Journal of Computational Physics 334 (2017) 419–441

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A moving mesh interface tracking method for simulation of liquid–liquid systems

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ARTICLE INFO

Article history:
Received 12 August 2016
Received in revised form 19 December 2016
Accepted 9 January 2017
Available online 11 January 2017

Keywords:
Interface tracking
Moving mesh
Liquid–liquid system
CFD
OpenFOAM

ABSTRACT

This manuscript presents a moving mesh interface tracking procedure, with a novel treatment for phase coupling. The new coupling strategy allows accurate predictions for the interface behaviour in a wide range of macroscopic properties with great potential to explore liquid–liquid systems. In this approach, governing equations are applied to each phase individually while the interface is represented by a zero-thickness surface that contemplates inter-phase jumps. These equations are described in an arbitrary Lagrangian–Eulerian finite volume framework. Computations consider the pressure-corrector *PISO* method. The new treatment for phase coupling incorporates the interfacial jump updates within the pressure/velocity calculations. Additionally, cell-centred values from both phases are considered when calculating convective and diffusive terms at the interface. The employment of *GGI* (Generalized Grid-Interface) interpolation provides conservative data mapping between surfaces for non-conformal meshes. The prediction capability of the new formulation is evaluated under different dominant effects governing interface motion. Simulated cases include gravity and capillary waves in a sloshing tank, three-dimensional drop oscillation for liquid–liquid systems and drop deformation due to shear flow. The numerical results show good agreement with analytical transient profiles of interface position. The procedure is able to successfully represent systems with similar macroscopic properties, i.e. density and viscosity ratios approaching unity, and a broad range of interfacial tensions.

1. Introduction

Multiphase systems are present in several fields such as polymer, petroleum, cosmetics and food industries. These systems are often encountered as dispersions where particles are suspended in a continuous medium. Processes as flotation and liquid–liquid extraction use the dispersion increased contact area to promote higher mass transfer rates [1,2]. Dispersed systems are also well-known products of the everyday, notwithstanding the actual development on sophisticated applications such as polymer blending [3] and nano-emulsions [4]. It is therefore essential to understand and predict the behaviour

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http://dx.doi.org/10.1016/j.jcp.2017.01.011

Nomenclature

a_0	initial disturbance on the interface
a_N	off-diagonal coefficients of the linear system
a_P	diagonal coefficients of the linear system
AP, BP	volume centroids on both sides of interface
AN, BN	centroids for neighbour volumes of (AP, BP)
B	minor axis of ellipsoid
C	closed curve bounding area element
Ca	capillary number
$\mathbf{d}$	distance vector
D_f	deformation parameter
$\mathbf{F}_S^\sigma$	interfacial tension force
$\mathbf{g}$	gravity acceleration
$\mathbf{H}$	terms from linear system $\mathbf{H} = -\sum_N a_N \mathbf{v}_N + \mathbf{r}_P$
H	height of fluid layer
L	major axis of ellipsoid
l	oscillation mode number
$\dot{m}$	mass fluid flow
$\mathbf{m}$	unit binormal vector
$\mathbf{n}_I$	interface normal vector
$\mathbf{n}$	outward pointing normal of control volume
N	neighbour control volume
P	analysed control volume
p	modified pressure as $p = p_{abs} - \rho(\mathbf{g} \cdot \mathbf{r})$
$\mathbf{r}$	position vector
R	radius
$\mathbf{r}_P$	source term of linear system
T	total simulated time
t	time
$\mathbf{t}$	unity tangent vector
$\mathbf{T}$	stress tensor
$\mathbf{v}$	velocity vector
V	volume
$\dot{V}$	volume flux due to mesh motion
W	width of sloshing tank
y_a, y_n	analytical and numerical interface profiles

Greek letters

$\mathbf{\Delta}_f$	vector parallel to $\mathbf{d}_{NP}$
Δ_p, Δ_v	pressure and velocity interfacial jumps
Δt	timestep size
η	density ratio
$\dot{\gamma}$	shear rate
κ	mean surface curvature
λ	viscosity ratio
μ	viscosity
ν	kinematic viscosity
ω	relative distance used during interpolations
$\phi_{r,f}$	relative mass flux evaluated at face-centres
ρ	density
σ	interfacial tension
ξ	error

Subscripts

A, B	indicates the side of the interface
abs	absolute
e	related to the edge
eff	effective
f	related to the face
N	centroid of neighbour control volume
P	centroid of control volume under analysis
S	related to the surface

Superscripts

n	new time step
o	last time step before n
oo	last time step before o

Acronyms

GGI	generalized grid interface
$PISO$	pressure implicit with splitting of operator

of such systems, what would allow the development of high quality products or the design of efficient equipments and operations.

An important aspect of dispersions is their high ratio between contact area and total volume, which gives a prominent role to the interfacial behaviour over the system properties. For systems composed only by fluids, this translates into the interface motion and deformation in response to flow along with the interplay among interfaces. These two features are closely related to the nature of the phases that govern the overall interaction strengths. Although both gas and liquid states are recognized as fluids, which obey the same laws of motion, their inherent degrees of cohesive forces lead to distinct behaviours when combining gas or liquid dispersed particles with the same continuous media. Since condensed phases are characterized by well-packed molecules with high cohesive forces, two liquid phases tend to interact more intensely than a gas–liquid combination.

In the continuum perspective, this leads to specific characteristics. For example, liquid–liquid systems always exhibit lower interfacial tension coefficients in comparison with the corresponding vapour–liquid system [5], which implies less work involved in expanding a drop's interface. Another distinct effect is the impact of momentum transfer upon the continuous phase velocity field. Due to its lower density, a bubble must present much higher speeds than a drop to significantly affect the velocity field of the continuous phase. Besides, bubbles usually exhibit negligible viscous effect compared to the medium in which they are immersed, as opposed to drops that can substantially contribute to the interfacial balance of shear stress because of their higher viscosity. In light of these observations, it can be concluded that two immiscible liquid phases display stronger two-way flow interactions when compared with a gas/liquid system, where the information flux is usually more expressive in one direction (i.e. from liquid to gas).

Besides the contrasting interdependence on the flow behaviour, the nature of the dispersed particles also influences the inter-particle forces [6]. This topic is of great importance because the interaction among individual particles has a direct