Numerical simulations of gas-focused micro jets

Grega Belšak[1], Božidar Šarler[1,2], Kenneth R. Beyerlein[3], Juraj Knoška[4], Luigi Adriano[5], Henry N. Chapman[3,4,6], Saša Bajt[5]

[1]Laboratory for Simulation of Materials and Processes,
Institute of Metals and Technology, Lepi pot 11, SI-1000 Ljubljana, Slovenia
email: grega.belsak@imt.si, bozidar.sarler@ung.si

[2]Laboratory for Multiphase Processes
University of Nova Gorica, Vipavska 13, SI-5000 Nova Gorica, Slovenija

[3]Center for Free Electron Laser Sciences,
Deutsches Elektonen-Synchrotron, Notkestraße 85, 22607, Hamburg, Germany

[4]Department of Physics, University of Hamburg, Luruper Chaussee 149, 22607, Hamburg, Germany

[5]Photon Science, Deutsches Elektronen-Synchrotron, Notkestraße 85, 22607, Hamburg, Germany

[6]Centre for Ultrafast Imaging, Notkestraße 85, 22607, Hamburg, Germany

ABSTRACT

The paper describes numerical modelling and simulation of gas-focused micro-jets used in delivery of samples in femtosecond crystallography, where the formation of a stable, thin, long and reliable jet represents an utmost priority [1]. Modelling is performed for axisymmetric arrangement of the nozzle and allows for coping with the dripping and jetting regimes [2]. Simulations are done for strongly coupled buffer liquid with the samples and the focusing gas. The liquid can be arranged as a single jet or as a configuration of a focusing liquid and buffer liquid. The later is advantageous since it allows for lower consumption of already scarce buffer. Numerical simulation of listed configurations is a highly complex task. It represents a great computational challenge due to the multiphase nature of the problem and the sub-micron size discretisation for high resolution and proper capturing of the flow. Additionally, in order to avoid numerical errors of the artificial outlet boundary the entire computational domain needs to be in the order of millimetre, which results in a very fine discretisation. The coupled gas-liquid models were solved with the open source computational fluid dynamics toolbox called OpenFOAM [3]. Two multiphase solvers were used, one of which needed to be modified in order to properly describe the interface between the focusing liquid and the gas. In this study three different incompressible physical models were considered and compared: a model without fluid focusing, a model that includes no-mixing of the two fluids (multiphaseInterFoam solver) such as water and oil, and a model where diffusion was permitted between the two liquids (modified InterMixingFoam solver), such as water and alcohol. It was found that in order to get the results independent of the choice of mesh, the finest cell size needed to be well below 0.5 μm. Parametric analysis was performed in order to study how the changing operating parameters of fluids and the nozzle geometry affect the jet formation. In particular we studied, how the flow rates of gas, focusing liquid and buffer are coupled with the jet length, diameter and its stability. In the physical model that accounts for diffusion the effects on the concentration profile through the jet were analysed. Findings of the simulations show that for the same set of parameters the jet is longest in the model with two fluids and diffusion, which is in good agreement with the obtained experimental data. In the future, also a three-dimensional model will be attempted that would allow to predict also the unstable whipping mode of the jet.

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