Explicit Numerical Simulation of Microfluidic Liquid Flows in Micro-Packed Bed

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A thesis submitted for the degree of Doctor of Philosophy

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Abstract

Microfluidic systems are of tremendous technological interest as demonstrated by their use in chemical analysis (so called 'lab-on-a-chip') and biochemical analysis (e.g. to detect biomarkers for disease), and in process intensification. Packed beds of micro-sized particles possibly utilized for enhancing heat and mass transfer in microfluidic devices, where the flow regime is normally laminar, as well as provide significant increases in surface area per unit volume for analytical chemistry and biochemistry, and for separation and purification. Whilst macro-scale packed beds have long been well understood, the same is not true of their microfluidic counterparts, which we term micro-packed beds or µPBs. Of particular concern is the effect that the small bed-to-particle diameter ratio has on the nature of the bed packing and the hydrodynamics of the flow within them. This lack of understanding stems in part from the challenges that are faced in experimentally assessing µPBs and the flow through to them. The study reported in this thesis addresses these concerns through a two developments. In the first body of work, a new method is proposed for the accurate reconstruction of the structure of a µPB from X-ray micro-computed tomography data for such beds. The porosity obtained from µPB was, within statistical uncertainty, the same as that determined *via* a direct method whilst use of a commonly used technique yielded a result that was nearly 10% adrift, well beyond the experimental uncertainty. This work particularly addresses the significant issues that arise from the limited spatial resolution of the tomography technique in this context. In the second part of the work reported here, a meshless computational fluid dynamics technique is used to study Newtonian fluid flow through µPBs, including determination of their permeability and the by-pass fraction due to wall effects, which are important in these beds. This use of a CFD allows determination of parameters that are difficult to determine experimentally because of the challenges faced in measuring the small pressure drops involved and the absence of the limited spatial and temporal resolutions of various imaging techniques. The meshless method used here also overcomes the challenges normally faced when seeking to discretise the complex three-dimensional pore space of the packed bed. The developments here open the way to studying more complex µPB configurations, and other processes within them such as non-Newtonian flows and mass and heat transfer.

Achievements

Three following papers were achieved from this work:

1) Navvab Kashani, M., Zivkovic, V., Elekaei, H., Biggs, M. J., *A new method for reconstruction of the structure of micro-packed beds of spherical particles from desktop X-ray microtomography images. Part A. Initial structure generation and porosity determination*, submitted to Chemical Engineering Science, Elsevier, 2015.
2) Navvab Kashani, M., Zivkovic, V., Elekaei, H., Herrera, L. F., Affleck, K., Biggs, M. J., *A new method for reconstruction of the structure of micro-packed beds of spherical particles from desktop X-ray microtomography images. Part B. Structure refinement and analysis*, submitted to Chemical Engineering Science, Elsevier, 2015.
3) Navvab Kashani, M., Elekaei, H., Zhang, H., Zivkovic, V., Biggs, M. J., *Explicit numerical simulation-based study of the hydrodynamics of micro-packed beds*, submitted to Chemical Engineering Science, Elsevier, 2015.

A part of this work was also presented in conference with the following titles:

1) Navvab Kashani, M., Zivkovic, V., Alwahabi, Z., Biggs, M. J., *Particle packing structure in a rectangular micro-capillary*, Chemeca 2012, 23-26 September 2012, Wellington, New Zealand.

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Abbreviations

BGAF	Basic Gradient Approximation Formula
CFD	Computational Fluid Dynamics
CT	Computed Tomography
DEM	Discrete Element Method
DGAF	Difference Gradient Approximation Formula
DNS	Direct Numerical Simulation
ENS	Explicit Numerical Simulation
FDM	Finite Difference Method
FEM	Finite Element Method
FVM	Finite Volume Method
HPC	High-Performance Computing
HT	Hough Transform
LBM	Lattice Boltzmann Method
LGA	Lattice Gas Automata
LOC	Lab-On-a-Chip
LoG	Laplacian of Gaussian
MC	Monte Carlo
MD	Molecular Dynamics
MRI	Magnetic Resonance Imaging
NMR	Nuclear Magnetic Resonance
NNP	Nearest Neighbouring Particles
NNPS	Nearest Neighbouring Particle Searching
PPE	Pressure Poisson Equation
PSD	Particle Size Distribution
Re	Reynolds Number
RMC	Reverse Monte Carlo
RTD	Residence Time Distribution
SA	Simulated Annealing
SD	Standard deviation
SGAF	Symmetric Gradient Approximation Formula
SPH	Smoothed Particle Hydrodynamics
3D	Three-dimensional
2D	Two-dimensional
μPB	Micro-Packed Bed
μTAS	Micro Total-Analysis-System

Nomenclature

a	[m/s^2]	Acceleration
A	[-]	Scalar quantity
A	[m^2]	Area
A_w	[-]	Wall correction parameter
B_w	[-]	Wall correction parameter
C	[m/s]	Sound speed
C_D	[-]	Drag coefficient
D	[m]	Bed diameter
D_{ij}	[m]	Particle-particle overlap
D_{iw}	[m]	Particle-wall overlap
d_{ij}	[m]	Minimum distance between particles in packed-bed
d_p	[m]	Sphere diameter
f	[-]	General function
F	[-]	Objective function
g	[m/s^2]	Gravitational acceleration
h	[m]	Cut-off distance (smoothing length)
I	[-]	Unit tensor
K	[-]	Number of sequential circular planes partitioning of a spherical particle
k	[m^2]	Permeability
K_1	[-]	Experimental coefficient in Reichelt model
L	[m]	Bed length
L_0	[m]	Initial distance between particles
M	[-]	Particle-to-bed size ratio
m	[kg]	Mass of particle
N	[-]	Number of computational cells
N_p	[-]	Number of SPH particles
P	[-]	Probability
P	[Pa]	Pressure
ΔP	[Pa]	Pressure drop
r	[m]	Position
r_{ij}	[m]	Distance between particles *i* and *j*
$\acute{r}$	[m]	Location of individual particle
R	[-]	Inter-plane resolution of x-ray microtomography
R_h	[m]	Hydraulic radius
R_O	[-]	Roundness
t	[s]	Time
t	[-]	Time step
Δt	[s]	Time step size
T	[K]	Temperature

u	[m/s]	Volume averaged fluid velocity
U_0	[m/s]	Superficial velocity
U_B	[m/s]	Bulk velocity
U_{max}	[m/s]	Maximum characteristic velocity
V	[m^3]	Particle volume
V	[m/s]	Velocity vector
W	[m^{-3}]	Smoothing kernel
x	[m]	Distance vector
$\mathbf{x}_{i0}$	[m]	Position of the particle in the initial 3d structure
$\overline{Z}$	[-]	Mean coordination number
γ	[-]	Coefficient for fluid properties
δ	[-]	Dirac delta function
ε	[-]	Porosity
ε	[-]	User-defined parameter in SPH particle-particle interaction model
η	[-]	Arbitrarily small quantity
μ	[Pa.s]	Dynamic viscosity
ρ	[kg/m^3]	Density
σ	N/m^2	Stress
τ	N/m^2	Shear stress
ϕ	[%]	Porosity
ξ	[-]	Random parameter
δx	[m]	Displacement
σ_i		Standard deviation
κ		Skewness
∇		Gradient operator

Subscript

i	Value for particle of interest
j	Value for neighbouring particles
b	Related to bed or bulk
D	Value for direct measurement
MC	From Monte Carlo
p	Value for particle
w	Related to wall
α	α-coordinate direction
β	β-coordinate direction

Superscript

α	Number of dimensions
β	Number of dimensions
*	Intermediate state

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