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Research paper

Numerical simulation of fast charge of natural gas on activated carbon in conjunction with variable velocity

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HIGHLIGHTS

- The fast charge of methane in activated carbon is optimized.
- The gas adsorption is described by the mass, momentum, and energy balances.
- The effect of pressure drop and inlet temperature on charge dynamics is investigated.
- The results show that the mass transfer in the adsorbent has a great impact on the gas speed during the adsorption process.

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ABSTRACT

This paper presents a numerical investigation of the dynamics of adsorption of pure methane in a packed column with activated carbon in order to optimize the fast charge process in adsorbed natural gas vessels. The investigation utilizes two main models. A model for the column that is described by mass, momentum, and energy balances in conjunction with the ideal gas equation and the monodisperse model for the adsorbent. The resulting equations are discretized by the finite-volume method. Several main findings were revealed from this investigation. Firstly, numerical results show that the mass transfer in the adsorbent has a great impact on the gas speed during the adsorption process. Secondly, the adsorbed mass of the column increases by reducing the gas inlet temperature. Lastly, it was observed that the saturation time in the column is a function of the applied pressure drop. In this case, the saturation time in the column varied between 500 and 1000 s. This range is considered satisfactory for the fast filling process of the column.

1. Introduction

Recently, the main concern of researchers and environmentalists seem to center around the emissions of gases that cause global warming. That is, the carbon dioxide that results from burning fossil fuels and deforestation. In order to reduce the high levels of carbon dioxide in the atmosphere, the use of clean fuels in addition to more efficient techniques for carbon capture have been proposed. In this context, natural gas (NG) emerges as a great alternative for application in automotive vehicles and industrial processes, since this fuel is available in large quantities and combustion gases from NG are much cleaner than other fossil fuels. However, there are several drawbacks in using NG in large-scale applications. One drawback is related to the high cost of storing and transporting natural gas [1]. Natural gas consists of about 95% methane – a gas that cannot be liquefied at ambient temperature since its critical temperature is about 191 K. Therefore, the technology of liquefied natural gas (LNG) is not convenient for application in automotive vehicles due to the cost and complexity of storage that uses cryogenic temperatures in the gas liquefaction process. Another technology used for the storage of natural gas is compressed natural gas (CNG). The main disadvantage of this technology is the high pressure used to store NG (20 MPa), which results in heavy and expensive tanks in order to support such high pressures [2].

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A promising technology for storing natural gas is adsorbed natural gas (ANG). Currently, microporous-activated carbon is the best adsorbent to be used in ANG vessels [3]. The adsorption of gas allows a reduction in pressure storage (3,5-4 MPa), while also having a storage capacity similar to that obtained with CNG. The reduction in the storage pressure allows the use of more efficient tanks in addition to reducing the cost of compressing the gas [4]. Pressure reduction would allow for lighter materials for manufacturing the tank, such as aluminum, as well as the use of different geometries other than cylindrical, which provides a greater versatility in the design of the storage system. Yet, two major drawbacks exist that currently prevents ANG technology to be used on a large scale. The first is related to the shape of the adsorption isotherm which prevents a linear response of the storage capacity relative to the pressure. The second is related to the negative impact of heat of adsorption in the process of charging and discharging the system.

During the charging step, the bed temperature increases, and therefore, the adsorbed mass decreases. Inversely, the bed temperature decreases and the mass retained in the vessel increases during the discharge. Ridha et al. [5] and Ridha et al. [6] showed these effects of the charging and discharging processes of ANG vessels, respectively. The heat of adsorption, during the process of charging and discharging, reduces the adsorption/desorption capacity of the ANG system; this reduction can reach nearly 25% of the capacity of the system under isothermal condition [7,8].

In order to minimize the effects of heat of adsorption on performance of ANG vessels, various solutions have been proposed in the literature [8–11]. However, these solutions require the insertion of accessories in the storage system that reduces the space available for gas storage and increases the design complexity of the vessel. The proposed solutions have serious limitations regarding the dissipation of the heat of adsorption due to the low thermal conductivity of the adsorbent. Santos et al. [12] and Santos et al. [13] suggested an approach to overcome the heat of adsorption for loading and discharging processes in ANG vessels. The approach uses forced convection between the gas and the adsorbent in order to increase the heat dissipation of the adsorption vessel, which reduces the negative impact of the adsorption heat on the performance of ANG vessels.

