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Research paper

Regression equations for predicting discharge performance of adsorbed natural gas storage systems

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HIGHLIGHTS

- Theoretical analysis of adsorbed natural gas storage reactors is carried out.
- The governing equations in non-dimensional form are solved numerically.
- Based on the results, regression equations for discharge are proposed.
- The regression equations cover a wide range of design and operating conditions.
- Proposed equations are useful in quick estimation of system performance.

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ABSTRACT

Simple regression equations are proposed to predict the discharge performance of adsorbed natural gas storage systems consisting of tubular reactors filled with MAXSORB III. The regression equations are obtained for discharge time and heat transferred in terms of few relevant and statistically significant non-dimensional numbers. The data required for regression analysis is generated by numerically solving the transient heat and mass transfer equations of adsorbed natural gas (ANG) storage system undergoing discharge under constant flow condition. The regression equations are compared with the values obtained from numerical simulations and it is observed that the difference between the two is well within 25% for all the parameters. Using the correlations it is possible to quickly estimate important performance parameters such as delivery capacity and energy to be supplied for a variety of tubular ANG reactors filled with MAXSORB III.

1. Introduction

A large number of studies are carried out in the past on developing suitable adsorbents for natural gas adsorption. Many researchers have carried out both theoretical and experimental studies on some newly developed activated carbons suitable for NG storage. Sun et al. [1] have measured the methane uptake on HKUST (Copper benzene-1,3,5-tricarboxylate,Cu-BTC MOF) for temperatures ranging from 120 K to 300 K and pressure up to 10 bar. They have also simulated the methane uptake data and its density distribution on HKUST-1 employing GCMC (grand canonical Monte Carlo) simulation and compared with experimental data. As Metal-organic frame work is a new class of adsorbent, Mason et al. [2] have presented a review on most important properties of six metal organic–frame works and an activated carbon, with a range of surface areas, pore structure, and surface area chemistries representative of the most promising adsorbent for methane storage. Bagheri and Abedi [3] have experimentally studied the methane adsorption on corn cob based activated carbon at four different pressures and two different temperatures. The maximum volumetric storage capacity for this activated carbon is found to be 160 (v/v) at 298 K and 1500 psi. Wang et al. [4] have measured the desorption characteristics of methane from Maxsorb II over a temperature range of 281–343 K and pressure up to 1.2 MPa and fitted the desorption data to Toth and Dubinin–Astakhov isotherm models. The Henry's law coefficients and their relations to isosteric heat of adsorption are also examined. Chakraborty et al. [5] have developed a thermodynamic frame work to capture the relation between the pore specific surface areas with the enthalpy of adsorption, which can be used as a guideline in developing advanced adsorbent and adsorbate pair. The important conclusion

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Nomenclature

A	area, m^2
A_r	area ratio
a	concentration, kg/kg
Bi	Biot number
C	specific heat capacity, J/kg K
C_p	specific heat at constant pressure, J/kg K
E	characteristic energy, J/mol
E_a	activation energy, J/mol
Fo	Fourier number
h	heat transfer coefficient, W/m^2 K
K_{so}	pre-exponent constant in the equation of kinetics of sorption, s^{-1}
L	length of the reactor, m
m	mass, kg
M	molecular weight, kg/kmol
N	number of grid points
$\dot{m}^*_{g,s}$	non-dimensional specific flow rate
n	index of isotherm equation
P	pressure, N/m^2
P_{no}	pressure number
P	p-value of the regression analysis
Q_{gen}	generation number
Q_{in}	non-dimensional heat transfer
Q	dimensional heat transfer, kJ
r	radius of adsorbent bed, m
R	non-dimensional radius
S	parameter that accounts for space occupied by enhancement material
R_u	universal gas constant, J/mol K
R_g	gas constant, J/kg K
T	temperature, K
t	time, s
th	bed thickness, m
U	overall heat transfer coefficient, W/m^2 K
v	specific volume, m^3/kg
V	volume, m^3
W_o	the limiting volumetric adsorbate uptake, m^3/kg
y	mass ratio, kg/kg
Z	compressibility factor

Greek symbols

ΔH	isosteric heat of reaction, J/mol
θ	non-dimensional temperature
ε	porosity
ρ	density, kg/m^3
λ	thermal conductivity, W/m K
η	efficiency
τ	rate constant parameter

Subscripts

a	adsorbed
b	boiling, bed
cr	critical
eff	effective
eq	equilibrium
f	fluid, fin, final
g	gas
gr	graphite
i	inner, initial
max	maximum
min	minimum
o	outer
p	particle
r	radial
ref	reference
s	saturation, specific, steel, solid
t	total
w	wall

Superscripts

*	non-dimensional

from this study is that the adsorbents with highly porous surfaces possess lower isosteric heats of adsorption during methane or hydrogen adsorption at room temperature. Birkett and Do [6] have reported a new method to determine the micropore size distribution by using adsorption data of methane in activated carbon under supercritical condition. This new method only uses information of the amount of methane loaded into the adsorption cell and the equilibrium pressure at the end of each dose and avoids the need of determining the void volume. Biloe et al. [7] have shown that the microporous properties of the activated carbon as well as its heat and mass transfer properties can reduce dramatically the performance of the ANG system. Using the Dubinin relation, Biloe et al have shown that the activated carbon must have highly microporous potential, very narrow microporosity, and an average micropore width of 1.5 nm–2.5 nm for charge and discharge steps respectively.

A large number of studies are carried out in the past on heat and mass transfer aspects of adsorbed natural gas (ANG) reactors suitable for compact storage of natural gas [8–17].

However, generalization of the results that allow the prediction of performance of ANG reactors under different design and operating conditions are not available in open literature. Using Buckingham-Π theorem Sacsa Diaz and Sphaier [18] have identified meaningful dimensionless groups required for the analysis of ANG reactors. They used the Langmuir isotherm model and did not consider kinetics of mass transfer. da Silva and Sphaier [19] have developed a dimensionless lumped formulation for performance assessment of adsorbed natural gas storage system. Sahoo and Ramgopal [20] have formulated a normalized heat and mass transfer model for constant pressure charging of an adsorbed natural gas storage system and developed regression equations for charging time, energy removed as well as maximum bed temperature. For on-board applications, the knowledge of discharge time, delivery capacity and the energy required to deliver the natural gas are important. However, accurate prediction of these parameters requires solution of the coupled partial differential equations that describe the mass, momentum and energy conservation equations. As this is time consuming, it would be useful if a simpler method is available for predicting the discharge characteristics under different design and operating conditions. In the present paper simple regression equations in dimensionless form are presented to predict the performance of tubular ANG reactors subjected to constant flow discharge.

Langmuir is the simplest of all the isotherm models, which describes monolayer type of adsorption [21–23]. The Langmuir model presumes homogeneous adsorbent surface with constant heat of