Validation of a computational model for a coupled liquid and gas flow in micro-nozzles

R. Zahoor[1*], J. Knoska[2,3], J. Gregorc[1], S. Bajt[4] and B. Šarler[1,5]

[1]Laboratory for Fluid Dynamics and Thermodynamics, Faculty of Mechanical Engineering, University of Ljubljana, Aškerčeva 6, 1000 Ljubljana, Slovenia
E-mail: rizwan.zahoor@fs.uni-lj.si, jurij.gregorc@fs.uni-lj.si, bozidar.sarler@fs.uni-lj.si

[2]Center for Free Electron Laser Science, DESY, Notkestraße 85, 22607 Hamburg, Germany
[3]Dept. Physics, University of Hamburg. Luruper Chaussee 149, 22761 Hamburg, Germany
E-mail: juraj.knoska@desy.de

[4]Deutsches Elektronen-Synchrotron DESY, Notkestraβe 85, 22607 Hamburg, Germany
E-mail: sasa.bajt@desy.de

[5]Laboratory for Simulation of Materials and Processes, Institute of Metals and Technology, Lepi pot 11, 1000 Ljubljana, Slovenia
E-mail: bozidar.sarler@imt.si

ABSTRACT

The work presents a numerical model for micro-jet focusing, where a coupled liquid and gas flow occurs in a gas dynamic virtual nozzle (GDVN). The micro-jets are efficient vectors of mass and momentum and find applications in countless scientific domains. The focus here is their use in serial femtosecond crystallography [1] as sample carriers for interaction with X-ray beam. For sample delivery the following performance criteria are necessary: the jet to be longer than 100 µm to avoid nozzle shadowing, the diameter smaller or equal to 1 µm to minimize background signal and the speed high enough that the same crystal sample is not exposed twice to the X-ray beam, operating at a frequency in the range 120 Hz - to few kHz. A comprehensive numerical investigation is carried out for operating parameters, nozzle geometry and types of focusing gases [2,3,4], where the present work focuses on numerical analysis of the jet velocities at the tip and their comparison with the experimental data. The coupled numerical model of GDVN considers a laminar two-phase, Newtonian, compressible flow, which is solved based on the finite volume method discretization and interface tracking with volume of fluid (VOF). Numerical solution is calculated with OpenFOAM based compressible interFoam solver, which uses algebraic formulation of VOF. A counter-gradient scheme is used to avoid the interface smearing. In experimental setup a 3D printed GDVN was inserted in a vacuum chamber with two windows used for illumination and visualization. Once the jet stabilized its velocity was estimated based on cross-correlation between the signals from two thin laser beams passing through the jet with a known separation distance. The computational and experimental study was performed for a constant liquid flow rate of 14 ul/min and the gas flow rate from 5 mg/min to 25 mg/min. The coupled numerical model correctly predicted the jet speed and shape as a function of the gas flow. The paper represents the first attempt of validation of the coupled micro-jet model with respect to variation of the focusing gas flow.

Keywords: gas dynamic virtual nozzle, micro-jet, jet shape, jet velocity, coupled numerical model

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