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Modelling the potential of adsorbed hydrogen for use in aviation

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ABSTRACT

A novel method for modelling the amount of hydrogen in high-pressure tanks containing varying quantities of adsorbent has been extended to allow calculation of the energy density and the specific energy of the storage system. An example calculation, using TE7 activated carbon beads as an adsorbent, has been conducted over a range of temperatures and compared to alternative energy storage methods, including conventional high-pressure methods. The results indicate that adsorption of hydrogen yields a higher energy density than direct compression up to a certain pressure, which is dependent on the temperature.

A preliminary comparison shows adsorbed hydrogen to be superior to battery storage technologies for both energy density and specific energy stored, although further calculations are required to expand the system boundaries used. Adsorbed hydrogen in a range of materials resulted in much lower energy density and specific energy than standard jet fuels such as kerosene, proving that advancement in the materials is required, especially intrinsic hydrogen storage capacity, before adsorption becomes a competitive energy storage technology for aviation.

1. Introduction

Hydrogen shows great potential as an energy store as it can be produced sustainably, it has the highest energy per unit mass of any chemical fuel, it is abundant in water and biomass, and only water is produced as a by-product when releasing the stored energy. However, hydrogen has a very low energy density per unit volume which is problematic when using it as an energy vector. To make hydrogen commercially viable the volumetric density (i.e. its mass per unit volume) needs to be vastly increased, particularly for applications where low mass and low volumes are required, such as in aviation. Physisorption of molecular hydrogen (H_2) in nanoporous materials is one promising method of doing this and may improve on conventional storage methods, such as liquid H_2 at low temperature (<-33 K) or high pressure gas (up to 70 MPa). Adsorptive storage is beneficial over chemisorption (storing hydrogen chemically bonded to other elements) in that it does not require large energy inputs to recover the stored hydrogen from the adsorbent, due to the relatively weak interaction between the adsorbent and hydrogen. However, because of these weak interactions, low temperatures are required in order to store large quantities of hydrogen.

Aviation is one industry within which emissions must be rapidly reduced. Using conventional jet fuel such as kerosene results in the production of 2–3 % of all global carbon emissions [1], as well as releasing short lived gases directly into the upper atmosphere, which results in an increase in the radiative forcing values of these gases and so causing large impacts on global warming [2–4].

Hydrogen has the potential to be a cleaner, safer fuel, whilst improving performance, lowering direct operating costs, and having a more favourable availability and economic impact compared to current jet fuels [5,6]. There have been various hydrogen prototype planes such as the Tupolev Tu-155 [7], the Antares DLR-H2 [8], the Boeing phantom eye [9] and the ENFICA-FC Rapid 200-FC [10], all of which have utilised the current conventional hydrogen storage methods of compression or liquefaction.

Physisorption of hydrogen has not been used in aircraft to date due to the immaturity of the technology. The potential issue with the use of physisorption of hydrogen over direct compression is the additional requirement of the adsorbent in the tank, as aircraft require very low weight technology [11].

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Nomenclature

V_c	(cm^3) container volume
V_B	(cm^3) bulk hydrogen volume
V_D	(cm^3) displaced volume
V_T	(cm^3) total adsorbate volume
V_F	(cm^3) volume of tank containing adsorbent
V_{BI}	(cm^3) volume of bulk hydrogen in the interstitial sites
V_{BC}	(cm^3) volume of bulk hydrogen in the tank containing no adsorbent
V_{BP}	(cm^3) volume of bulk hydrogen in the pores of the adsorbent
V_S	(cm^3) skeletal volume of the adsorbent
V_P	(cm^3) open pore volume
V_A	(cm^3) adsorbate volume
f	(–) fill factor
x	(–) packing factor of adsorbent
Θ_A	(–) fractional filling of the pore
υ_P	($cm^3\ g^{-1}$) specific pore volume
m_S	(g) mass of the adsorbent
m_H	(g) mass of hydrogen
ρ_B	($g\ cm^{-3}$) density of bulk hydrogen
ρ_A	($g\ cm^{-3}$) density of adsorbate
ρ_S	($g\ cm^{-3}$) skeletal density
E_H	(MJ) energy available
m_W	(g) mass of the system
m_S	(g) mass of the adsorbent
b	(MPa^{-1}) affinity parameter
c	(–) heterogeneity parameter
Z	(–) compressibility factor
P	(MPa) pressure
P_B	(MPa) break-even pressure
M	($g\ mol^{-1}$) molar mass
R	($cm^3\ MPa\ K^{-1}\ mol^{-1}$) gas constant
T	(K) temperature

In order for the benefits of adsorptive storage of hydrogen to be quantified, there is a need for a method for calculating the amount of energy stored *via* hydrogen per unit volume and per unit mass of the system. This equation has been derived, from which the comparison between compressed hydrogen and physisorbed hydrogen can be made, and additionally can be loosely compared to other potential aircraft propulsion systems including kerosene, lithium-ion batteries and lead-acid batteries.

