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Computational fluid dynamics simulation of fluid particle fragmentation in turbulent flows ☆

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ABSTRACT

A simulation methodology is presented that allows detailed studies of the breakup mechanism of fluid particles in turbulent flows. The simulations, based on large eddy and volume of fluid simulations, agree very well with high-speed measurements of the breakup dynamics with respect to deformation time and length scales, and also the resulting size of the daughter fragments. The simulations reveal the size of the turbulent vortices that contribute to the breakup and how fast the interaction and energy transfer occurs. It is concluded that the axis of the deformed particle and the vortex core axis are aligned perpendicular to each other, and that breakup sometimes occurs due to interaction with two vortices at the same time. Analysis of the energy transfer from the continuous phase turbulence to the fluid particles reveals that the deformed particle attains it maximum in interfacial energy before the breakup is finalized. Similar to transition state theory in chemistry this implies that an activation barrier exists. Consequently, by considering the dynamics of the phenomenon, more energy than required at the final stage needs to be transferred from the turbulent vortices for breakup to occur. This knowledge helps developing new, more physical sound models for the breakup phenomenon required to solve scale separation problems in computational fluid dynamics simulations.

1. Introduction

Multiphase flows are frequently encountered in the chemical, food, and process industries. In many cases the industrial processes are operated in the dispersed flow regime to ensure a good contact between the phases. By operating the processes at turbulent conditions the interfacial area can be controlled. The interfacial area is affected by the energy in the turbulent vortices that exert a disruptive stress which can fragment each fluid particle into two or more entities, resulting in an increased mass transfer area. Simultaneously, coalescence between the fluid particles may occur which counteracts fragmentation and reduces the interfacial area. In order to design new multiphase flow processes and predict the interfacial mass transfer area these two phenomena must be understood. Whereas flow field and turbulence can be simulated with computational fluid dynamics (CFD), there is a problem with separation of scales, i.e. fluid particles on micro to millimeter scale and the process on meter scale, that prevents CFD simulations of the breakup and coalescence phenomena. Instead CFD subgrid models are needed to predict the breakup rate, the number of fragments formed, the daughter size distribution and

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Nomenclature

A	interfacial area (m^2)
C	phase function (–)
d	fluid particle diameter (m)
$\mathbf{F}_i$	interfacial tension force (N)
g	gravitational acceleration ($m\,s^{-2}$)
p	pressure ($N\,m^{-2}$)
$\mathbf{S}$	strain rate (s^{-1})
$\mathbf{u}$	velocity (ms^{-1})
γ	normalized interfacial energy (–)
κ	curvature (m^{-1})
μ	dynamic viscosity ($N\,m^{-2}\,s$)
ρ	density ($kg\,m^{-3}$)
σ	interfacial tension ($N\,m^{-1}$)
$\mathbf{\Omega}$	rotation rate (s^{-1})

Subscripts

c	continuous phase
d	dispersed phase

also models for the coalescence rate. The framework needed to predict the size distributions using CFD and population balance modeling is well established and the algorithms are included in some of the commercial codes. Recent advances include development of a mathematical framework to include also higher order breakup, i.e. fragmentation into more than two daughter particles [1], and methodologies for making the computations efficient by calculating the moments of the size distributions [2]. By using CFD simulations combined with population balance modeling, to account for the breakup and coalescence phenomenon, the evolution of the dispersed phase size distribution can be quantified and the performance predicted at different operating conditions even for novel equipment [3]. However, the accuracy of the simulations relies on the choice of the breakage and coalescence models, since these give different predictions. Despite the fact the two phenomena have been studied for several decades and that numerous models have been proposed in the literature, the understanding of the phenomenon is not good. Liao and Lucas have recently reviewed the various assumptions used when deriving models for breakup and coalescence in turbulent flows [4,5].

Breakup of fluid particles occurs when the external disruptive stress caused by the continuous phase turbulence exceed the stabilizing stresses at the interface due to interfacial tension plus the stabilizing viscous stress of the fluid inside the particle. When the disruptive stress dominate the particle starts to stretch and deform, leading to formation of a neck that subsequently contracts, and finally two or more fragments are formed. A few years ago the author presented measurements of single fluid particle breakup in turbulent flows that shows that the breakup occurs within a few milliseconds [6]. This short time scale is comparable to the lifetime of the vortices, and indicates that breakup occurs due to interaction with single turbulent vortices. However this could not be proven experimentally since enough temporal and spatial resolution of the continuous phase turbulence could not be obtained. Another basic question is whether vortices smaller or larger than the fluid particles control the breakup rate. Currently there is no consensus in the literature if vortices larger than the fluid particle contribute to breakup. Some of the most popular models in the literature assume that only vortices smaller than and equal to the size of the fluid particles contribute to the breakup. It has been shown that relaxing this criterion in these models, significantly affects the predicted breakup rates, at some conditions more than an order of magnitude [7]. Consequently, models sensitive to these limits of integration are tunable and their description of the phenomenon might not be physically correct. Most breakup models have in common they contain one or more criteria for when breakup occur. Often the models contain a criterion for energy, i.e. breakup only occurs if the turbulent kinetic energy of the vortex exceeds a critical value. This critical value can be the interfacial energy of the mother particle, or the mean value of the increase in interfacial energy at cases of equal-sized breakup and the case of a very small and one large in binary breakup [8]. It can also be defined as the increase in interfacial energy resulting from the breakage [9].

In this work we assess if CFD simulations can be used to study the interaction between fluid particles and the turbulent vortices, and shed light on the mechanisms behind fluid particle breakup. This requires the model resolves the disruptive and cohesive stresses accurately. For this purpose we use a combination of large eddy simulations (LES) and volume of fluid (VOF) simulations in this study. CFD simulations based on DNS-VOF and LES–VOF formulations have been used in many multiphase flow studies. Li and co-workers used VOF simulations to analyze the breakup of viscous drops, subjected to shearing between parallel plates under laminar flow conditions [10]. Gotaas and co-workers studied collision outcome between liquid droplets [11]. The VOF model was also used by Lubin who studied air entrainment in breaking waves by using a combination of VOF and large eddy simulations [12]. A combination of LES and VOF was also used by Lacanette and coworkers to

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