



Numerical modeling and experimental validation of fractional heat transfer induced by gas adsorption in heterogeneous coal matrix



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ABSTRACT

Despite one fundamental issue in the adsorption theory of coalbed methane, little is known about the thermodynamic properties of gas adsorption in a porous coal matrix. In this work, considering the heterogeneity of pore structure and the exothermic characteristics of gas adsorption, a fractional heat conduction model with an unsteady volumetric heat source is proposed to study the heat transfer process induced by gas adsorption in a heterogeneous coal matrix. The heat conduction equation with a fractional time derivative is discretized by using an implicit numerical method based on the generalization of a standard finite-difference scheme. First, to validate the fractional heat conduction model, gas adsorption experiments on a microcalorimeter were carried out on 5 g coal samples of 0.3 mm diameter at 25 °C. The experimental heat flux with initial adsorption pressures of 3.23 bar, 5.83 bar and 9.77 bar increases rapidly from zero to peak values of 7.17 mW, 12.05 mW and 16.81 mW in less than 7 min (i.e., fast thermal diffusion stage) and then decreases slowly to zero again in approximately 2 h (i.e., slow thermal diffusion stage). It is revealed that for all tested gas pressures the fractional heat conduction model with a fractional order $\alpha = 0.86$ can reproduce the experimental process of heat flux with better accuracy than the Fourier law-based model (i.e., $\alpha = 1$), suggesting that anomalous thermal diffusion is the governing heat transfer process of gas adsorption in the coal matrix. Second, the spatial distribution and temporal evolution of temperature patterns with different model parameters are numerically simulated. It is found that the time to reach the peak temperature decreases from 760 s at the center of the coal particles to 490 s at the boundary. Finally, the parametric sensitivity of the thermodynamic properties of gas adsorption such as temperature, heat flux and integral adsorption heat is discussed in detail. Particularly, it is shown that as one of the most important thermodynamic parameters, the integral heat is very sensitive to the fractional order α . In the case of 3.23 bar, if α increases from 0.75 to 1, while other model parameters remain unchanged, the integral heat could be enhanced from 1.1 J/g to 8.5 J/g.

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1. Introduction

With the increasing development of coalbed methane (CBM) and carbon dioxide sequestration for enhanced coalbed methane (CO₂-ECBM) recovery, gas storage and transport in coal reservoirs has received considerable attention [1–3]. Coal seams differ significantly from conventional gas reservoirs in that most gas in coal seams is originally adsorbed on the surface area of the porous coal matrix rather than stored as free gas [4]. Consequently, gas adsorption and desorption within the porous coal matrix plays a

dominant role in the geological and engineering evaluation of coalbed methane resources, including the determination of methane content of in situ coal seams and the extent of gas recovery for commercial exploitation [5,6].

Studies on the dynamic behavior of gas adsorption in the porous coal matrix have been published extensively in the literature and include theoretical, experimental and numerical methods. Generally, gas adsorption is considered to be concentration-driven, which can be described by diffusion theory [7]. In terms of the pore diameter of coal matrix and the mean free path of gas molecules, three different diffusion mechanisms were identified for gas adsorption in porous coal matrix, including bulk diffusion, Knudsen diffusion and surface diffusion [8]. Most experimental works investigated the adsorption isotherms and their relationships with coal properties and experimental conditions [9], such as pore

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Nomenclature

T	coal temperature, °C	τ	rate constant, s^{-1}
T_0	temperature constant, °C	κ	thermal diffusivity, m^2/s
Q_s	volumetric heat source, W/m^3	M	amount of adsorbed gas at time t , kg/m^3
H_{int}	adsorption heat, J/kg	M_∞	amount of adsorbed gas at equilibrium, kg/m^3
H_{total}	total heat released, J	S	total surface area of coal particles, m^2
c_p	specific heat capacity, $J/kg \cdot K$	D	fractional thermal diffusivity $\kappa \sigma_t^{1-\alpha}$, m^2/s^α
q	flux of heat conduction, J/m^2	P	adsorption parameter
q_{max}	maximum heat flux, J/m^2	t	temporal coordinate, s
u	excess temperature $T - T_0$, °C	r	radial coordinate
u_{max}	maximum temperature, °C	r_0	radius of coal particles, m
N_r	mesh number of spatial domain	p	gas pressure, Pa
N_t	mesh number of temporal domain	p_0	initial pressure, Pa
Δt	discrete time step	p_∞	equilibrium pressure, Pa
Δr	discrete space step	\tilde{p}	normalized pressure
		m	total mass of coal, kg
<i>Greek symbols</i>			
$\Gamma(\cdot)$	Gamma function	<i>Subscript</i>	
ρ	coal density, kg/m^3	i	discrete time index
λ	heat conductivity, $W/m \cdot K$	j	discrete space index
α	order of fractional derivative	0	initial
λ_α	fractional heat conductivity, $J/m \cdot K \cdot s^\alpha$	∞	equilibrium
σ_t	auxiliary parameter, s		

