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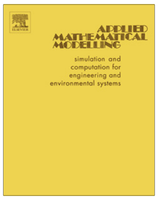

Analytical modeling of non-Fickian wave-diffusion of gas in heterogeneous media

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The coauthor dedicates this paper to the memory of David Ross Boyd Professor Emeritus Maurice L. Rasmussen, a great mathematician, a creative and practical engineer, an outstanding researcher, and a dedicated teacher.

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ABSTRACT

An isothermal transient-state non-Fickian diffusion model is developed and analytically solved for description of gas dissolution in locally heterogeneous media suddenly exposed to a high pressure gas. The full-, short-, and long-time analytical solutions are used to establish the significance of the non-Fickian gas dissolution in heterogeneous media compared to the Fickian diffusion assumption. Parametric studies are carried out by means of the special analytical-solutions obtained for gas transport in the semi-infinite and finite-thickness heterogeneous media involving a delay time. The profiles of concentration and diffusion flux obtained for the non-Fickian wave-diffusion case are compared with the Fickian pure-diffusion case. The initial propagation of a right-running wave and its reflection from the wall are illustrated for the concentrations and diffusion fluxes. The small-time behavior is shown to be inherently wave-like and the discontinuity wave front propagates into the medium with the speed decreasing with time. For small times, the differences between the wave- and pure-diffusion cases are found to be significant depending on the magnitude of the delay time. For sufficiently large times, the wave behavior dies out and the wave solutions approach the equilibrium pure-diffusion solutions, except very near the decaying wave front. The formulations presented in this paper are of practical importance because they can be instrumental in determination of the diffusivity, interface surface mass-transfer coefficient, and rate of dissolution of gases in heterogeneous medium. A parameter estimation method is also proposed and elaborated for estimation of the diffusion and interface surface mass-transfer coefficients from measured pressure decay data.

1. Introduction

Modeling of gas dissolution in a locally heterogeneous medium is a complicated task which results with wave diffusion because of non-Fickian transport involving time delay. Various examples of practical importance can be found in the natural and engineering systems where the non-Fickian effects should be considered for accurate description and proper modeling [1–4]. For example, Das [5] emphasizes that the behavior of some systems such as the Brownian species motion in a potential field, the ionic species diffusion in superionic conductors under inertial effect, and the neutron diffusion in nuclear reactors,

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Notation

A	cross-sectional area of the test tank, L^2
D	gas diffusivity in the heterogeneous medium, L^2/T
c	gas mass concentration of the heterogeneous medium, M/L^3
H	thickness of the gas column, L
J	gas mass flux, M/L^2/T
k	interface mass-transfer coefficient, L/T
L	thickness of the heterogeneous medium, L
M	molecular weight of gas, M/mol
p	pressure, M/L/T^2
Q	cumulative gas mass, per unit cross section area, dissolved in the heterogeneous medium, M/L^2
R	universal gas constant, ML^2/mol/θ/T^2
x	distance measured from the gas–heterogeneous medium interface into the heterogeneous medium, L
t	time, T
T	temperature, θ
x	distance measured from the gas–heterogeneous medium interface, L
v	$\sqrt{D/\tau}$, wave speed of sound, L/T
V	volume, L^3
w	gas mass fraction of the heterogeneous medium, dimensionless
Z	real-gas deviation factor, dimensionless

Greek

β	isothermal coefficient of expansion, dimensionless
τ	delay time, T
ρ	density, M/L^3
λ	root of Eq. (3.21), dimensionless
ϕ	fugacity coefficient of the dissolving gas in the heterogeneous medium, dimensionless

Subscripts

D	dimensionless
g	gas
LT	long-time
ST	short-time
o	initial or reference state

Superscripts

*	equilibrium state

and the associated species fluxes at absorbing boundaries, can be described adequately by a non-Fickian type diffusion equation.

The conventional Fickian law of diffusion describes the spontaneous transport of species in a carrying-medium because of concentration gradients under the conditions of local thermodynamic equilibrium. A medium is considered at local thermodynamic equilibrium only when its constituents are at equilibrium with each other. This requires the fulfillment of two critical conditions. First, a medium under external factors should be able to approach equilibrium much faster than its macro parameters and, second, the relaxation to local equilibrium should occur sufficiently faster than relaxation to global equilibrium [2,3]. Thus, the conventional Fickian model cannot describe a wave-like transfer of species mass by diffusion involving a time delay (relaxation) in heterogeneous medium because often these conditions are not fulfilled. The relaxation time induces traveling jump discontinuities in diffusing species mass concentration profiles. Such behavior has been observed in various non-Fickian transfer processes [6]. However, the non-Fickian conditions are mostly prevalent for short-times but disappear later for long-times as attested by the analyses carried out by Chen and Liu [7] and in the present paper.

The internal structure of some heterogeneous medium may cause considerable retardation in the flux of diffusing species because it requires a certain amount of time, referred to as delay or relaxation time, in order to attain a local thermodynamic equilibrium. Under such conditions, attaining local thermodynamic equilibrium is not an instantaneous but a gradual process because of delay in the flux caused by the different scales (for example, nano, micro, or medium types) of the various internal features existing in heterogeneous medium, such as pointed out by Civan and Sliepcevich [8] and Civan [9] for freezing and thawing of moist soils. Consequently, several studies, including by Abarzhi [3] and Liu et al. [10], have demonstrated that the conventional Fickian law of diffusion is incapable of describing the diffusion phenomenon in locally nonequilibrium medium. For example, the natural and synthetic fibrous materials have been reported to indicate sharp fronts in dye

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