EXPERIMENTAL AND NUMERICAL INVESTIGATIONS OF GAS–LIQUID AND GAS–LIQUID–LIQUID FLOWS IN MICROCHANNELS

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by

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Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy

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Dedicated to My Parents, Wife and My Sons.

Certificate

This is to certify that the thesis entitled ***"Experimental and Numerical Investigations of Gas-Liquid and Gas-Liquid-Liquid Flows in Microchannels"***, being submitted by **V. M. Rajesh** to the Indian Institute of Technology Delhi, is worthy of consideration for the award of the degree of **Doctor of Philosophy** and is a record of the original bonafide research work carried out by him under my guidance and supervision. The results contained in the thesis have not been submitted in part or full, to any other University or Institute for the award of any degree or diploma.

I certify that he has pursued the prescribed course of research.

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Abstract

In chemical process industry; the need of cost competitive, energy efficient and environmentally benign processes initiated the development of micro-structured reactors and process equipment. Microreactors offered the controlled fluid manipulations and were used to perform the reactions in microchannels with typical dimensions of tens of micrometers up to a millimeter. Microreactors have broadly been employed to intensify chemical and biological processes, because of significant increase in quick analysis of products, reduction in sample volume and reactant consumptions. Microreactors enhanced the reactor performance and functionality by integrating the different components (microchannels) on to individual reactors. The high surface-area-to-volume ratio of microreactors leads to enhanced heat and mass transfer and interfacial transport phenomena. As a consequence, high conversion and selectivity can be achieved in comparison to conventional reactors.

The present thesis focused on experimental and numerical investigations on gas−liquid and gas−liquid−liquid flows in microchannels. Gas−liquid two−phase flows experiments were performed to investigate the effect of flow rates of continuous (water) and dispersed phases (air) on flow regimes, formation mechanisms of air bubbles/slugs and their corresponding lengths in T− and Y−junction microchannels. High speed imaging experiments were performed to identify and to map the gas−liquid−liquid flow regimes and to understand the effect of flow rates of continuous (kerosene) and dispersed phases (air and water), addition of surfactant in aqueous phase with various concentrations on the flow regimes,

formation mechanisms of air bubbles/slugs and water drops/slugs and also their lengths. Experiments were also performed to control the generation of air bubbles and water drops with embedded capillary needles of different sizes for air and water inlets. This particular study was done to investigate the effect of inlet distributors on three−phase flow regimes, formation mechanisms of bubbles and drops and their corresponding lengths. A variety of interesting three-phase gas−in−water−in−oil emulsions were also generated using flow focusing devise to increase the interfacial area of air bubbles per unit volume of water slug in continuous oil phase.

In addition to the experiments, numerical simulations of three−dimensional (3D) gas−liquid microchannel flow using the volume-of-fluid (VOF) method, as implemented in OpenFOAM were performed. Simulations were performed for a 1) prediction of gas−liquid flow regimes and their formation mechanisms in T−and Y−junction microchannels, and 2) the prediction of lengths of air bubbles/slugs. In addition, an unified correlation was developed to predict the lengths of air bubbles and slugs in T− and Y−junction microchannels.

For the first time, 3D VOF simulations were also performed to simulate the gas-liquid-liquid flows in a T−junction microchannel using the commercial CFD solver Fluent 14.0. The predictive capability of VOF method was tested to predict the three phase gas−liquid−liquid flow regimes. The numerical predictions for two−phase (gas−liquid) and three−phase (gas−liquid−liquid) flow regimes, formation mechanisms of bubble/drop or slugs and their corresponding lengths showed an excellent agreement with the experimental data. The results presented in this thesis will be important to understand the hydrodynamics of three−phase gas−liquid−liquid flows in microchannels which in turns to device microreactor systems for catalytic reactions involving gas−liquid−liquid flows.

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Nomenclature

Notations

U_G	superficial velocity of gas phase, m/s
U_L	superficial velocity of liquid phase, m/s
Q_{water}	volumetric flowrate of water, m^3/s
Q_{oil}	volumetric flowrate of oil, m^3/s
d_h	hydraulic diameter, mm
Ca	capillary number, (Ca=$\mu * U/\sigma$)
Ca_{oil}	capillary number for oil phase-defined at 1^{st} T-junction as $Ca_{oil} = \mu_{oil} U_{oil}/\sigma_{ail-oil}$ and at the 2^{nd} T-junction as Ca_{oil}= $\mu_{oil} U_{oil}/\sigma_{water-oil}$
A_{GI}	cross sectional area of gas inlet distributor, mm^2
A_{ch}	cross sectional area of channel, mm^2
we_{water}	weber number of water, (we_{water} = $d_h U^2_{water} \rho_{water})/\sigma_{water-oil}$)

we_{air}	weber number of air, (we_{air}= $d_h U_{air}^2 \rho_{air}$ $/\sigma_{air-oil}$))
ρ_{air}	density of air
$\rho_{air-oil}$	density of air and oil, kg/m^3

d	diameter of channel, m
D	channel depth, m
w	channel width, m
H	channel hight, m
L	length of main channel/solution domain, m
F	frequency of bubble of slug formation, 1/s
T	bubble formation period, s
R	curvature
g	gravitational constant, m/s^2
n	surface normal vector
P	pressure, Pa
t	time, s
U	superficial velocity, m/s
u	mean liquid velocity, m/s
Re	Reynolds number ($=\rho * d * U/\mu$)
W_i	gas inlet

Greek letters

α	volume fraction, dimensionless

μ	molecular visocity, Pa.s
θ	contact angle
ρ	density, kg/m^3
σ	surface tension, N/m
ϕ	line constant
ε	gas hold-up or volumetric fraction
Υ	ratio of gas inlet width and channel width
β	geometrical angle of entry of gas in main channel at junction

Subscripts

g, G, Air	gas phase
l, L, liquid	liquid phase
oil	oil phase
B	bubble
a	axial curvature
r	radial curvature
L	laplace
Ch	channel
GI	gas inlet
GI	gas inlet distributor
air−oil	air and oil

Acronyms

SDS	Sodium Dodecyl Sulfate
PMMA	Polymethyl methacrylate
VOF	Volume-of-Fluid
OpenFOAM	Open Field Operation and Manipulation