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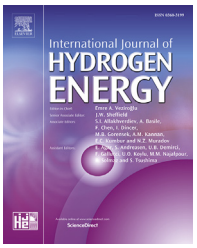

One-dimensional metal-hydride tank model and simulation in Matlab–Simulink

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ABSTRACT

A model has been developed for a metal-hydride tank for hydrogen storage, based on linked modular mathematical models in Simulink®. The objective of the work was a tank-level model suitable for incorporation into a whole-of-system model, implying modest computing demands and reduced complexity. Finite-element analysis was not used. Because the apparent kinetics of a practicable metal-hydride tank is dominated by heat flow originating in the enthalpy of hydrogen absorption/desorption, particular attention was paid to modelling the effective thermal conductivity, based on a detailed description of the thermal resistance between hydride particles. The model was tested against our own experimental data for a pair of tanks with 6.4 kg total hydrogen capacity, and compared with a published 2D model and published experimental data. In all cases, the new model performed very well. The incorporation of a physical model of the effective thermal conductivity means that the tank model can also be used as a research tool to investigate ways of improving tank performance by altering the physical characteristics of the metal-hydride itself to achieve an optimal thermal design and enhanced reaction kinetics.

Introduction

Hydrogen storage is a key enabling technology for the advancement of hydrogen and fuel cell technologies in applications including stationary power, portable power, and transportation. Relative to other fuels, hydrogen has a very high gravimetric energy density (120 MJ kg^{-1} LHV) but a very low volumetric energy density at ambient temperature and pressure (96.4 MJ m^{-3} LHV). To match the gravimetric and volumetric energy densities of gasoline (44 MJ kg^{-1} and 32 GJ m^{-3} respectively), a hydrogen fuel tank would need to contain 35 mass% hydrogen compressed to 4 times liquid density.

The storage problem has been resolved in commercially available fuel-cell electric vehicles by compressing gaseous hydrogen to 70 MPa for small vehicles and 35 MPa for buses. This solution is unlikely to be feasible for larger storage units (say >100 kg H_2), however, because of high cost and low volumetric density.

While solid-state hydrogen storage achieves gravimetric energy densities that are unacceptably low for use in automobiles, it can achieve high volumetric energy density at near-ambient pressures [1]. Nickel-metal hydride batteries were the first commercial success for solid-state hydrogen storage [2]. Metal-hydride energy storage is beginning to be used in public off-grid buildings *e.g.* the Sir Samuel Griffith Centre, Griffith University, Brisbane, Australia [3], with 120 kg

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Glossary

a_H	Hertzian contact radius, m
a_L	Radius of macro-contact, m
b	Specific gas constant
c	Vickers microhardness coefficient
C_p	Specific heat capacity, J kg^{-1} K^{-1}
D	Diameter, m
d_v	Indentation diagonal depth, m
E	Activation Energy, kJ mol^{-1}
E'	Effective elastic modulus, GPa
F_n	Force, N
F	Reacted fraction
H/M	Hydrogen to metal ratio per formula unit or per metal atom; *i.e.* [0–6] or [0–1] for $LaNi_5$
H_v	Vickers microhardness, GPa
H_c	Contact microhardness, GPa
h_f	Heat transfer coefficient of fluid, W M^{-2}
k_B	Boltzmann constant, 1.38 × 10^{-23} J K^{-1}
k	Thermal conductivity, W m^{-1} K^{-1}
Kn	Knudsen number
K_r	Reaction rate coefficient
κ	Rate constant
K_p	Permeability, m^2
LHV	Lower heating value
l_m	Molecular mean-free path
$\dot{m}$	Rate of mass absorbed or desorbed, kg m^{-3}
M	Gas parameter
N	Coordination number
Nu	Nusselt number
n	Pre-exponential factor
s	Solid
p	Particle
eff	Effective
eq	Equilibrium
in	Initial
ref	Reference
sat	Saturation
su	Supply
tn	Tank
P	Pressure, Pa
Pr	Prandtl number
r	Radial coordinate, m
R_g^*	Universal gas constant, 8.3144 J mol^{-1} K^{-1}
Re	Reynolds number
R	Radius of sphere, m
R_c	Thermal contact resistance, Ω
R_s	Micro-contact thermal resistance, Ω
R_L	Macro-contact thermal resistance, Ω
R_g	Micro-gap thermal resistance, Ω
R_G	Macro-gap thermal resistances, Ω
T	Temperature, K
V	Volume, m^3
ρ	Density, kg m^{-3}
v	Velocity, m s^{-1}
ε	Porosity
t	Time, s
w	Weight percent, %
τ	Ratio of expansion
σ	Surface roughness, m
α_T	Thermal accommodation coefficient
γ	Adiabatic exponent
μ	Dynamic viscosity, kg m^{-1} s^{-1}

Subscripts

a	Absorption
d	Desorption
f	Fluid
g	Gas

H_2 capacity (≈2 MW-h electric equivalent) and the Henn-na Hotel, Nagasaki, Japan [4].

The advantages of metal-hydride storage in these situations come from (i) the decoupling of power and energy ratings, which makes it advantageous for long-term storage compared to batteries [5]; (ii) its ability to be tuned for low operating pressure suitable for direct coupling to an electrolyser (~1 MPa); (iii) excellent safety coming from the low pressure and relatively slow kinetics of hydrogen release; and (iv) high volumetric energy density. For example, the classic intermetallic hydride $LaNi_5H_6$ contains only 1.4 mass% hydrogen, but has a 100%-dense volumetric capacity of approximately 115 kg m^{-3} at room temperature and <1 MPa pressure [6] compared to 70.8 kg m^{-3} at 20.3 K and 0.1 MPa for liquid hydrogen.

The design of a system involving any modality of hydrogen storage requires modelling of its characteristics and interactions with the rest of the energy system. Modelling hydrogen storage in a metal hydride (MH) is a complex multi-physics problem, which involves compressible gas flow in a porous MH bed, coupled with heat transfer and reaction kinetics. For example, the enthalpy of formation of $LaNi_5H_6$ is ≈30 kJ mol^{-1}, so charging 1 kg of hydrogen releases ≈15 MJ of heat, compared to the stored energy of 120 MJ LHV. This heat must be managed, preferably via thermal storage and use in another process. The key point from the modelling perspective is that the effective thermal conductivity of MH beds is very poor owing to their porosity and inter-particle contact resistance. Various values have been reported for the measured effective thermal conductivity of a $LaNi_5$ powder bed (with porosity ≈0.5), the most reliable representative value probably being 1.32 W m^{-1} K^{-1} [7], compared to >30 W m^{-1} K^{-1} for a solid composite compact of $LaNi_5$ [8]. As a result of the poor thermal conductivity, the observed reaction kinetics for absorption and desorption of hydrogen is dominated by heat flow [9]. Realistic thermal modelling, especially of the thermal conductivity, is therefore essential to build a quantitative model of MH storage.

This paper continues a series in which mutually compatible modular models of the components of an energy system, specifically one incorporating solar-derived hydrogen [3], are presented. One overall objective is to link the suite of component models together to form a whole-of-system model and simulation that can realistically predict the behaviour of a

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