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# A comparison of experimental and simulated propagators in porous media using confocal laser scanning microscopy, lattice Boltzmann hydrodynamic simulations and nuclear magnetic resonance

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#### Abstract

Confocal laser scanning microscopy has been used to obtain 3D optical image stacks of packings of glass ballotini in various fluorescent dye-containing fluids inside a 3D micromodel. The fluids' refractive index was matched to that of the glass ballotini so that clear images at an appreciable depth ( $\sim$ 400 µm) inside the packings were obtained. The lattice Boltzmann method was then used to produce 3D velocity fields through the 3D image stacks of the packed ballotini. These have been used in conjunction with a stochastic random-walk algorithm to produce simulated displacement propagators, which have been shown to be in qualitative agreement with experimental propagators, obtained using nuclear magnetic resonance, of water flowing through the exact same micromodel. © 2005 Elsevier Inc. All rights reserved.

Keywords: Propagators; CLSM; Flow simulation

### 1. Introduction

This work combines and exploits the high spatial resolution of confocal laser scanning microscopy (CLSM), the ability of lattice Boltzmann (LB) simulations to describe the flow field in extremely complex geometries and nuclear magnetic resonance (NMR) to quantify the local pore-scale displacement for an entire sample in order to study transport processes in 3D micromodels as are employed in oil industry research. Refractive index (RI)-matched random packings of 100-µm-diameter borosilicate ballotini in fluorescent-dyed fluids have been imaged inside a 3D micromodel using CSLM. LB hydrodynamic simulations have been conducted on the 3D CLSM image stacks, and the resulting velocity fields have been used in conjunction with a stochastic random-walk algorithm [1] to generate simulated displacement propagators. The simulated propagators have been compared with experimental displacement

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propagators, acquired using NMR, for flow through the exact same packings as those imaged using CLSM. The effect of simulation volume on the resulting propagators has thus been investigated.

## 2. Experimental setup

The CLSM images were obtained using a Zeiss LSM 510 confocal microscope with a  $10 \times /0.3$  Plan NEOFLUAR lens. CLSM positively images the fluorescence emitted by fluorescent dyes, which are dissolved in a fluid phase occupying the pore space. The fluids in this work contained Rhodamine B fluorescent dye and were excited by the 543 nm line of a He–Ne laser. Potassium thiocyanate (65% w/w) solution was used in the imaging due to the importance of RI-matched systems for our application. In all images that were used in the production of masks for LB simulations, the isotropic resolution was 3.6 µm per pixel, with image dimensions of  $256 \times 256 \times 126$  voxels.

Experimental displacement propagators were acquired on a Bruker 2-T superconducting magnet with a 310-mmdiameter horizontal bore and a radio frequency probe of

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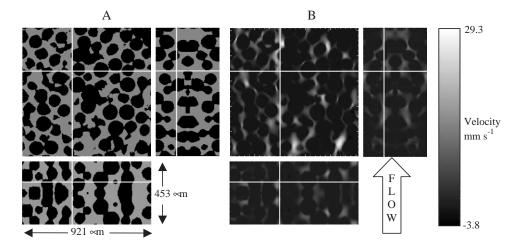


Fig. 1. (A) 3D CLSM image of 100 µm ballotini and the resulting (B) 3D flow field following LB simulation.

60 mm internal diameter. The <sup>1</sup>H operating frequency was 85.2 MHz. The propagators were acquired using an alternating pulsed gradient stimulated echo sequence [2], for a range of evolution times ( $\Delta$ ) of 50 ms–1 s, with applied-gradient duration ( $\delta$ ) of 4 ms, a maximum gradient strength of 0.0781 G cm<sup>-1</sup> and fluid interstitial velocities of 545 and 778 µm s<sup>-1</sup>.

#### 3. Simulations

The LB method was used to simulate hydrodynamic flow through 3D arrays, obtained from "clean" (noise voxels caused by the imaging process had been removed) CLSM image stacks. Simulations were conducted on 3D arrays of various sizes, the largest having dimensions of  $256 \times 256 \times 126$  voxels. The Reynolds numbers of the simulations were matched to those of the water in the corresponding experimental propagators.

The stochastic random-walk algorithm was applied to a particular volume inside the 3D LB hydrodynamic flow field. The algorithm subjects particles to a convective jump, based on their position in the flow field, and then allows the particles to undergo a random diffusive jump. This process is iterated a fixed number of times for each particle, and the ensemble displacements recorded as a probability distribution — a propagator.

## 4. Results and discussion

In order to obtain clear, resolved images of the ballotini packings over an appreciable depth, it was necessary to match the RI of the fluid in which the ballotini was immersed to the RI of the ballotini (~1.5). The imaging is highly sensitive to differences in RI — a mismatch of ~0.01 in RI has quite a severe effect on image quality. An example of a 3D CSLM image is shown in Fig. 1(A), the resulting LB flow field (shown only in the superficial flow direction) is shown in Fig. 1(B).

For simulations in which one dimension is very shallow [e.g., a single layer (2D) image], a large peak at zero displacement is seen in the resulting simulated propagators, as a function of  $\Delta$ , compared with the corresponding experimental propagators. We believe that this is caused by a reduction in the connectivity of the pore space. As the

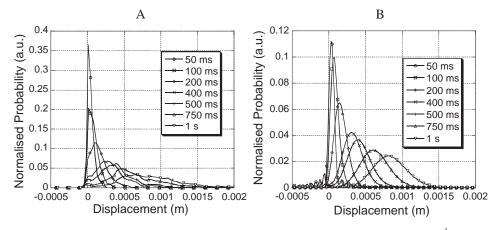


Fig. 2. Comparison of (A) simulated and (B) experimental displacement propagators, for interstitial velocity of 778 mm s<sup>-1</sup>, through 100  $\mu$ m ballotini for a range of  $\Delta$ .

depth of the simulation increases, the connectivity between pores increases because the fluid can now move in three "full" dimensions. The resulting propagators for a simulation lattice of  $256 \times 256 \times 126$  are shown in Fig. 2(A), and the corresponding experimental propagators are shown in Fig. 2(B). There is qualitative agreement, particularly bearing in mind that the CSLM image represents less than 1% of the total packing volume sampled by NMR when producing the experimental propagators. The broader distribution produced by the simulations is attributed to the CSLM image being necessarily near the top of the packing and hence being both partially ordered (due to edge effects) and "partially exposed" on the surface.

## 5. Conclusions

It is necessary to immerse the packed glass ballotini with a fluid that has an RI that matches that of the ballotini in order to acquire useful images at an appreciable depth inside the packing. The simulated propagators describe the key characteristics of the experimental propagators. However, the simulations must be performed over an appreciable depth in order for there to be a good agreement between the simulated and experimental propagators.

#### Acknowledgments

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