A crucial assumption in the study of ANG systems is that the natural gas consists of pure methane. In this case, large variations in the gas velocity and pressure are observed in the bed due to the intense mass transfer in the adsorbent. These variations affect the displacement of the mass and temperature fronts, and consequently, the saturation time of the ANG vessel. Taking into account the momentum balance in the modeling process is fundamental to the correct description of the charge dynamics of the ANG vessel. In this work, the fast charge of natural gas in a column of activated carbon, open on both sides, is investigated in order to optimize the adsorbed natural gas into the activated carbon column. A detailed discussion is presented to improve Santos et al. [12] analysis, where the assumption of constant velocity was considered in the development of the numerical model. In particular, the mass transfer and friction effects on the velocity and pressure profiles during the fast charge process will be a focus of discussion.

2. Mathematical model

Fig. 1 shows the configuration investigated. In order to perform the analysis, a single column filled up with activated carbon and open on both sides is considered. The natural gas flows from one side of the column to the other. The constitutive equations are based on the mass, momentum, energy balances [14,15], and the ideal gas equation. Next, we show the model along with the initial and boundary conditions for the column and the adsorbent material.

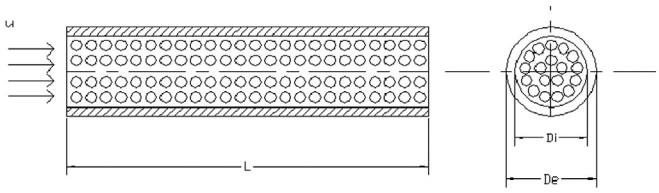

Fig. 1. Activated carbon-packed column.

2.1. Column model

For the column model, the following assumptions are considered:

- Radial effects are neglected.
- Natural gas is constituted of pure methane.
- Sorbate behaves as an ideal gas.

Under the above assumptions, the column model is constituted by the continuity equation, momentum equation, energy equation, and the ideal gas equation. The respective equations follow below:

$$\frac{\partial \rho_f}{\partial t} + \frac{\partial}{\partial x}\left(\rho_f u\right) = -\frac{1-\varepsilon}{\varepsilon}\frac{\partial \overline{q}}{\partial t}, \tag{1}$$

$$\frac{\partial}{\partial t}\left(\rho_f u\right) + \frac{\partial}{\partial x}\left(\rho_f\, u\, u\right) = -\frac{\partial p}{\partial x} - \frac{150\mu}{d_p^2}\frac{(1-\varepsilon)^2 u}{\varepsilon^2} - \frac{1.75\rho_f}{d_p}\frac{(1-\varepsilon)u^2}{\varepsilon}, \tag{2}$$

$$\frac{\partial}{\partial t}\left(\rho_f T_f\right) + \frac{\partial}{\partial x}\left(\rho_f\ u\ T_f\right) = \frac{\partial}{\partial x}\left(\frac{\lambda_f}{cp_f}\frac{\partial T_f}{\partial x}\right) + \frac{6h_p}{d_p}\frac{(1-\varepsilon)}{\varepsilon cp_f}\left(T_s - T_f\right) + \frac{2U_g\left(T_\infty - T_f\right)}{\varepsilon R_i cp_f}, \tag{3}$$

$$\rho_f = \frac{p}{R_g T_f}, \tag{4}$$

where ρ_f is the density of gas (kg/m^3), p is the pressure (Pa), T is the temperature (K), λ is the thermal conductivity (W/m K), ε is the bed porosity, R_g is the ideal gas constant (J/kg K), c_p is the specific heat at constant pressure (J/kg K), d_p is the pellet diameter (m), U_g is the overall heat transfer coefficient (W/m^2 K), R_i is the internal column radius (m), and subscript f denotes the fluid phase.

In order to study the adsorption process, it is assumed that an overcooled gas stream with constant temperature (T_{in}) and pressure (p_{in}) is suddenly forced into an activated carbon-packed column, which is initially saturated with gas at a temperature (T_0) and a pressure (p_0). The initial conditions used in the adsorption step are the last values of temperature and pressure obtained at the ending of the desorption process. The outlet pressure is kept at p_0. Details of the methane desorption in activated carbon can be found in Santos et al. [13]. Therefore, the following initial and boundary conditions are applied to the bed equations:

$$p(x, t=0) = p_0; \quad T_f(x, t=0) = T_0; \quad u(x, t=0) = u_0, \tag{5}$$