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Accurate phase-shift velocimetry in rock

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ABSTRACT

Spatially resolved Pulsed Field Gradient (PFG) velocimetry techniques can provide precious information concerning flow through opaque systems, including rocks. This velocimetry data is used to enhance flow models in a wide range of systems, from oil behaviour in reservoir rocks to contaminant transport in aquifers. Phase-shift velocimetry is the fastest way to produce velocity maps but critical issues have been reported when studying flow through rocks and porous media, leading to inaccurate results. Combining PFG measurements for flow through Bentheimer sandstone with simulations, we demonstrate that asymmetries in the molecular displacement distributions within each voxel are the main source of phase-shift velocimetry errors. We show that when flow-related average molecular displacements are negligible compared to self-diffusion ones, symmetric displacement distributions can be obtained while phase measurement noise is minimised. We elaborate a complete method for the production of accurate phase-shift velocimetry maps in rocks and low porosity media and demonstrate its validity for a range of flow rates. This development of accurate phase-shift velocimetry now enables more rapid and accurate velocity analysis, potentially helping to inform both industrial applications and theoretical models.

1. Introduction

Fluid flow through porous media, such as rock or sand packs, is found in a wide range of industrial and natural processes ranging from chemical reactors to petroleum recovery. Knowledge of the flow properties in these media can be crucial in understanding transport processes and developing accurate transport models. Nuclear magnetic resonance based approaches enable the complexity of local flow processes within the system to be characterized, moving our understanding of flow beyond bulk average macroscopic descriptions. NMR based approaches have been used to, for example, explore simultaneous flow of oil and water in sandstone [1], unpick complexities in nanoparticle transport behaviour in rock [2], map organic pollutant transport in fractures [3] and image heavy metal removal in bio-film mediated ion exchangers [4]. The Pulsed Field Gradient Nuclear Magnetic Resonance (PFG NMR) experiment originally proposed by Stejkal and Tanner [5], has long been used to non-invasively study flow and diffusion properties [6]. Furthermore, localised measurement of flow properties can be achieved by combining PFG with an imaging module to give PFG velocimetry also known as Magnetic Resonance Velocimetry (MRV). The resulting spatial maps of velocity provide a rich insight into the transport and structural properties of optically opaque systems.

There are two main methods of PFG velocimetry, namely propagator velocimetry and phase-shift velocimetry. Propagator velocimetry consists of resolving the probability distribution of displacements for each voxel. These are slow to acquire, requiring at least 8 [7] and up to 128 [8] gradient encoding steps (or $\boldsymbol{q}$ values). Phase-shift velocimetry is faster, requiring only two gradient encoding steps to measure the average velocity in each voxel. Indeed, phase-shift velocimetry is at least 4 times faster than propagator velocimetry, and is thus a highly desirable alternative when experiments can have time durations of days.

In the application of PFG velocimetry to porous media, it is useful to distinguish two regimes. In the first regime, where the imaging voxel size is smaller than the typical pore size, e.g. bead packs, both of the PFG methods are used and found to be reliable [9]. In the second regime, where the voxel size is greater than the typical pore size, e.g. sandstone rock [10], though there have been reports of quantitative phase-shift velocimetry [11], it has been generally advised to use the more time consuming propagator method [12], as numerous issues have been reported with the use of phase-shift velocimetry. These issues can be broadly categorised as:

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1. Measured average velocity values not agreeing with values calculated from the known flow rate and porosity. Lower values than expected are reported at higher flow rates [13] making the relationship of measured velocity to the imposed flow rate non-linear [14,15].
2. Standard deviation of voxel velocities exceeds the expected values. This effect becomes stronger at lower flow rates [16] with a large proportion of the voxels unexpectedly indicating negative velocities [15].
3. Measured velocity can vary with experimental PFG parameters. Several authors have shown that at fixed flow rate, different velocity values are measured when different gradient strengths (G) [12] or observation times (Δ) [15] are used.

