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Monitoring water transport in sandstone using flow propagators: A quantitative comparison of nuclear magnetic resonance measurement with lattice Boltzmann and pore network simulations

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ABSTRACT

A comparison of advective displacement probability distributions (flow propagators) obtained by nuclear magnetic resonance (NMR) experiment with both lattice Boltzmann (LB) and pore network (PN) simulations is presented. Here, we apply all three methods to the exact same sample for the first time: we consider water transport in a Bentheimer sandstone. The LB and PN simulations are based on X-ray micro-tomography (XMT) images of a small rock sample; the NMR experiments are conducted on a much larger rock core-plug from which the small rock sample originated. Despite the limited size of the simulation domains, good agreement is achieved between all three sets of results, verified quantitatively by comparison of the low order moments of the flow propagators. We are concerned primarily with validating the simulations at high liquid flow rates (>10 ml min^{-1}) in high permeability sandstone, ultimately for future application to geological carbon sequestration studies. Under these conditions the LB simulation is found, as expected, to be more robust than the PN model due primarily to the reduced requirement to manually tune the simulation lattice to match the petro-physical properties of the rock.

1. Introduction

A considerable proportion of potable water comes from underground freshwater aquifers close to the Earth's surface. These aquifers can suffer water quality reduction due to saltwater intrusion as a consequence of over-exploitation and rising sea levels. Large saline aquifers which are present at greater depths also offer potential sites for the geological sequestration of carbon dioxide (CO_2) [1–4]. Therefore, understanding the transport properties of water in underground rock formations is a critical requirement. In general, fluid flow through rock is important for oil, gas, and mineral extraction [5–7], contaminated land clean-up [8], and disposal of hazardous waste such as nuclear fuel [9]. Measuring flow in these optically opaque systems has traditionally been limited to techniques such as analysis of tracer breakthrough [10,11] or bulk pressure drop measurements [12], most of which are conducted in small laboratory-scale (sub-metre) samples of cored reservoir (rock) material or ideal porous media. However, these bulk measurements provide little or no information on the distribution of advective displacements within the porous sample.

Nuclear magnetic resonance (NMR) allows fluid transport to be probed non-invasively in optically opaque systems. NMR offers several advantages over the methods mentioned above, including acquiring signal directly from the moving water nuclei without the need to inject tracer material, and the ability to observe the relative contribution of diffusion and advection to transport over different length and time scales. In particular, NMR pulsed field gradient (PFG) techniques [13] now comprise a standard set of methods for observing molecular self-diffusion in both bulk liquids and saturated porous media [14].

One of the applications of PFG NMR is the measurement of a probability distribution of advective displacements averaged across the sample over a given time interval: the so-called "flow propagator" experiment [15,16]. Flow propagators have been used to quantify single fluid-phase flow in porous media, with most studies focusing on the Stokes' regime of a single fluid-phase (usually water) flowing through glass bead packs [17–23] as a proxy for reservoir rock or chemical reactors. Several studies have also focussed on water transport in rock core-plugs [24–30]. Rapid methods of obtaining NMR flow propagators are available, as reviewed by Mitchell and Johns [31], although we are not concerned here with speed of acquisition. The NMR propagator is best suited to the measurement of displacements much larger than the length-scale associated with molecular self-diffusion. Accordingly, NMR

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propagators have been applied to a pore-scale morphological study of CO_2 ganglia formation in a bead pack due to capillary forces (residual trapping), a process that readily occurs at comparatively high flow rates [32]. Here, then, we consider high flow rates appropriate for such CO_2 sequestration, and attempt to validate two simulation methods against experiment for use in future studies of geological carbon sequestration. Such high volumetric flow rates (e.g., >10 ml min^{-1}) are also relevant for mass-transport near the well-bore of oil and gas reservoirs, or water aquifers in general. Despite the advantages of the NMR flow propagator, the measurement is limited to studying advection over the sample length (less than 100 mm, typically) that will fit within the confines of the magnet geometry. To predict the fluid flow behaviour that will occur in a reservoir through many kilometres of rock formation, it is necessary to turn to simulations. Closure laws are then required in order to up-scale the laboratory-scale measurements to reservoir-scale simulations.

To predict macroscopic flow across reservoirs reliably, it is first necessary to understand transport observed on the micro-scale. Reservoir-scale simulations operate typically on pre-defined functions (closure laws) to predict ingress and egress of fluid from large (super-metre) formation segments. The behaviour within these reservoir segments may be based on pore-scale simulations, although this scale-up process is difficult and represents an area of on-going research in reservoir modelling [33]. Here, we are concerned with these pore-scale computational methods of modelling flow phenomena that can be directly compared against the experimental NMR flow propagator measurements. Two approaches for modelling fluid flow in porous media at the micro-scale used widely at present are lattice Boltzmann (LB) and pore network (PN) simulations. LB methods utilise an exact representation of the porous material and are often preferred because of their relatively straight-forward implementation for simulating flow in heterogeneous media [34]. LB is, however, computationally expensive and limited in terms of the domain (sample) size over which flow can be simulated. NMR flow propagators have been used previously to validate LB results for flow through ideal porous media, with favourable quantitative comparisons obtained between experimental and simulated propagators [26,32,35–39].

