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Pore-scale numerical investigation into the impacts of the spatial and pore-size distributions of organic matter on shale gas flow and their implications on multiscale characterisation

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ABSTRACT

Owning to their differences in surface properties and pore geometry, pores of predominant submicron sizes in organic and inorganic matter of gas shale incur different gas flow and transport behaviours. Those differences can manifest at sample scales differently depending on the spatial distributions of shale organic and inorganic matter, and the pore-size distributions in these types of matter. Therefore, understanding the impacts of variable configurations of them on the gas flow is essential to guide progressive subsampling in multiscale shale characterisation that is required for modelling shale gas flow at the first place. This article reports a pore-scale numerical investigation into the impacts of combinations of three end-member spatial arrangements of the organic matter and two contrasting sets of organic and inorganic pore-size distributions at variable organic fractions on gas flow using pore-network modelling. A unified pore-network flow model for shale gas that captures a comprehensive set of gas flow and transport mechanisms is developed in this work to calculate the effective gas apparent permeability at reservoir conditions. In terms of the mean permeability at each selected organic fraction, the largest differences are found to appear at a high fraction above 25% across all the arrangements, and the upper bound can reach more than two orders of magnitude greater than the lower bound. The results suggest that subsampling ought to focus on subdomains where organic fractions are high, organic and inorganic pores differ in size, and distinct flow-enhancing or baffling arrangements of organic matter are present.

1. Introduction

"Gas shale" refers to rock successions that consist of significant intervals of rock with dominantly mud-sized fine particles, with significant organic or kerogen content, and in which the spatial arrangements of organic and inorganic matter are expressed at multiple scales. The organic- and inorganic-matter pores are typically ultra-small with varying modes of genesis and with diverse surface chemistry [1–3]. As a result, gas flow in gas shale pore space exhibits non-Darcy flow behaviours, coupled with significant effects associated with gas molecule interactions on organic and inorganic surfaces [4–10]. Pore-scale modelling of shale gas materials can capture the full range of shale gas flow and transport mechanisms that occur in submicron pores, and provides crucial insights about how complex sub-scale gas flow behaviours can manifest in a composite fashion at the sample scale. Knowledge about both are of critical importance in making reliable predictions of shale gas properties by forward modelling and inversion from laboratory measurements, given the heterogeneous nature of gas shale at scales that are still smaller than the sizes that can be used in laboratory measurements.

Recent advances in high-resolution imaging allow accurate characterisation of most submicron pores in shale, but only on a sample volume that is several orders of magnitude smaller than would be required for reconstructed models to be representative [11]. This is due mainly to the mutual constraint between the size of the field of view, and the image resolution, applying to all imaging techniques. A multiscale image-based pore-grain characterisation and simulation framework has been proposed to circumvent this limitation by selective subsampling at increasingly finer resolutions, progressively [12,13]. The multi-scale approach calls for suitable techniques and procedures to answer the critical question: where should we undertake subsampling, at a given scale?

Selection of subdomains for subsampling ought to focus on identification of those subdomains in which any mischaracterisation can lead

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to significantly different predictions of gas flow behaviour. Since shale gas flow behaves very differently in organic and inorganic pores, due to their differences in surface chemistry and pore geometry, a mischaracterisation is expected to have a large impact if it fails to correctly identify the existence and arrangement of organic matter in that subdomain. Despite the recognition of the critical impact that the textural characteristics at submicron pore scales have on shale gas flow, little has been given to the issue of selection of subdomains within the framework of the coarser-scale (mm-cm size) architecture of the material. The aim of the work reported here is to link the known submicron arrangements of organic and inorganic matter in such subdomains to their impact on the local gas flow, and to identify the implications of these configurations relative to subdomain siting.

Organic and inorganic pores are known to possess significant differences in pore sizes and surface chemistries that give rise to complex gas flow behaviours. Being predominantly submicron-size [1–3], the pores of intra-/inter-granular organic matter are usually less than 100 nm in diameter [14,15], while inorganic pores are generally larger than organic ones, although the opposite can be true [16]. In such small pores, the mean free path of gas becomes more comparable to the characteristic length of the pores, and as a result, gas flow no longer is characterised by the Darcy and slip flow regimes, and instead, occurs primarily within transition flow regimes. In nano-pores, gas molecules are transported through Knudsen diffusion [4,6–8,10]. In addition, gas adsorption takes place on pore surfaces, where the surface concentration of the gas molecules is mainly a function of the chemical compositions of the pore-bounding solid phases, but also is dependent on pore geometry and pore-surface morphology, along with in-situ pressure and temperature. Adsorbed gas on the surface of a pore reduces the pore space available for non-adsorbed or free gas molecules to flow in that pore [5,9], but the adsorbed gas may also diffuse along the surface in a direction towards a lower concentration of gas molecules [17]. Moreover, shale gas critical pressure (P_c) and critical temperature (T_c), which define the point where gaseous and liquid phase boundaries of a fluid vanish, may vary with the pore size in the confined space [18–20]. This can result in significant changes in fluid properties and therefore impacts on the fluid flow behaviour. Although all the gas flow and transport mechanisms, and the gas phase behaviours, can take place in both organic and inorganic pores, the gas adsorption and surface diffusion occur mostly on organic surfaces, because organic matter is often a much stronger adsorbent than inorganic matter, and it has a large specific surface area to adsorb a significant quantity of gas molecules [21]. Therefore, the difference between the gas transport potentials in the pore systems of organic matter and in those of the inorganic matter is primarily controlled by the gas adsorbability and surface diffusivity, as well as any contrast in the pore-size distributions.

