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Simulation study on the outlet flow dynamics of a hydride-based hydrogen storage canister for medical use

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ABSTRACT

In recent years, hydrogen molecule as therapeutic antioxidant was found to be useful for the treatment of a number of diseases. To supply hydrogen safely and reliably in the hospital, a patent-pending system was proposed by the authors, including a canister filled with metal hydride, a gas mixing chamber and some other components. The outlet flow of the canister must be controlled within certain accuracy to assure the medical effect of the hydrogen intake, thus was investigated in this work. The mathematical model of hydrogen release process, which couples porous flow, heat and mass transfer was solved using a commercial software package COMSOL Multiphysics 3.5a. The outlet flow dynamics are tested in the cases of convective heating and electrical heating, and great differences are found. For the case of electrical heating that provides constant heat flux, the mass flow rate of H_2 showed little temporal variation after the initial transient. Moreover, under certain conditions a PI control strategy was successfully applied to regulate the valve openness for keeping a constant flow rate of H_2.

1. Introduction

Hydrogen, due to some unique properties, has been found useful on a number of occasions, e.g. fuel. However, it was only recently that people discovered the tremendous potential of molecular hydrogen in therapy use. The understanding of the biological role of molecular hydrogen has experienced a long process, and is yet to be complemented.

Molecular hydrogen used to be thought of as an inert gas in the biological sense. Some early researchers reported the effects of high pressure (~1 MPa) hydrogen on treating certain diseases [1,2], yet received little attentions, probably because of the difficulty in using high pressure hydrogen in the hospital. Later on 2007, Ohsawa et al. [3] presented an experimental study in cell-free systems in a rat middle cerebral artery occlusion model, showing the selective reduction of

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Nomenclature

A	parameter in P–C–T equation
B	parameter in P–C–T equation, K
C_d	reaction rate constant, s^{-1}
C_p	specific heat capacity, $J\ kg^{-1}\ K^{-1}$
C_V	flow coefficient
E_d	activation energy for dehydriding reaction, $J\ mol^{-1}$
F	volumetric force term, $N\ m^{-3}$
h	heat transfer coefficient, $W\ m^{-2}\ K^{-1}$
ΔH	reaction enthalpy, $J\ mol^{-1}$
$\dot{m}$	mass source term of reaction, $kg\ m^{-3}\ s^{-1}$
M	molecular weight, $g\ mol^{-1}$
$\vec{n}$	normal vector
p	pressure, MPa
q_h	heat flux exerted on the hydrogen storage canister, $W\ m^{-2}$
q_m	outlet mass flow rate of H_2, $kg\ s^{-1}$
q_s	setting value of hydrogen mass flow rate, $kg\ s^{-1}$
q_v	volume flow rate at normal state, $m^3\ s^{-1}$
r	r-coordinate, mm
R	rangeability of valve
R_g	universal gas constant, $J\ K^{-1}\ mol^{-1}$
ΔS	reaction entropy, $J\ mol^{-1}\ K^{-1}$
t	time, s
T	temperature, K
$\vec{U}$	velocity vector, $m\ s^{-1}$
v	vertical component of hydrogen gas velocity, $m\ s^{-1}$
W	mass, kg
x	pressure drop ratio
X	reacted fraction
Y	expansion factor
z	z-coordinate, mm
Z	compressibility factor

Greek symbols

δ	proportional band
ε	volume fraction
η	dynamic viscosity, Pa s
θ	hysteresis factor in P–C–T equation
κ	permeability, m^2
κ_{dv}	dilatational viscosity, Pa s
λ	thermal conductivity, $W\ m^{-1}\ K^{-1}$
ρ	density, $kg\ m^{-3}$
ϕ	plateau flatness factor in P–C–T equation
ϕ_0	plateau flatness factor in P–C–T equation

Subscript

0	initial
b	bulk, back
eff	effective
ed	equilibrium state for dehydriding reaction
f	heat transfer fluid
g	hydrogen gas
in	integral control
max	maximum
min	minimum
v	void space in the MH bed

poisonous radicals by the molecular hydrogen under mild conditions. Since then, many follow-up studies were conducted to explore the application potential of molecular hydrogen as therapeutic gas. Encouragingly, either in the form of gas or saline solution, molecular hydrogen was confirmed effective in treating some very tricky diseases, e.g. ischemia reperfusion injury [4,5], pressure ulcer [6], early neurovascular dysfunction [7]. Since hydrogen is easily available and produces no side effects, the treatment method seems to have a bright future.

To supply hydrogen safely and reliably for therapy use, a patent-pending system was proposed by the authors [8], whose working principle is detailed in Section 2. The hydrogen is stored in the form of intermetallic metal hydride, which features compactness, good security and long-term storage. On the other hand, the relatively high price and heavy weight of the MH based hydrogen storage system seem acceptable for the stationary use in the hospital. Therefore, the proposed system is promising for practical use, supposing that the medical effects of molecular hydrogen on human body can be further understood, both qualitatively and quantitatively.

It should be noted, however, that the therapeutic effect of hydrogen is dose-dependent [3], and the existing studies were mostly conducted with the mass flow rate of hydrogen kept constant. Nevertheless, as revealed by some investigations in the literature [9–11], the dehydriding reaction, through which molecular hydrogen is discharged and used in the concerning hydrogen supply system, is generally highly transient. In other words, the reaction rate tends to change temporally due to many factors, e.g. heat transfer. Therefore, it is meaningful and interesting to check whether and how the mass flow rate of hydrogen can be controlled within certain accuracy for such a metal hydride based hydrogen supply system. In this manuscript, we established a mathematic model for the working process of the hydrogen storage canister, and a commercial package COMSOL Multi-physics 3.5a was used to solve it. The abovementioned flow control issues were discussed based on the simulation results under various heating modes and valve characteristics.

2. Working principles of the hydrogen supply system

The schematic of the hydride based hydrogen supply system is shown in Fig. 1, and the working principle is described as follows:

The hydrogen is stored in a canister (1) filled by metal hydride powders (2), and some heat exchange facilities (3) are provided for the canister, either internally or externally. Through a three-way valve (6), the hydrogen storage canister can be connected to a gas mixing chamber (9) in the downstream, or a hydrogen source (in Fig. 1 a hydrogen