structure [10], temperature [11] and moisture [12]. Furthermore, several mathematical models have been proposed to reproduce the experimental data and predict the quantity of desorbed gas, such as the equilibrium model [13], unipore diffusion model [14] and bidisperse diffusion model [15].

In addition to mass transfer in the process of gas adsorption, heat transfer induced by gas adsorption occurs simultaneously. Gas adsorption by coal is essentially the interaction between the molecular structure of coal and gas molecules, which is normally an exothermal process [16]. Thus, heat transfer is an intrinsic characteristic of the gas adsorption process, and directly reflects the energy state of gas molecules on the surface adsorption field of coal. Experimentally, Taraba [17] measured the heat of adsorption by studying the competitive adsorption of methane and carbon dioxide. Using a microcalorimeter, Zhou et al. [18] measured the adsorption microheat of coalbed methane on coal with different chemical functional groups. Theoretically, Bülow et al. [19] proposed a method for calculating the heat of adsorption by using the Clausius-Clapeyron equation. Using the Dubinin-Radushkevich equation, Day et al. [20] calculated the adsorption heat of carbon dioxide on coal. Gawor and Skoczylas [21] established a heat conduction equation for the process of gas adsorption and discussed the kinetics of adsorption rate of carbon dioxide on coal. These studies, excluding [21], mainly concentrated on the estimates of adsorption heat under adsorption equilibria, but until now little is understood about the process of heat transfer. One of the difficulties in modeling the heat transfer process induced by gas adsorption is how to establish an appropriate governing equation for heat balance in the coal matrix. This is because coal has a heterogeneous pore structure with pore size varying from a few angstroms to over a micrometer [10].

Recently, partial differential equations with fractional derivatives have been successfully applied to thermal processes in physics, chemistry, geology, etc. [22–25]. Particularly, the application of fractional derivatives allows for more accurate results in modeling thermal systems based on diffusion processes and for those with complex structure. Zheng et al. [26] proposed an improved heat conduction model with a Riesz fractional Cattaneo-Christov flux that considered the effects of relaxation time, fractional

parameter and convection velocity. Povstenko [27] and Jiang and Xu [28] proposed a type of fractional Fourier model that considered the nonlocal time-dependence between the heat flux vector and the temperature gradient. Sierociuk [29] presented results of modeling the heat transfer process in heterogeneous media by using fractional calculus. Based on the fractional Fickian law, Cheng and Ma [30] used a diffusion model to study the fractal heat and mass transfer in a fluidized bed. Suzuki et al. [31] developed a fractional heat transfer model to describe the anomalous heat diffusion in porous and fractured reservoirs.

Overall, in sharp contrast with the rich knowledge on mass transfer during gas adsorption, the study of heat transfer induced by gas adsorption is far less advanced, although it is of great significance to the deep understanding of adsorption characteristics [32]. Motivated by this fact, the purpose of this work is to develop a heat conduction model with a fractional derivative to study the heat transfer process of gas adsorption in a heterogeneous porous coal matrix. Numerical modeling and laboratory experiments are conducted to validate the fractional model. Furthermore, the temporal evolution and spatial distribution of temperature patterns in the coal matrix and the effects of model parameters on the thermodynamic properties of gas adsorption are discussed.

2. Modeling heat transfer with fractional derivative

2.1. Mathematical formulation of fractional heat conduction

As mentioned in the introduction, gas adsorption by coal is not only a mass transfer process but also a heat transfer process, i.e., gas adsorption is essentially a spontaneous and exothermic process. In this work, the changes in temperature in the coal matrix induced by gas adsorption are assumed to be governed by the theory of heat conduction. It is also assumed that (i) coal particles are spherically symmetric in shape; (ii) the convective flow in macropores is negligible; (iii) the heat released during the adsorption process can be treated as an internal heat source.

The governing equation of heat conduction with a heat source is expressed as

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