2. Materials and methods

All materials and methods used in this work are equivalent to those in our previous work [12].

3. Theory and calculation

3.1. The new model for a tank filled with an adsorbent

We have previously derived a method for comparing the amount of hydrogen stored in a set volume when using varying quantities of adsorbent, which can be depicted as a design curve [13]. These equations have been altered to account for a density variation within the pores of nanoporous materials, as described in our previous work [12], which we believe to be a more accurate representation of the hydrogen in the pores. The development of this model presented here includes a factor to account for the hydrogen in the intergranular space, as observed in Fig. 1, where V_C represents the volume of the container, V_B is the volume of the bulk hydrogen, V_D is the displaced volume, V_T is the total volume of the adsorbent, and V_F is the volume of the tank containing the adsorbent (V_T plus intergranular volume). The bulk hydrogen contribution can be separated into the following volumes: V_{BI} is the volume of the bulk hydrogen in the interstitial sites between the adsorbent, V_{BC} is the volume of the bulk hydrogen in the section of the container containing no adsorbent and V_{BP} is the volume of the bulk hydrogen in the pores of the adsorbent. The skeletal volume of the adsorbent including the closed pores is V_S, the open pore volume is V_P, and the volume of the adsorbate is V_A. f is the fill factor indicating the ratio of the volume of the tank containing the adsorbent to the total volume of the tank, x is the packing factor of the adsorbent, indicating the ratio of the total volume of the adsorbent to the total volume of the adsorbent plus intergranular space, Θ_A is the fractional filling of the pore i.e. the ratio of the adsorbate volume to the pore volume, and υ_P is the pore volume per unit mass of the adsorbent, m_S, after degassing.

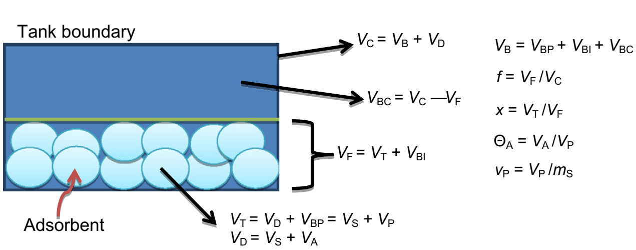

Fig. 1. Representation of the nomenclature used to calculate the amount of hydrogen in a tank containing adsorbent.

Using this nomenclature, the following derivation for the total amount of hydrogen within a tank containing adsorbent is achieved,

$$m_H = \rho_B V_B + \rho_A V_A \quad (1)$$

where m_H is the mass of hydrogen, ρ_B is the density of bulk hydrogen and ρ_A is the density of the adsorbate:

$$m_H = \rho_B V_{BC} + \rho_B V_{BI} + \rho_B V_{BP} + \rho_A V_A \quad (1a)$$

$$m_H = \rho_B (V_C - V_F) + \rho_B (V_F - V_T) + \rho_B (V_P - V_A) + \rho_A V_A \quad (1b)$$

$$m_H = \rho_B V_C (1 - f) + \rho_B (f V_C - x f V_C) + \rho_B (V_P - V_A) + \rho_A V_A \quad (1c)$$

$$m_H = \rho_B V_C (1 - f x) + \rho_B \upsilon_P m_S (1 - \Theta_A) + \rho_A \upsilon_P m_S \Theta_A \quad (1d)$$

where υ_P is the specific pore volume. The mass of the adsorbent can be varied and so the following substitution is required

$$m_S = \rho_S V_S \quad (2)$$

where ρ_S is the skeletal density

$$m_S = \rho_S (V_T - V_P) \quad (2a)$$

$$m_S = \rho_S (V_T - \upsilon_P m_S) \quad (2b)$$

Rearranging Eq. (2b) gives

$$m_S = \frac{V_T \rho_S}{1 + \upsilon_P \rho_S} \quad (2c)$$

Substituting Eq. (2c) into Eq. (1d) gives

$$m_H = \rho_B V_C (1 - f x) + \rho_B \upsilon_P \frac{V_T \rho_S}{1 + \upsilon_P \rho_S} (1 - \Theta_A) + \rho_A \upsilon_P \frac{V_T \rho_S}{1 + \upsilon_P \rho_S} \Theta_A \quad (3)$$