Open-source CFD Digital Twin Model for High-Throughput Droplet Microfluidic Devices

1 CONTEXT

Digital twins are digital replicas of physical systems. In particular, a CFD (computational fluid dynamics) digital twin is a numerical representation of fluidic phenomena. For droplet microfluidics, fluidic interactions result in droplet formation at the crossing of immiscible phases. Uniform (monodisperse) droplets generated, have applications in pharmaceutical synthesis, diagnostics, cell analysis and other fields. Generating monodisperse droplets (typically < 5% coefficient of variation for volume) with various loads inside at high generation rates (typically >5 kHz) is technically challenging. Challenges include tuning flow parameters and junction geometry optimization to achieve the desired droplet volumes with adequate flow stability. Having a reliable, general-purpose, open-source digital twin would greatly simplify the design and parameter optimization process. The thesis project focuses on implementing a droplet generator digital twin in OpenFOAM (i.e. open source CFD software), as well as validating it on experimental data found in the literature. Furthermore, to demonstrate the utility of the digital twin, an existing or new droplet generator geometry (e.g., step emulsification geometry) should be optimized using it, to find the maximum possible generation rate and droplet size range. Optionally, the finalized device design may be fabricated via 3D printing and tested experimentally. The thesis topic can be taken by MSc students. Upon successful completion of all MSc thesis objectives, results will be used in project PRG620 and potentially published in scientific literature. Objectives for the thesis semester are highlighted, and the preceding objectives are for the master seminar.

2 OBJECTIVES

- Review existing literature on high-throughput microfluidic droplet generators and understand the fundamentals of microfluidics
- Get familiar with droplet microfluidics experiments and CFD simulation, as well as OpenFOAM
- Select and configure appropriate multiphase solver in OpenFOAM: evaluate performance of Volume of Fluid (VOF) method, select appropriate meshing method, droplet tracking algorithm and implement droplet size calculation in simulation
- Implement simulation of published experimental droplet generator setup, analyze error between simulation and experimental data
- [thesis semester] Assess and compare performance of existing technological solutions to the problem of high monodispersity associated with high-throughput droplet production in microfluidic devices
- [thesis semester] Set up a droplet generation simulation based on an initial high-throughput droplet production device (existing or novel design)
- [thesis semester] Parametric study of the device geometry to modify the initial design of the device geometry and/or include the nozzle type to meet the project requirements for droplet production rate and monodispersity (coefficient of variation)
- [thesis semester, optional] Make the final design with an SLA 3D printer.
- [thesis semester, optional] Experiment with the step emulsifier and compare the results to simulation results.

3 PREREQUISITES

- Prior knowledge of Fluid mechanics is an advantage
- Prior knowledge of CAD is an advantage
- Prior knowledge of CFD simulation tools is an advantage
- Interest in microfluidics and Lab-on-a-Chip research
- Self-motivation and the ability to work independently

4 REFERENCES

1. Mora, Angel & Silva, Ana & Lima e Silva, Sandro Metrevelle. (2019). Numerical study of the dynamics of a droplet in a T-junction microchannel using OpenFOAM. Chemical Engineering Science. 196. 514-526. 10.1016/j.ces.2018.11.020.
2. Fatehifar, M.; Revell, A.; Jabbari, M. Non-Newtonian Droplet Generation in a Cross-Junction Microfluidic Channel. Polymers 2021, 13, 1915. https://doi.org/10.3390/polym13121915
3. Stolovicki, Elad & Ziblat, Roy & Weitz, David. (2017). Throughput enhancement of parallel step emulsifier devices by shear-free and efficient nozzle clearance. Lab on a Chip. 18. 10.1039/C7LC01037K

5 CONTACTS

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Thomas Johann Seebeck Department of Electronics supports equal opportunities; female students are particularly encouraged to contact us.