Studies have found that the spatial distribution of organic matter can exhibit diverse and heterogeneous patterns. Using Ar-ion-beam milling and scanning electron microscopy (SEM), Loucks et al. [22] analyse the spatial distributions of organic matter, and pore sizes and connectivity, on Barnett shale samples from the Fort Worth Basin, Texas, USA, and categorise them into three end-member patterns: A) organic matter is concentrated in continuous layers; B) organic matter is sparser, but still mostly laterally continuous; C) organic matter is sparse and discontinuous, or disseminated. Those authors postulate that permeability pathways within the Barnett shale are primarily governed by the arrangement of organic matter in A) and/or B), because these configurations contain the most-connected organic pores. Strong evidence from other studies [11,23–25] suggests that the spatial arrangements of organic matter are expressed at multiple scales, ranging from a few microns or larger as “characteristic” length scales [11].

The key concern, from a subsampling point of view, is to identify subdomains where the spatial arrangements and pore-size distributions of the organic matter, relative to those of the inorganic matter, and the manner of the inter-connectivity of organic and inorganic pore spaces, may enable efficient and preferential gas flow [22,26,27]. In order to understand how important the spatial arrangements of organic matter might be, still within the submicron scale, and thus how important it might be to characterise the sample elements that contain organic matter, it is necessary to determine whether the submicron configurations of organic matter do have a significant impact on the local flow properties. This can be explored numerically using pore-scale models that represent those types of configurations.

In this work, the pore-network modelling approach is taken because it is computationally efficient for simulating gas flow, especially when one needs to consider many pore networks that are based on sets of parameters. A unified pore-network flow model is developed in this work to calculate the steady-state effective gas apparent permeability – the “effective permeability” in shorthand hereafter – at in-situ conditions, for a set of stochastic pore network models. This unified model accounts for viscous flow with a slip boundary condition, and Knudsen diffusion on both organic and inorganic pore elements, and adsorption, desorption and surface diffusion in organic pore elements only, as well as phase property changes, as a result of the changes of critical pressure and temperature in the pore space. To capture detailed gas flow behaviours that occur at submicron pores, pore network models are built on a domain volume of a few microns in each dimension so that the spatial arrangements of organic matter, relative to inorganic matter, and all the submicron pores, can be modelled explicitly. This gas flow model is then applied to a set of 360 pore-network models to analyse the influence of the spatial distributions of organic and inorganic matter, and the pore-size distributions of these elements, relative to their impacts on effective permeability. Three sets of 120 pore-network models each have been stochastically constructed from a base shale pore network, which defines a single topology used for all pore networks herein, by distributing organic matter to sets of pores in a way that captures one of the three end-member patterns, A-B-C, respectively. That base model is reconstructed from a real shale sample, and defines a realistic topology of the pore system. Three log-normal pore-size distributions, denoted as O-PSD-1, O-PSD-2 for organic (O) pore-size distributions (PSD) and IO-PSD, for inorganic (IO) pore-size distributions (PSD), of which the means of the former two are greater and smaller than that of the third, respectively, are applied to each set. This divides each set of 120 models into two groups, Groups 1 and 2, prescribed with O-PSD-1 and IO-PSD, and O-PSD-2 and IO-PSD, respectively, so that there are 60 models in each group. Each group of 60 models is divided into 6 subsets of 10 models, each at one of six organic-element fractions, denoted as N_f, between 5% and 30%. Note that due to the density difference between organic and inorganic matter, a fraction as high as 30% is not unrealistic. Using the pore-network method described herein, the results of the flow simulations are then analysed in terms of sample mean and standard deviation of effective permeability calculated for each set of 10 models at each N_f to quantify their upper and lower bounds across the different configurations of combined spatial arrangements and pore-size distributions.

The authors of this article are not aware of any other work that has been carried out close to what has been outlined above, although the spatial patterns considered here are so simple that they tempt one to estimate the bounds by treating organic and inorganic matter as two different types of continuums and then applying suitable average techniques. Note that the intention of this work is to explore the potential flow impact of spatial distributions of organic matter to gain an understanding about the range of the impact without focusing on the realism of pore network models. However, the outlined pore-scale approach does enable one to consider different realistic pore topologies and geometries of shale pores by replacing the base model with more realistic ones. That extension of the work will be undertaken in a later work in conjunction with advanced multiscale imaging and characterisation.

This paper is organized as follows. In Section 2, a pore-network flow model and a solution procedure are developed, with detailed formulations of every mechanism given in Appendix B, which follows Appendix