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Principle-based design of distributed multiphase segmented flow

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ABSTRACT

The design of systems incorporating multiphase flows remains a significant challenge for applications including lab-on-chip and microreactors. Segmented two-phase flow is used for the purpose of distributing biological samples from one site to many, enhancing heat and mass transport over laminar single phase flow and rapid chemical synthesis. This paper examines hierarchical designs, regularly utilised in such applications, that transport a segmented gas–liquid flow over an area with maximal thermodynamic performance. Fundamental design rules, predicted using the constructal method, minimize flow resistance of elemental bifurcations. The predicted geometric configuration follows an alternative to the established Murray's law (or Hess–Murray law) when the global pressure difference is dominated by short liquid slugs and dispersed gas phase. Breakup of phases in the junction region was examined numerically with a volume-of-fluid approach to develop a general criteria where junction losses are non-negligible. Although this loss is periodic, the interfacial pressure during the necking stage of the dispersed phase dominates. Using the findings for an elemental bifurcation, multiple scale hierarchical configurations for combined fluid and heat transport were assessed. The multiple scale tree-shaped design can be advantageous for low thermal resistance and pumping power requirements compared to a single scale serpentine layout. The principle-based method and results can reduce the design space in high-fidelity investigations of microscale segmented flows.

1. Introduction

Research on systems which involve multiphase transport, and in particular segmented flow without phase change, cover a broad range of applications including biofluidics [1], microreaction [2], bubble logic [3] and heat exchange technologies [4]. Such widespread applications take advantage of segmentation for a number of reasons. Controlled manipulation of small volumes in compartments which are separated from an outer environment benefits process throughput and homogenisation, while also preventing contamination issues. Indeed, compartmentalisation of a liquid is core to one of the most fundamental principles of nature, the formation of cells and the development of multicellular organisms. Through decoupling cell internal chemistry from outer environmental conditions, such compartments have supported the evolution of life [5]. Homogenisation is a key factor for reproducible products in microreactors, and is achieved through the unique control of enhanced heat and mass transport that features in segmented flows at low Reynolds numbers and mini- and microscales. This wide range of applicability has led to increased research interest on transport phenomena of segmented flows.

Previous studies have provided an insight into both the fluid mechanics and heat transport characteristics due to flow segmentation [6–13], with a focus on a single channel configuration. The design of higher complexity systems which can carry segmented multiphase mixtures across the working area of a device and enhance transport phenomena is currently a major challenge, but necessary for advancement of the previously discussed applications. In multiphase systems, design and prediction of performance characteristics using high-fidelity numerical approaches is typically limited to simplified configurations. This limitation is mainly attributed to challenges resolving interfaces between dissimilar phases and the multiple length scales that exist. It remains a challenge to accurately predict and resolve the interface, leading to the development of a number of continuum numerical methods including volume-of-fluid with interface reconstruction, level-set and front tracking [14]. For segmented flows in a channel, the large disparity of length scales is also evident as the film thickness can be $\delta \sim 0.01D$ or less [15]. It is unsurprising therefore, that combined numerical and experimental approaches such as that recently presented by Khodaparast et al. [16] are necessary to make confident high-fidelity predictions.

While numerical approaches supplemented with experiment provide a detailed spatio-temporal insight into complex multiphase

