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A least-squares method with direct minimization for the solution of the breakage–coalescence population balance equation

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Abstract

A least-squares method with a direct minimization algorithm is introduced to solve the non-linear population balance equation that consists of both breakage and coalescence terms. The least-squares solver, direct minimization solver together with a finite difference solver are implemented for comparisons. It is shown that the coalescence term introduces a strong non-linear behavior which can affect the robustness of the numerical solvers. In the comparison with the least-squares method, the direct minimization method is proved to be capable of producing equally accurate results, while its formulation is better conditioned. In the case of a non-linear population balance equation system, the direct minimization method converges faster than the standard least-squares method.

Keywords: Population balance equation; Least-squares method; Direct minimization; QR decomposition

1. Introduction

The population balance is a widely used tool in engineering, with applications including crystallisation, pharmaceutical manufacture, pollutant formation in flames and growth of microbial and cell populations. A general population balance equation (PBE) consists of terms such as breakage, coalescence, growth and transport. Bubble breakage depends on the balance between external stresses that disrupt the bubble and surface/viscous stresses that resist the bubble deformation [6]. Coalescence may result from velocity difference in gas–liquid and liquid–liquid systems, and from surface properties of the particles in solid–liquid and solid–gas system [6].

In practical chemical processes, bubbles/droplets can pass through regimes where subsets of the population balance terms are dominant [3]. In general, the bubble coalescence is more complex than the bubble breakage since it involves the interaction between two bubbles and the intervening liquid film from the continuous phase [6]. Numerically, the coalescence term in the PBE is non-linear and could result in a complex convergence behavior.

Using the population balance model the dispersed phase is commonly treated using a density function, DF, which is a function of time, property and spatial position. Solution of the density function is necessary to determine the properties

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Nomenclature

$\mathcal{A}$	bilinear operator
b	breakage function
b_c	equivalent coalescence rate
$\mathcal{B}$	total rate of breakage
c	coalescence function
$\mathcal{C}$	total rate of coalescence
C_1, C_2	constants
f	function, distribution function
f_l	nodal value
f_N	solution in X_N space
$\mathcal{F}$	continuous linear operator
g	source term
G	problem definition function
h	redistribution function
$\mathcal{J}$	objective function
k	index of the iteration step
k_0	parameter
L	parameter defined in test case
$\mathcal{L}$	linear operator, population balance operator
$\mathcal{L}_b$	breakage operator
$\mathcal{L}_c$	coalescence operator
N	degree of the polynomials
$\mathcal{Q}, \mathcal{R}$	matrices from QR decomposition
s	internal coordinate
v	a function in X
w	quadrature weights
X	function space
$\mathcal{X}_\Omega$	mapping between function and standard domain
Y	mapped function space

Greek letters

α	coalescence rate parameter
δ	difference between two successive iteration steps
ε	perturbation, error
θ	relaxation parameter
$\mathbf{\Lambda}$	diagonal weights matrix
ξ	independent variable, internal coordinate
$\hat{\xi}$	independent variable in the standard domain
Φ	basis function
Ω	domain of the system

Abbrevations

DF	density function
DM	direct minimization
FDM	finite difference method
GL	Gauss–Legendre
GLL	Gauss–Lobatto–Legendre
LSM	least-squares method
PBE	population balance equation