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Study of Immiscible Liquid-Liquid Microfluidic Flow using SPH-based Explicit Numerical Simulation

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A thesis submitted for the degree of Doctor of Philosophy

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November 2015

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Hamideh Elekaei Behjati

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Abstract

Microfluidic devices are utilized in a wide range of applications, including micro-electromechanical devices, drug delivery, biological diagnostics and micro-fuel cell systems. Of particular interest here are liquid-liquid microfluidic systems; which are used in drug discovery, food and oil industry amongst others. Increased understanding of the fundamentals of flows in such devices and an improved capacity to design them can come from modelling. In the case of liquid-liquid flows in microfluidic systems, it is necessary to explicitly model the behaviour of the individual liquid phases. Such explicit numerical simulation (ENS) as it is termed requires advanced numerical methods that are able to evaluate flow involving multiple deforming fluid domains within often complex boundaries. Smoothed Particle Hydrodynamics (SPH), a Lagrangian meshless method, is particularly suitable for such problems. This use of a CFD allows determination of parameters that are difficult to determine experimentally because of the challenges faced in microfabrication. The study reported in this thesis addresses these concerns through development of a new SPH-based model to correctly capture the immiscible liquid-liquid interfaces in general and for a microfluidic hydrodynamic focusing system in particular. The model includes surface tension to enforce immiscibility between different liquids based on a new immiscibility model, enforces strict incompressibility, and allows for arbitrary fluid constitutive models. This work presents a detailed study on the effects of various flow parameters including flowrate ratio, viscosity ratio and capillary number of each liquid phase, and geometry characteristics such as channel size, width ratio, and the angle between the inlet main and side channels on the flow dynamics and topological changes of the multiphase microfluidic system. According to our findings, both flowrate quantity and flowrate ratio affect the droplet length in the dripping regime and a large viscosity ratio imposes an increase in the flowrate of the continuous phase with the same capillary number of the dispersed phase to attain dripping regime in the outlet channel. Also, increasing the side channel width causes longer droplets, and the right-angled design makes the most efficient focusing behaviour. This study will provide great insights in designing microfluidic devices involving immiscible liquid-liquid flows.

Achievements

Three following papers were achieved from this work:

1) Elekaei Behjati, H., Navvab Kashani, M., Biggs, M. J., *Modelling of Immiscible Liquid-Liquid Systems by Smoothed Particle Hydrodynamics*, to be submitted to Computational Mechanics, 2015.
2) Elekaei Behjati, H., Navvab Kashani, M., Zhnag, H., Biggs, M. J., Smoothed Particle Hydrodynamics-based Simulations of Immiscible Liquid-Liquid Microfluidics in a Hydrodynamic Focusing Configuration, to be submitted to Physics of Fluids, 2015.
3) Elekaei Behjati, H., Navvab Kashani, M., Zhnag, H., Biggs, M. J., Effects of Flow Parameters and Geometrical Characteristics on the Dynamics of Two Immiscible Liquids in a Hydrodynamic Focusing Microgeometry, to be submitted to Physics of Fluids, 2015.

Acknowledgements

Over the past four years, I was inspired and supported by many people without whom I would never have been able to finalize this dissertation. This section is therefore dedicated to all those people who have shared their time, enthusiasm and expertise with me, admitting that I will never be able to thank enough those whom I am indebted the most. I would like to express my deepest gratitude and appreciation to all of them.

I would like to start by thanking my principal supervisor, Prof Mark J. Biggs for his ongoing advice and support during the entire course of my PhD study. Mark, your expertise and detailed critical comments on every part of my research, pushed me to think deeper about my research and shape my ideas. I am also very grateful to the other members of the supervision team, A/Prof Zeyad Alwahabi and Dr Hu Zhang for their valuable feedback and supports.

During the four years of my PhD, I have been lucky to discuss my research and collaborate with many bright people. In particular, I wish to extend my appreciation to Dr Milan Mijajlovic. Milan, thanks for your occasional support in computer coding and programming.

