Paper ID: 77244
oral
student

IAF MICROGRAVITY SCIENCES AND PROCESSES SYMPOSIUM (A2)
Science Results from Ground Based Research (4)

Author: Mr. Vishal Hugar
R V College of Engineering, Bengaluru, India, vishalhugar.ae21@rvce.edu.in

Mr. Shivayya Hiremath
R V College of Engineering, Bengaluru, India, shivayyach.ae20@rvce.edu.in
Ms. Shruthishree S
R V College of Engineering, Bengaluru, India, shruthishrees.ch21@rvce.edu.in
Prof.Dr. Ravindra Kulkarni
R V College of Engineering, Bengaluru, India, ravindraskulkarni@rvce.edu.in
Ms. Sejal Jain
R V College of Engineering, Bengaluru, India, sejaljain.ae20@rvce.edu.in

A NUMERICAL ANALYSIS IN HYBRID CONTINUUM-MOLECULAR DYNAMICS OF MICROFLUIDIC FLOWS THROUGH FLUIDIC CARD GEOMETRIES

Abstract

Microfluidics is a vast and important field, its applications ranging from molecular biology to microelectronics; with vast applicability in space technology. Microfluidics cards – with channels and wells – are used for microbiological experiments in space whose results have massive implications. As is the norm for modern engineering projects, any microfluidics card must go through rigorous analysis and simulation before prototyping and production. Computational fluid dynamics (CFD) uses numerical methods to analyze fluid flows. However at a certain flow scale, continuum dynamics cannot be accurately applied to fluid flows. In such instances, the use of Molecular Dynamics simulations would be more pertinent as they would more accurately simulate the "flows" at sub-micro and nano scales. Molecular dynamics (MD) is a simulation technique used to analyze the motion and interaction of atoms and molecules. Though accurate, MD simulations tend to be extremely computationally expensive and time consuming. This limits their use in modeling entire micro and nano-scale flows. The two methods of CFD and MD can be coupled by modeling a flow wherein a majority is governed by continuum mechanics, a small critical region is governed by MD, and an overlapping hybrid region which interfaces the CFD and MD regions. The foreseen advantages of this is the reduced computational cost over a purely MD simulation, and increased accuracy and precision in critical regions over a purely CFD simulation. CFD and MD simulation methods can be coupled by using Open FOAM (CFD simulation tool) as a base, and calling upon LAMMPS (MD simulation tool). This paper focuses on the hybrid CFD – MD simulations of flow over certain geometries in microfluidic cards. Flows in microfluidic cards face a unique set of challenges that often need special characterization. The flow around these unique geometries and flow regimes specific to microfluidic cards have been analyzed in this paper through a hybrid continuum-molecular dynamics numerical simulation. Furthermore, this hybrid analysis has been compared to traditional CFD methods to identify the advantages it offers, and to realize the situations in which the use of a hybrid method would be most appropriate.