OpenQBMM - A Next-Generation Open-Source Computational Fluid Dynamic Code for Polydisperse Multiphase Flows in Science and Engineering

Alberto Passalacqua†, Rodney O. Fox††, Simanta Mitra∗

†Department of Mechanical Engineering, ††Department of Chemical and Biological Engineering, ∗Department of Computer Science

Period of performance: October 1, 2014 – September 30, 2017

2016 NSF – SII PI Meeting

CONTRIBUTION

OpenQBMM is an open-source suite of codes, based on OpenFOAM® for multiphase reacting flows. Target applications are:

- Turbulent reacting flows
- Gas-liquid flows
- Gas-solid flows

THE COMPUTATIONAL FRAMEWORK

The computational framework that will be implemented relies on quadrature-based moment methods (QBMM) and high-order realizable numerical schemes to guarantee the moment realizability accuracy of the results.

QUADRATURE-BASED MOMENT METHODS

Multiphase reacting flows can be described by solving a generalized population balance equation, whose unknown is the number density function (NDF). To reduce the computational cost, transport equations are obtained for the moments of the NDF. These equations are closed using Gaussian quadrature formulae, which allow the calculation of the source terms in the moment transport equations.

QBMM allow the NDF to be reconstructed either with a weighted sum of Dirac delta functions or of non-negative kernel density functions, in case a continuous form of the approximate NDF is desired for accuracy.

YEAR 1: POPULATION BALANCE EQUATION

A PBE solver, suitable to simulate flows at low particle concentration, with particles of small size, incapable of significantly affecting the fluid motion was developed and published during year 1 of the project. An example verification and validation case showing the time evolution of the particle size in a process involving aggregation and breakup of particles is shown in the figure.

SOFTWARE DISTRIBUTION AND COMMUNITY

The developed software package is distributed under the GNU GPL 3 license, with documentation and tutorials.

EDUCATION AND COMMUNITY INVOLVEMENT

Three graduate students supported: David Williams, Ehsan Madadi, Jeffrey Heylmann.

External contributions to code and algorithm development from:

- Frédérique Laurent-Nègre, École Centrale Paris
- Matteo Icardi, University of Warwick

CONTACTS

- Website: www.openqbmm.org – E-mail: openqbmm@outlook.com
- GitHub: https://github.com/OpenQBMM
- Follow us on Twitter: @OpenQBMM

This work is supported by the National Science Foundation of the United States, under the SI2 – SSE award NSF – ACI 1440443.