2014)

## Figures used in the abstract

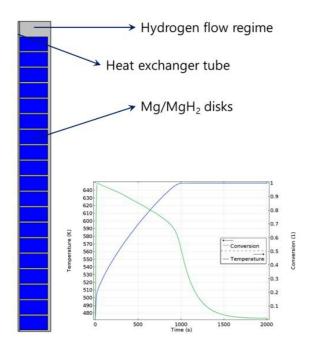


Figure 1: Geometry for magnesium hydride reactor and temperature/conversion graph