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Nomenclature

Variable	
A	area, [m^2]
a, b, c, C_i	constants, [–]
Ca	capillary number, [–]
C_p	specific heat capacity, [J/kg K]
D	diameter, [m]
D_h	hydraulic diameter, [m]
f	friction factor, [–]
h	heat transfer coefficient, [W/m^2 K]
H	height, [m]
k	thermal conductivity, [W/m K]
K_a, K_b	interface curvatures, [m^{-1}]
L	length, [m]
$\dot{m}$	mass flow rate, [kg/s]
n	number of turns/bifurcations, [–]
Nu	Nusselt number, [–]
NTU	number of transfer units, [–]
p	non-dimensional pressure $= PD/\sigma$, [–]
P	pressure, [Pa]
Q	heat transfer rate, [W]
r	radius of disc, [m]
R	resistance
R_a, R_b	interface radii, [m]
Re	Reynolds number, [–]
S	serpentine spacing, [m]
Sv	svelteness $= A^{1/2}/A_p^{1/2}$, [–]
t	time, [s]
T	temperature, [K]
U	two-phase velocity $= U_l + U_g$, [m/s]
U_l	liquid velocity, [m/s]
U_g	gas velocity, [m/s]
V	volume, [m^3]
$\dot{W}$	pumping power, [W]
x, y	coordinates, [m]
x, y	generic diameter, length ratio, [–]

Greek	
α	liquid fraction $= U_l/(U_l + U_g)$, [–]
β, γ	bifurcation angles, [°]
Γ	junction/channel loss ratio, [–]
δ	film thickness, [m]
δ_n	neck thickness, [m]
ϵ	void fraction $= U_g/(U_l + U_g)$, [–]
ε	effectiveness, [–]
θ	non-dimensional variable, [–]
λ, ζ	Lagrange multiplier, [–]
Λ	mesh parameter, [m]
μ	viscosity, [kg/m s]
ξ	volume fraction, [–]
ρ	density, [kg/m^3]
σ	surface tension, [N/m]
τ	non-dimensional time $= Ut/D$, [–]
ϕ, ψ	aggregate functions
φ	constant, [–]

Subscript	
amb	ambient
b	bubble
cv	convective
i	branch number
in	inlet
jc	junction
max	maximum
min	minimum
opt	optimum
0	entrance branch
p	channel perimeter
s	slug
seg	segmented
th	thermal
v	viscous
w	wall

Other	
$.^*$	non-dimensional thermal length, [–]
$\tilde{.}$	non-dimensional quantity, [–]
$\hat{.}$	dispersed/continuous ratio, [–]

flows, there is often a substantial cost in resources and time. This regularly makes it impractical for real systems, particularly at early design stages when there is a wide design space to investigate. Preliminary design approaches for pressure-driven microfluidic networks, such as that presented by Oh et al. [17], highlights the practical level of fidelity and simplifications that are regularly introduced in the design of complex concentration- and flow-dependent systems that comprise of junctions connected by capillaries.

Hierarchical designs are particularly useful for transporting segmented multiple phase flows as it can maintain phase segmentation while also providing a controlled distribution from a single source (input) to many users or locations (output). This configuration is therefore regularly used in microreactors [5,18] and lab-on-chip devices [19–21]. Hoang et al. [18] presented an example of a hierarchical design for parallel production of bubbles, formulating guidelines for stable operation including breakup and the production of uniform bubbles. This device used an assembly of multiple T-shaped bifurcations for parallelized production of bubbles and segments. Pressure-driven lab-on-chip devices similarly benefit from the use of bifurcated microchannels to create massively parallel analysis [19] through droplet splitting [20,21] and merging [21].

High-fidelity simulations, experiments and even less expensive circuit analogy approaches [17] suffer from a common disadvantage which is the need to investigate many design variations. The designer provides the configuration and iterates towards a final solution using a *Trial and Error* approach, supplemented with additional methods such as design of experiments [22] to limit the required number of trials. A more efficient way is to predict configuration, give direction for the high-fidelity methods, and narrow the design space.

The constructal method [23] is a principle-based approach that can be used to predict valuable design rules which provide thermodynamically optimal configuration, or geometric structure. An aim of this study is to demonstrate that even for complex multiphase transport, it is benefical to utilize such principle-based approaches to inform design. Bejan et al. [24] introduced constructal design for single phase flows that originate at a point and bath an area using a bifurcated construct. The authors confirmed Murray's well-established design rule for diameter ratio in laminar flow [25], also referred to as the Hess–Murray law [23]. Furthermore, geometric design rules were predicted for length ratio and the turbulent flow regime. These design rules for single phase flow have since been