I am more thankful than I can say to Mrs Jacqueline Cookes, Mrs Marilyn Seidel and Mr Ron Seidel. Mrs Jacqui, you have been always nice and kind to me, that made me feel at home. You have been a cheerful caring friend for me. Your honesty, experience and kindness make you a person with whom talking is nothing else but a pleasure. I have learnt a lot from you that will never forget. Marilyn and Ron, I am not able to describe your big hearts in a few words, I can just wholeheartedly thank you both for all the endless support I have received from you. You all made my PhD journey much more enjoyable. Thanks for everything.

The Government of Australia and the University of Adelaide are gratefully acknowledged for providing me Adelaide Scholarships International (ASI) for my study in Australia. The cluster super-computational facilities and high-performance computing (HPC) system for this work were provided by *eResearch SA organization,* which is warmly appreciated.

I am deeply indebted to my loving parents, who have always been encouraging me to continue my education and broaden my mind. Dad, thank you for your infinite support. Mum, you created a home environment that encouraged me to study and learn. Words cannot describe how grateful I am for your never ending love and care and all you have done for me. Without your support, I would never achieve what I have today. I am also thankful to my caring brothers, Majid, Habib and Mehdi, and my lovely sisters, Zahra and Shabnam, for all their support, accompany, and encouragement during my PhD study overseas. Likewise, I would like to thank my parents-in-law for their support, inspiration and influence.

Finally, and above all, I cannot begin to express my unfailing gratitude and love to my best friend, my dear husband, Dr Moein N. Kashani. Moein, you have always supported me through every step of this long journey, and have constantly encouraged me when the tasks seemed arduous and insurmountable. Without you, I would never have had the inspiration and motivation to complete this dissertation. Thank you for your warm presence in my life.

Hamideh Elekaei Behjati

November 2015

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Abbreviations

Ca	Capillary Number
CAD	Computer Aided Design
CFD	Computational Fluid Dynamics
DNS	Direct Numerical Simulation
DPD	Dissipative Particle Dynamics
ENS	Explicit Numerical Simulation
Eo	Eotvos Number
FDM	Finite Difference Method
FEM	Finite Element Method
FVM	Finite Volume Method
HPC	High-Performance Computing
LBM	Lattice Boltzmann Method
LGA	Lattice Gas Automata
LOC	Lab-On-a-Chip
LoG	Laplacian of Gaussian
LSM	Level Set Method
MD	Molecular Dynamics
Mo	Morton Number
NNPS	Nearest Neighbouring Particle Searching
Oh	Ohnesorge Number
PPE	Pressure Poisson Equation
Re	Reynolds Number
SD	Standard deviation
SPH	Smoothed Particle Hydrodynamics
VOF	Volume of Fluid
µTAS	Micro Total Analysis System
3D	Three-dimensional
2D	Two-dimensional

Nomenclatures

a	[m]	Length of the major axis of the ellipsoid
A	[m^2]	Area
b	[m]	Length of the minor axis of the ellipsoid
c	[-]	Colour function
C_D	[-]	Drag coefficient
g	[m/s^2]	Gravitational acceleration
h	[m]	Cut off distance
I	[-]	Unit tensor
L_0	[m]	Initial distance between particles
m	[kg]	Mass of particle
N_p	[-]	Number of SPH particles
P	[Pa]	Pressure
ΔP	[Pa]	Pressure drop
r	[m]	Position
R	[m]	Radius of droplet
r_{ij}	[m]	Distance between particles *i* and *j*
t	[s]	Time
t	[-]	Time step
Δt	[s]	Time step size
u	[m/s]	Volume averaged fluid velocity
U	[m/s]	Superficial 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
γ	[-]	Interfacial tension
δ	[-]	Dirac delta function
ε	[-]	Thread thickness
ε	[-]	Immiscibility model parameter
η	[-]	Density ratio
λ	[-]	Viscosity ratio
μ	[Pa.s]	Dynamic viscosity
ρ	[kg/m^3]	Density
σ	N/m^2	Stress
τ	N/m^2	Shear stress
ξ	[-]	Channel width ratio
∇		Gradient operator

Subscript

c	Value for continuous phase
i	Value for particle of interest
j	Value for neighbouring particles
j	Value for jetting
d	Value for droplet
p	Value for particle
w	Related to wall
α	α-coordinate direction
β	β-coordinate direction
*	Intermediate state

Superscript

α	Number of dimensions
β	Number of dimensions
*	Dimensionless value

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