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A pore network model for simulating non-ideal gas flow in micro- and nano-porous materials

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ABSTRACT

The capability to simulate real gas flow in porous materials with micro- and nano-meter-scale pores is of importance in many applications, such as gas extraction from shale reservoirs, and the design of gas-based fuel cells. A node-bond pore-network flow model (PNFM) has been developed for gas flow where it is the only fluid phase. The flow conductance equation includes the usual Darcy flow terms, and additional terms that capture the contributions from slip flow to Knudsen diffusion. With respect to the case for a non-ideal gas, the extra contributions, which are necessary, to the coefficients of the Darcy and Knudsen terms, are expressed in terms of reduced temperature and pressure, using van der Waals's two-parameter principle of corresponding states. Analysis on cylindrical pores shows that the coefficient deviates from that of the non-ideal gas case by more than 80% in the Darcy term, while between −80% and 150% in the Knudsen term, when the physical states approach to the critical state of the fluid. Although the deviations become smaller when the states are away from the critical state, they remain relatively large even at conditions relevant to practical applications. The model was applied to a pore network of a realistic 3D shale model to show slippage and Knudsen effects on the predicted permeability and the sensitivity to pore sizes. Simulations were carried out for methane under the operational conditions of typical shale-gas reservoirs, and nitrogen under the conditions of laboratory experiments. The results show that the ratio of gas and Darcy permeability correlates positively and strongly with the pore size but inversely with the gas pressure and Tangential Momentum Accommodation Coefficient (TMAC) in the slip term, which can impact gas permeability disproportionally. The results are in favour of controlling the rate of gas depressurisation to avoid early depletion in shale gas production. The methane permeability is shown to be 30% greater, relatively, than that when the ideal gas law is applied, even under normal field operational conditions, while the nitrogen permeability can only approximate the methane permeability within a certain range of field operational conditions when the slip flow is not dominating.

1. Introduction

In the energy arena, there is a need to understand and calculate the flow of gas in porous materials. This subject has been studied intensively in recent years for such purposes as predicting gas production from unconventional reservoirs, and designing gas-based fuel cells. In both of these exemplar areas of study, the crucial issue is to understand how gas passes through porous media that are dominated by pores whose sizes are in the micro- and nano-meter scales. Gas flow has long been known to behave differently in such confined spaces due to increased interactions between gas molecules and the pore-wall surface [1,2]. The physics that govern gas flow in such settings have been studied experimentally and numerically at microscopic scales (see [3] for a review). It is generally understood that gas flow may be broadly classified into one of several flow regimes, ranging from continuum, to slip, to transitional, to Knudsen diffusion [4], depending on the pore sizes, the gas properties, and other aspects that are discussed in this paper. Mathematical models of gas flow have been developed that capture the key physics of the physical phenomena that arise in these micro- and nano-porous materials [5–9].

Such microscopic or pore-scale models have been used to invert laboratory experimental results, so estimating the macroscopic properties that are the main interest in practice [10–12]. Clearly, the success of this approach critically depends on whether the laboratory experiments can be carried out under such conditions that allow inference of the in situ properties reliably and robustly. In practice, the ideal experimental conditions are difficult to achieve, and it may not be possible to obtain representative samples at

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suitable sizes. For example, it is well-known that gas shale cores are extremely difficult to preserve in their in situ conditions, as trapped gas may expand to crack otherwise intact rock samples when they are lifted to the surface, and this leads to erroneous pressure and flow-rate measurements [13]. Also, laboratory techniques are difficult to employ for small-sized samples, such as the hydrophobic microporous layer (MPL) that is inserted between the gas diffusion layer (GDL) and the catalyst layer (CL) at the cathode of a hydrogen polymer electrolyte membrane fuel cell (PEMFC). The MPL can dramatically improve water management, so enhancing the efficiency of the battery and prolonging its lifespan; however, because a MPL is only a few microns thick, its properties are difficult to measure directly [14]. For these materials, and others, there is a need to develop property estimation methods that are suited to the particulars of materials with ultra-small pores but not completely dependent on laboratory measurements.

Recent advances in high-resolution imaging technology have made it possible to characterise pores and solids, as well as the details of the pore structures of a porous material [15–18]. Using such pore-structure models, numerical simulations can be carried out to predict macro-scale phenomena, expressed in terms of transport and mechanical properties [19–22]. This so-called digital core analysis (DCA) approach has great potential to expand our database of material properties, without relying on expensive, or in some cases, impossible, laboratory measurements. Within the DCA approach, a trade-off is often needed between using full information of the pore-solid structures, or implementing full microscopic physics, in order to make the computation tractable. To simulate pore-scale fluid flow, the Navier–Stokes and Cahn–Hilliard, and LB models for two-phase fluid flow, can be applied to 3D image-based pore-structure models of only the size of a few hundred voxels in each direction even when using high-performance computers. Even for a simple reservoir-quality sandstone, the limited model size is equivalent to only a small proportion of a typical sample used in the laboratory and the model may be too small to derive reliable and robust properties.

