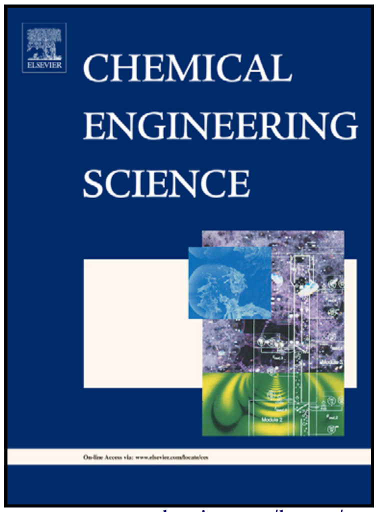

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PII: S0009-2509(15)00429-7
DOI: http://dx.doi.org/10.1016/j.ces.2015.06.021
Reference: CES12424

To appear in: *Chemical Engineering Science*

Received date: 9 February 2015
Revised date: 28 May 2015
Accepted date: 11 June 2015

Cite this article as: Daniel Deising, Holger Marschall, Dieter Bothe, A Unified Single-Field Model Framework for Volume-Of-Fluid Simulations of Interfacial Species Transfer applied to Bubbly Flows, *Chemical Engineering Science,* http://dx.doi.org/10.1016/j.ces.2015.06.021

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A Unified Single-Field Model Framework for Volume-Of-Fluid Simulations of Interfacial Species Transfer applied to Bubbly Flows

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Abstract

Most methods for Direct Numerical Simulations of interfacial species transfer across fluid interfaces suffer from poor stability, accuracy and/or the loss of conservativeness or boundedness properties. In literature this is often attributed to shortcomings in the 'numerics'. This paper presents a single-field *model*, termed *Continuous Species Transfer (CST)* model. The resulting numerical method is virtually void of above problems.

In detail we shall set out the model's derivation procedure which is based on the Conditional Volume-Averaging technique and thus *guides* our consistent Finite Volume discretisation practice. The CST method enables the simulation of species transfer in two-phase flows in a realistic range of Henry coefficients and diffusivity ratios in the context of algebraic Volume-Of-Fluid (VOF) interface capturing techniques, given a sufficient resolution of the concentration boundary layer with at least four to five computational cells. Beside setting out the mathematical and numerical foundation of the CST method, we present a sound validation study. The CST method is then applied to the case of interfacial species transfer from single rising bubbles in quiescent liquids. Our method development and numerical simulations have been based on OpenFOAM®, in particular its algebraic VOF solver family `interFoam`.

Key words: Interfacial mass transfer, Single rising bubble, Conditional Volume-Averaging, Computational Fluid Dynamics, Volume-Of-Fluid method, OpenFOAM

1. Introduction

In various industrial applications based on dispersed two-phase systems, e.g. in spray towers and bubble columns used in chemical engineering, detailed knowledge of the hydrodynamics like fluid particle interactions, induced turbulence, rise velocities and fluid particle size distributions are of fundamental importance. However, especially for applications in the chemical industry,

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