These issues have effectively made phase-shift velocimetry unreliable for use with porous media like rocks, where voxel sizes can be greater than the typical pore size. In this work, we clearly characterise the above mentioned problems, identify their underlying causes and propose concrete solutions for producing accurate phase-shift velocimetry measurements in rocks and porous media.

1.1. PFG NMR velocimetry

PFG NMR velocimetry consists of making the phase of the NMR signal sensitive to translational motion. This is achieved by applying a pulsed field gradient of amplitude G during a time δ, imposing spatially dependent phase shifts to the spins. For a spin moving along the path $\boldsymbol{r}(t)$, the induced phase is given by:

$$\varphi(t) = \gamma \int_0^t \boldsymbol{G}(t) \cdot \boldsymbol{r}(t) dt \tag{1}$$

After an observation time Δ, rephasing gradients are applied to the system. By choosing parameters such as $\delta \ll \Delta$ (narrow pulse approximation), one can neglect displacements that occurred during δ. Then, for a spin starting at $\boldsymbol{r_0}$ and ending at $\boldsymbol{r_0} + \boldsymbol{R}$, the resulting phase-shift is given by $\gamma\delta\boldsymbol{G} \cdot \boldsymbol{R}$. At this stage, to describe phase modulation due to molecular motion, it is often convenient to introduce the wave vector $\boldsymbol{q} = \gamma\delta\boldsymbol{G}$. The wave vector $\boldsymbol{q}$ is the conjugate of spin displacement in the same way that the wave vector $\boldsymbol{k} = \int_0^t \boldsymbol{g}(t)dt$ is the conjugate of spin position in an imaging experiment [17]. The combination of velocity encoding and imaging allows to measure phase-shift for each voxel in the sample.

The NMR signal resulting from a spatially resolved PFG NMR experiment can be expressed by:

$$S(\boldsymbol{k}, \boldsymbol{q}) = \int \int \rho_\Delta(\boldsymbol{r}, \boldsymbol{R}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{i\boldsymbol{q}\cdot\boldsymbol{R}} d\boldsymbol{r} d\boldsymbol{R} \tag{2}$$

Moran [18] showed that, for a spin at position $\boldsymbol{r}$ with a displacement $\mathbf{R}$ during the time Δ, spin density $\rho(\boldsymbol{r})$ could be generalised to a joint density function, $\rho_\Delta(\boldsymbol{r}, \boldsymbol{R})$, defined as:

$$\rho_\Delta(\boldsymbol{r}, \boldsymbol{R}) = \rho(\boldsymbol{r}) P_\Delta(\boldsymbol{R}, \boldsymbol{r}) \tag{3}$$

where $P_\Delta(\boldsymbol{R}, \boldsymbol{r})$ is the normalised probability distribution function of spin displacements over the period Δ, also called a propagator. By applying the velocity encoding gradients along a single direction (for example z) and considering a displacement Z of each spin during the time Δ, the combination of Eqs. (2) and (3) gives the NMR signal for a voxel situated at position $\boldsymbol{r}$ as:

$$S(\boldsymbol{r}, q) = \rho(\boldsymbol{r}) \int P_\Delta(Z, \boldsymbol{r}) e^{iqZ} dZ \tag{4}$$

Defining the average velocity of each spin during Δ as $\bar{v} = \frac{Z}{\Delta}$, it is possible to rewrite Eq. (4) as:

$$S(\boldsymbol{r}, q) = \rho(\boldsymbol{r}) \int P_\Delta(\bar{v}, \boldsymbol{r}) e^{iq\bar{v}} d\bar{v} \tag{5}$$

If the time integral of the velocity encoding gradient is zero, this integral is independent of spin position and $S(\boldsymbol{r}, q)$ is the Fourier transform of the velocity-density function $P_\Delta(\bar{v}, \boldsymbol{r})$.

