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A model for the flow of gas mixtures in adsorption dominated dual porosity reservoirs incorporating multi-component matrix diffusion
Part I. Theoretical development

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Abstract

A matrix-fracture transfer function for multi-species gas flow with adsorption behavior is presented. This transfer function is developed from the extended Fick's law and therefore the coupling effect of mutual-diffusivity is included in the representation. The transfer function is formulated based on an *exac*t formal solution of a set of linear partial differential equations for matrix blocks with regular geometry, and is expressed in the form of a series expansion with history-dependent integrals. This series, at first order, reduces to a simple algebraic expression that is of an equivalent computational efficiency in comparison with the extended Warren–Root model in which the mutual-diffusion effect is not present.

The presented transfer function is compared with the Warren–Root relationship and it is shown that the Warren–Root model is a limiting case of the new model. It is also shown how the new model can be applied to reservoirs where gas is stored within the porosity rather than as an adsorbed phase.

Keywords: Gas reservoir; Matrix-fracture transfer function; Gas adsorption; Multi-species diffusion; Porous medium; Reservoir simulation

1. Introduction

Gas flow in certain types of geological formations may involve two physically different but coupled migration processes; one is for larger scale distributed networks of natural fractures, and the other is for much finer porous structures of local matrix blocks between the fractures (Kolesar and Ertekin, 1986; Gray, 1987; Shi and Durucan, 2003, etc.). A common approach to representing these dual-porosity media is to assume that Darcy-flow is the dominant mechanism within the fracture networks and that diffusive transport dominants the matrix. That is, the movement of gas through the fractures can be described by Darcys' law and driven by pressure gradients, whilst gas transport within the matrix blocks is a diffusion process which may involve several different mechanisms, subject to the pore size and gas properties (Shi and Durucan, 2003). For the diffusion process the gradient of gas concentration for each species, rather than total pressure, is the primary driving force. In addition, in certain types of the dual-porosity media, such as coal, gases within the matrix may be stored as an adsorbed phase such that the adsorption behavior also plays an important role in the flow process.

Many existing approaches used for gas flow in dual porosity media concern that only one species is present and have been developed following the concept proposed by

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Barenblatt and Zheltov (1960) (Warren and Root, 1963; de Swann, 1977; Najurieta, 1980; Moench, 1984; Zimmerman and Bodvarsson, 1989; Chen, 1990; Dykhuizen, 1990; Zimmerman et al., 1993; Lim and Aziz, 1995; Choi et al., 1997; Civan and Rasmussen, 2001; Rangel-German and Kovscek, 2006, etc.). Of these the Warren–Root model (Warren and Root, 1963) is the classic approach and has been widely adopted for oil and gas reservoir simulation and groundwater contaminant transport.

For multi-species gas flows in dual-porosity media with adsorption behavior, as is the case of enhanced coalbed methane recovery (ECBM) or CO_2 sequestration in coal, an extension to the Warren–Root model is used with a pseudo steady-state assumption of adsorption on the surfaces of matrix blocks (Kolesar and Ertekin, 1986; Kolesar et al., 1990a,b). With this approach, the Warren–Root model is applied to each individual component and, for each component representation, an independent constant, called characteristic "adsorption time" or "diffusion time", is introduced. Such a representation can be written as,

$$Q_i = -\frac{\mathrm{d}\bar{C}_i}{\mathrm{d}t} = -k_\mathrm{s}\frac{C_i^\mathrm{s} - \bar{C}_i}{\tau_i}, \quad (i = 1, 2, 3, \cdots, N_\mathrm{C}), \tag{1}$$

where Q_i is the exchange rate of the gas species i between the fractures and matrix, C_i is the concentration of gas species i, $\bar{C}_i$ is its mean value within a matrix block, and C_i^s denotes the concentration of component i adsorbed on the boundary of a matrix block, k_s is known as the shape factor (Zimmerman et al., 1993; Lim and Aziz, 1995; Rangel-German and Kovscek, 2006, etc.) and N_C is the total number of gas species concerned. Discussion of shape factor is beyond the scope of this text, as we are only focused on the effect of multi-diffusivity in this study. Physically, the characteristic time, τ_i, in Eq. (1) can be written as $\tau_i = \frac{a_\mathrm{M}^2}{\tilde{\mathrm{D}}_\mathrm{M}^{(i)}}$, $(i = 1, 2, 3, \cdots N_C)$, where a_M is an effective characteristic length associated with the matrix block concerned (e.g., Zimmerman et al., 1993; Zimmerman and Bodvarsson, 1995; Lim and Aziz, 1995; Lu and Connell, 2006, etc.), and $\tilde{D}_\mathrm{M}^{(i)}$ is the effective diffusion coefficient of species i, which will be further addressed in the following sections.

However Eq. (1) assumes that for a multi-species gas flow there are no interspecies interactions on the diffusion process. In fact, for a general multi-species diffusion process in a porous matrix, the transport of gases follows the extended classical Fick's law which can be described by (Allen et al., 1988)

$$\phi_m \rho_i \boldsymbol{j}_i = -\left(\frac{\phi_m}{\Gamma}\right)\sum_{k=1}^{N_C} D_{ik}\nabla C_k, \tag{2}$$

where $\boldsymbol{j}_i$ is the diffusive mass flux, ϕ_m the porosity of the solid, ρ_i the density of component i, and Γ denotes the tortuosity of the porous matrix, while D_{ik} $(i,k = 1,2,3,\cdots, N_C)$ stands for the matrix of the molecular diffusion coefficients in the porous medium and it shall be referred to in this text as the mutual diffusion coefficients.

Eq. (2) indicates that the mass flux of a gas species during a multi-species diffusion process is not only determined by its diagonal term (main-term) and its concentration but also influenced by the other species present through the off-diagonal terms (cross-term) in $\{D_{ik}\}$. However, those off-diagonal terms of $\{D_{ik}\}$ are not present in Eq. (1). Therefore, Eq. (1) is mathematically equivalent to considering a *self-diffusion* process of each component in a porous medium merely, while the interactions among gases are omitted. Theoretically, these interactions may have, subject to specific values of those cross terms, significant impacts to the transport process of gases (Bear, 1972; Cussler, 1984).

This series of two papers present a modified dual-porosity representation, which is developed from the extended Fick's law expressed by Eq. (2) and thus includes a rigorous description of the multi-component diffusion process. This new representation is formulated in terms of solving a set of fully coupled linear multi-component diffusion equations in porous media. Therefore both the diagonal diffusion coefficients and their off-diagonal counterparts are included in the transfer function. Besides, since the presented transfer function is obtained on the basis of an *exact* formal solution, it does not give rise to additional inaccuracies due to invoking simplifications or assumptions with the relevant boundary conditions. The representation of the model is expressed in the form of a series expansion with the first term being algebraic and higher order ones being of an integral form. Thus, this transfer function, when substituted into the Darcy flow equations for fracture continua as a sink/source term, leads to a system of integro-(partial) differential equations. The differential terms of flow equations are for the Darcy flow in large fractures while integrals in time for the transport of gases within matrix blocks. Consequently, a new numerical algorithm is required to implement this model for reservoir simulations.

In this text, theoretical development of the model is presented. Important characteristics of the model are also investigated analytically and discussed here. In the second part of the study (Lu et al., submitted for publication) a numerical algorithm for the model is presented and numerical examples are demonstrated there.