NUMERICAL SOLUTION OF BIVARIATE POPULATION BALANCE EQUATION USING AN OPEN-SOURCE FINITE ELEMENT CFD FRAMEWORK

A THESIS

submitted by

DEEPAK KUMAR SINGH

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of

MASTER OF SCIENCE

(by Research)

Supervisor: DR GAURAV BHUTANI

SCHOOL OF ENGINEERING

INDIAN INSTITUTE OF TECHNOLOGY MANDI

MAY 2021

DECLARATION

This is to certify that the thesis titled "**Numerical solution of bivariate population balance equation using an open-source finite element CFD framework**", submitted by me to the Indian Institute of Technology Mandi, for the award of the degree of Master of Science (by Research), is a bona fide record of the research work carried out by me under the supervision of **Dr Gaurav Bhutani**. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

Place: Mandi

Date: 20 MAY 2021

Deepak Kumar Singh

THESIS CERTIFICATE

This is to certify that the thesis titled “**Numerical solution of bivariate population balance equation using an open-source finite element CFD framework**”, submitted by **Deepak Kumar Singh** to the Indian Institute of Technology Mandi, for the award of the degree of Master of Science (by Research), is a bona fide record of the research work done by him under my supervision. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

Dr Gaurav Bhutani

Date: 20 MAY 2021

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ABSTRACT

The population balance equation (PBE) is an established mathematical framework to explain the evolution of polydisperse multiphase systems. The employment of a bivariate or multivariate PBE model, characterized by two or more internal coordinates, is required to analyse a variety of systems. The direct quadrature method of moments (DQMOM), a computationally economical and favourable numerical method for the PBE–computational fluid dynamics (CFD) coupling, can be conveniently applied for solving bivariate or multivariate PBEs. In the past, DQMOM has been implemented in a few commercial finite volume CFD packages to solve bivariate PBEs. However, to date, no open-source CFD package contains this numerical technique for solving the bivariate PBEs as a standard implementation. In this work, for the numerical solution of the bivariate PBE the DQMOM is for the first time implemented in an open-source CFD code—Fluidity. This efficient numerical framework is a highly-parallelised finite element (FE) CFD code that allows for the use of mesh adaptivity on fully-unstructured meshes. To evaluate the accuracy of the bivariate PBE solution using DQMOM in the present FE framework, various test cases to solve spatially homogeneous bivariate PBEs with aggregation, breakage, growth and dispersion (diffusion in phase space) were simulated and verified against analytical solutions, resulting in excellent agreement. Benchmarking, by comparison with the Monte-Carlo method solutions from the literature, with realistic kernels in a gas-liquid system for simultaneous bivariate aggregation and breakage was also performed to show the feasibility of this implementation for realistic applications. This open-source framework demonstrates its impressive potential in the case of bivariate PBE and can be exploited for the simulation of the complex polydisperse multiphase system.

TABLE OF CONTENTS

Table of Contents (continued) **Page**