PN models seek to represent the structure of a porous medium as an idealised set of pore bodies (nodes) and interconnecting throats (bonds) [40–43]. Early PN models were based on a regular lattice structure that did not account for the complexity of real heterogeneous porous materials and were thus mainly used for qualitative studies [42]. In recent years, the use of geologically realistic pore networks for predictive modelling has become possible [44–46]. These networks are extracted from three-dimensional (3D) images of rock acquired using various techniques ranging from process based models which simulate the formation of geological materials, to experimental methods including image reconstruction from two-dimensional (2D) thin-sections or 3D X-ray microtomography (XMT) [47,48]. PN models have been used previously to predict NMR flow propagators [49,50] over small displacements. Although PN simulations have been used to predict larger displacements [51], these probability distributions have not been validated against experimental results. PN simulations are more computationally efficient than LB simulations, so limitations on simulation domain size may be less restrictive. However, network extraction from tomography data can be costly and slow; additionally, skilled, manual intervention is generally required to tune the porosity and transport properties of the resultant network and remove non-physical nodes.

The sample volumes that can be reproduced by either LB or PN methods are smaller, by two orders of magnitude or more, than those explored by NMR. However, NMR has one disadvantage in the limited time-scale of the measurement: due to spin relaxation, the displacement of ^{1}H nuclei in water can be monitored only over a maximum observation time of $\Delta \leqslant 5$ s. Longer observation times can be achieved by interrogating other resonant nuclei, e.g. ^{13}C [21], but that is not an option for the water flow considered here. Transport of liquid in a large reservoir can occur very slowly, on the order of 10^{-4} cm s^{-1}. At such low volumetric flow rates, the propagator is Gaussian-like where the distribution shape is determined by diffusion. In studies of pipe flow or advection through a non-porous glass bead pack [17–21] (i.e., no stagnant liquid), low flow rates are monitored by observing a shift in the mean displacement. However, in tortuous porous media such as rocks, the volume of stagnant spins provides a persistent Gaussian-like distribution with zero mean displacement and a width determined by the liquid diffusion coefficient. Therefore, for the NMR measurement to be sensitive to flow the advective displacement must be significant compared to diffusive dispersion during Δ. Accordingly, it is not possible to explore flow rates relevant to oil recovery with NMR propagators due to the limited observation time [24]. Instead, we chose to apply the high flow rates (and corresponding large displacements) more relevant to residual trapping during CO_2 sequestration [32].

In the work presented here, we consider the use of XMT images of sandstone rock to provide direct simulation lattices for LB simulations and indirect pore networks for PN modelling of liquid flow. The resultant 3D flow fields are used to generate flow propagators for both methods, which are then validated against PFG NMR measurements of propagators in the same sandstone rock cores. Although we do not consider the NMR data to constitute a "gold standard" in displacement measurements, PFG NMR is one of the few techniques able to quantify, in situ, the average distribution of advective displacements and is therefore readily compared to simulations of the same. To the best of our knowledge, this represents the first direct comparison of PN and LB simulations of displacement propagators for flow through porous media.

2. Theory

The flow propagator is a probability distribution $P(\zeta,\Delta)$ of molecular displacement ζ over the observation time Δ. The application of a magnetic field gradient of strength g_z causes nuclear spins (here, ^{1}H) to precess at different frequencies depending on their spatial position within the sample. After a time δ, individual spins have acquired a phase relative to spins precessing at the Larmor frequency ($\omega = \gamma_r B_0$). After a time Δ, a gradient of strength $-g_z$ is applied to rewind the phase encoding. If a spin has remained stationary during Δ, then its phase is restored. However, if the spin has moved from position $\mathbf{r}(0)$ to $\mathbf{r}(\Delta)$, then the phase reversal is incomplete. The net phase shift is

$$\phi = \gamma_r \delta \mathbf{g} \cdot [\mathbf{r}(\Delta) - \mathbf{r}(0)], \tag{1}$$

where γ_r is the gyromagnetic ratio of the spins and $\mathbf{g}$ is the gradient vector (we are concerned here only with the component in z). This phase shift can be written as $\phi = 2\pi \mathbf{q} \cdot \mathbf{R}$ where $\mathbf{q}$ is the magnetization wave vector, such that $\mathbf{q} = \gamma_r \delta \mathbf{g}$, and $\mathbf{R} = \mathbf{r}(\Delta) - \mathbf{r}(0)$ is the displacement vector. We are concerned with advective displacements $\zeta = R_z$, i.e., the z-component of $\mathbf{R}$. This observed NMR signal is proportional to the ensemble average over all encoded spins (equivalent to the integral over all positions) and is described by the Fourier transform (FT) of the probability function [15]

$$S(q) = \int P(\zeta,\Delta) \exp[2\pi i q \zeta] \mathrm{d}\zeta, \tag{2}$$

where q is the magnitude of $\mathbf{q}$. To determine $P(\zeta,\Delta)$ it is necessary to obtain $S(q)$ across an appropriate bandwidth of q-space by varying g_z and performing an inverse FT of $S(q)$. To provide a quantitative