A common approach to this difficulty is to simplify a large and detailed pore-structure model into a pore network consisting of pore nodes connected by pore bonds. Each of these elements is associated with a set of attributes that together characterise the effective geometry of the pore space it represents. The spatial location of each element is specified explicitly by its coordinates, allowing the network to capture the topology and geometry of highly irregular pore space. On such a pore network, multi-phase fluid flow may be simulated efficiently by assuming that phase displacement takes place quasi-statically by capillary pressure drives, or dynamically by considering other forces. For determining the bulk fluid flow of one phase in a network, the flow conductance needs to be calculated for each element. For two/three-phase flow under quasi-static conditions, phase displacement is determined by a set of rules derived from hydro- and thermo-dynamic principles [23]. The network-based DCA approach has been used to calculate the macroscopic flow properties for conventional reservoir rocks (e.g. coarse-grained sandstone) and carbonate rocks [24–27], as well as for GDL and CL [28]. The increasing capability to image micro-/nano-pores using nano-X-ray tomography, Focused/Broad Ion Beam milling and Scanning Electron Microscopy (F/BIB-SEM), has, in recent years, led to the potential to extend the network-based DCA technique to nano-porous materials, such as shales and MPL. However, few existing pore-network flow models are capable of simulating gas flow across the full range of flow regimes, and even fewer have the ability to deal with non-ideal gases that have pressure–volume–temperature (PVT) relationships significantly different from that of the ideal gas.

The objective of this work is to develop a pore network flow model that is capable of simulating gas flow when taking into account the effects arisen from non-Darcy flows, the slip flow, transitional flow, and Knudsen diffusion, and the differences between non-ideal and ideal gas in PVT and viscosity. Several models that claim to work across the full flow regimes are reported in the literature [4–7] and are adopted to model gas flow in applications such as gas production in shale gas reservoirs [12,29,30] and fuel cell design [14]. In this work, the model proposed by Javadpour [7], for gas flow in sub-micron and nano-meter pores, is adopted to develop the pore network flow model. That model is basically a superposition of the Darcy model, a first-order Maxwellian's slip-wall model [2,31], and a model for Knudsen diffusion [6,9,32]. Sakhaee-Pour and Bryant developed a PNFM that considers the slip flow and gas ad-/de-sorption, but not the Knudsen diffusion, and for ideal gas only [33]. Very recently, Mehmani et al. [62] developed a network model that takes into account of the slip and Knudsen effects and applied that model to study the impacts of pore geometry constraints on the gas flow in shale matrix for ideal gas only. Thus, the model described in this paper is an assembly of methods derived from prior works, augmented by consideration of non-ideal gas behaviour in non-circular pores.

Based on the adopted gas flow model that superposes the slip and Knudsen terms upon the Darcy term, full formulations of the apparent permeability and flow conductance are developed where each term is expressed explicitly, and the coefficients encapsulate the effect in PVT relationships between non-ideal and ideal gases and in viscosity arising from state dependencies. Each coefficient is expressed generically in the space of van der Waals' reduced pressure and temperature, making it possible to analyse the behaviours in relation to an ideal-gas counterpart for any non-ideal gas.

This paper is organised as follows. Section 2 reviews some unique characteristics of gas flow, and a mathematical model [7] for simulating gas flow behaviours in pores that occur at both micro- and nano-meter scales. With that model, the apparent gas permeability and the flow conductance are formulated each as a summation of Darcy, slip and Knudsen terms, while the extra contributions of non-ideal gas, with respect to the ideal gas, are incorporated as coefficients to the respective terms, expressed as a relationship of van der Waals' reduced temperature and pressure. This formulation enables a quantitative analysis of these contributions to flow along a cylindrical pore. Section 3 discusses how the classical network flow model is extended, using the formulation developed in Section 2, to network elements with non-circular cross-sections, and describes some key implementation issues and solution strategies related to the nonlinear pressure equations. Section 4 applies the proposed PNFM to a realistic 3D model reconstructed from 2D sections of a gas shale sample to explore the importance of the pore characteristics, and the impact of gas properties on methane permeability under operational conditions, and nitrogen permeability under laboratory conditions, which is often used in experiments aimed at estimating in situ gas permeability. This is followed by a section comprising a discussion and conclusions.

2. A gas flow model, apparent permeability and flow conductance for a cylindrical capillary

Gas flowing in small pores behaves differently, depending on its pressure and temperature, and the pore dimensions. The Knudsen number $k_n = \lambda/l_{ch}$ is used to determine to which, of four flow regimes, the gas flow belongs [4]. Here λ is the mean free path – the average distance that a particle travels between two consecutive collisions, and is defined as: $\lambda = \frac{k_B T}{\sqrt{2}\pi d^2 p}$ where k_B, T, p and d are Boltzmann constant (J/K), temperature (K), pressure (Pa) and the diameter of the gas particles (m), respectively. λ is therefore