1.1.1. Propagator velocimetry

One approach to measure velocity, called propagator velocimetry, consists in acquiring $S(\boldsymbol{r}, q)$ for several q values, or q-steps, and then apply an inverse Fourier transform in order to obtain the propagator $P_\Delta(\bar{v}, \boldsymbol{r})$. The number of q-steps and their size has to be selected appropriately so as to cover the velocity range found in each voxel and get the desired propagator resolution. Typically a minimum of q steps has to be used, which leads to significant experimental times, even when using fast acquisition sequences [19].

1.1.2. Phase-shift velocimetry

In another approach, velocity is related to the phase of the signal resulting from a PFG measurement. First, by inserting the expression of the ensemble averaged velocity for a voxel, $V(\boldsymbol{r}) = \int \bar{v} P_\Delta(\bar{v}, \boldsymbol{r}) d\bar{v}$, into Eq. (5) one obtains:

$$S(\boldsymbol{r}, q) = \rho(\boldsymbol{r}) e^{iqV(\boldsymbol{r})\Delta} \int P_\Delta(\bar{v}, \boldsymbol{r}) e^{iq(\bar{v} - V(\boldsymbol{r}))\Delta} d\bar{v} \tag{6}$$

If the velocity density function is symmetric around the mean velocity $\bar{v}$ then the integral in Eq. (6) is real and the phase of the resulting signal is found to be proportional to the average velocity, $V(\boldsymbol{r})$, and the resulting phase is given by:

$$\varphi(\boldsymbol{r}) = \gamma\delta G \Delta V(\boldsymbol{r}) \tag{7}$$

In theory, by subtracting two phase images taken at equal Δ times, and with equal but opposite G values one can obtain a map with intensities proportional to velocity [20]. The second G value phase image cancels eddy current related phase contributions that are independent of q. This $\Phi(\boldsymbol{r}) = \varphi_2(\boldsymbol{r}) - \varphi_1(\boldsymbol{r})$ map is easily transformed into a velocity map using Eq. (8):

$$\Phi(\boldsymbol{r}) = \gamma\delta(G_2 - G_1)\Delta V(\boldsymbol{r}) \tag{8}$$

In practice, the measured phase-shift $\Phi(\boldsymbol{r})$ is affected by additional experimental parameters. The phase-shift effectively measured at any voxel $\boldsymbol{r}$ of a phased image can be expressed as [21]:

$$\Phi(\boldsymbol{r}) = \gamma\delta(G_2 - G_1)\Delta V(r) + \alpha(\boldsymbol{r}) + \theta(\boldsymbol{r}) \tag{9}$$

where $V(\boldsymbol{r})$ is the average velocity of spins, γ is the gyromagnetic ratio, $\alpha(\boldsymbol{r})$ corresponds to phase contributions that depend of q and $\theta(\boldsymbol{r})$ is phase shift caused by noise.

By acquiring a phase-shift map at zero flow, $\Phi_0(\boldsymbol{r})$, it is then possible to remove phase contributions that are not flow related. The resulting phase-shift can then be rewritten as:

$$\Phi(\boldsymbol{r}) - \Phi_0(\boldsymbol{r}) \simeq \gamma\delta(G_2 - G_1)\Delta V(\boldsymbol{r}) + \theta(\boldsymbol{r}) - \theta_0(\boldsymbol{r}) \tag{10}$$

The noise related phase-shift error is related the uncertainties in the measurement of the x and y components of the nuclear magnetisation in the rotating frame [22]. For an uncertainty ΔS in each direction, phase error can be estimated by [12]:

$$\theta = \Delta S / S \tag{11}$$

θ is therefore reciprocal of the signal-to-noise ratio (SNR). This makes SNR an important parameter to consider since $\theta(\boldsymbol{r}) \ll \gamma\delta G \Delta V(\boldsymbol{r})$ is a condition for producing accurate velocity maps.

Phase-shift velocimetry relies on the linear relation between the phase of the NMR signal and the imposed velocity-encoding gradient, which enables to use Eq. (10) for the production of a velocity map. But it has been shown in rocks that this phase-gradient linearity gets compromised as gradient increases [12], with the linear range becoming smaller at higher flow rates. Working at lower flow rates is not a solution, since the imparted