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On the interfacial roughness scale in turbulent stratified two-phase flow: 3D lattice Boltzmann numerical simulations with forced turbulence and surfactant

R. Skartlien [a,e,f,*], E. Sollum [b,a], F. Fakharian [c,a], T.L. Palmer [d]

[a] FACE – The Multiphase Flow Assurance and Innovation Center, P.O. Box 40, N-2027 Kjeller, Norway
[b] Norwegian Institute for Air Research (NILU), P.O. Box 100, N-2027 Kjeller, Norway
[c] Technische Universität München, Arcisstraße 21, 80333 München, Germany
[d] Department of Physics, University of Oslo, P.O. Box 1048, Blindern, N-0316 Oslo, Norway
[e] Institute for Energy Technology (IFE), P.O. Box 40, N-2027 Kjeller, Norway
[f] Department of Chemical Engineering, NTNU, N-7491 Trondheim, Norway

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ABSTRACT

Numerical 3D simulations of turbulent, stratified two-phase shear flow with a surfactant laden interface were used to test and develop a phenomenological interfacial roughness scale model where the energy required to deform the interface (buoyancy, interfacial tension, and viscous work) is proportional to the turbulent kinetic energy adjacent to the interface.

The turbulence was forced in the upper and lower liquids in the simulations, to emulate the interfacial dynamics without requiring (prohibitively) large simulation domains and Reynolds numbers. The addition of surfactant lead to an increased roughness scale (for the same turbulent kinetic energy) due to the introduction of interfacial dilatational elasticity that suppressed horizontal motion parallel to the interface, and enhanced the vertical motion.

The phenomenological roughness scale model was not fully developed for dilatational elasticity in this work, but we proposed a source term that represents surfactant induced pressure fluctuations near the interface. This source term should be developed further to account for the relation between surfactant density fluctuations and turbulence adjacent to the interface. We foresee that the roughness scale model can be used as a basis for more general interfacial closure relations in Reynolds averaged turbulence models, where also mobile surfactant is accounted for.

Introduction

The development of a better understanding of turbulence near deformable interfaces has been a long standing research challenge, and experiments and numerical simulations have already revealed many important aspects of the structure of the interface and the adjacent turbulence (e.g., Lugt and Ohring, 1992; Tsai, 1996; Lombardi et al., 1996; Fulgosi et al., 2003; Guo and Shen, 2010). The interfacial fluctuations respond to the turbulent kinetic energy, length scales and vortex structures in the fluids adjacent to the interface (e.g., Rein, 1998; Hong and Walker, 2000; Brocchini and Peregrine, 2001a; Brocchini and Peregrine, 2001b; Smolentsev and Miraghaie, 2005; Hunt et al., 2011) and the turbulence is affected by the interfacial properties (elasticity, viscosity and energy), posing a two-way interface-turbulence coupling. For rigid or stiff interfaces, the turbulence structures resemble those of wall bounded flow, while more flexible interfaces with low energy content are easily deformed by the fluid motions, and the turbulence structures resemble those in the fluid interior, outside boundary layers.

The turbulence-induced interfacial roughness scale in stratified gas/liquid or liquid/liquid flow is an important quantity with respect to the hydrodynamic coupling between the phases. Many two-phase turbulence models for pipe and channel flow rely on interfacial friction models to predict the turbulent (axial) momentum flux transported over the interface from one fluid to the other. In Reynolds averaged models, such as k–ϵ models, one adopts an interfacial friction model that is often modelled in terms of a roughness scale (e.g., Durbin et al., 2001; Berthelsen and Ytrehus,

* Corresponding author at: FACE – The Multiphase Flow Assurance and Innovation Center, P.O. Box 40, N-2027 Kjeller, Norway. Tel.: +47 63 80 64 67; fax: +47 63 81 11 68.
E-mail address: roar.skartlien@ife.no (R. Skartlien).

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2005; Biberg, 2007; de Sampaio et al., 2008), and it is of importance to develop reasonable roughness scale models that can respond to the length, time and energy scales of the turbulence near the interface. Perhaps the most obvious natural system where the roughness scale is central, is the coupling between the ocean surface and the overlying wind (e.g., Charnock, 1955; Wu, 1980; Fernando, 1991). For example, the driving of hurricanes depends on the roughness scale (friction) but also entrainment (heat exchange by sea-spray or droplets) (e.g., Bao et al., 2011).

Earlier, we derived a phenomenological roughness scale model by assuming proportionality between the energy needed to deform the interface and the turbulent kinetic energy adjacent to the interface (Skartlien et al., 2014). Brocchini and Peregrine (2001a,b) formulated a Reynolds averaged model for the free surface layer, accounting for the interfacial fluctuations via an intermittency factor or a volume fraction profile, that can also be expressed in terms of a probability distribution (pdf) for the interface level, of the type developed in Skartlien et al. (2014). Mathematical models for the intermittency factors were discussed for the gravity dominated scarred or "scarified" regime, and the wavy regime. The entraining, "splashing" regime was modeled by a Gaussian pdf as function of distance from the mean interfacial level, and with a specified width in the interfacial layer. A similar Gaussian approach was invoked by Hong and Walker (2000) in a unified Reynolds averaged turbulence model that contained the interfacial layer as part of the model domain, rather than a boundary condition. However, the width of the interface was specified as an input parameter that was calibrated to experimental data.

A similar pdf approach for the interface layer was invoked by Skartlien et al. (2014), but in terms of a Boltzmann type of pdf, which was a function of the interfacial energy, and the interfacial energy was modelled in terms of gravitational and interfacial tension contributions, given a certain geometrical model for the interfacial deformations. Viscous losses in the adjacent fluids under interfacial deformation were accounted for in an approximate way. The thickness or roughness scale, or the RMS value of the interfacial fluctuations, was obtained by assuming equality between the average interfacial energy and a measure of the local turbulent kinetic energy near the interface. This model was tailored to turbulence controlled interfaces with entrainment, and it was tested against volume fraction profile data for gas/liquid pipe flow. The modelled roughness scale could be recast in terms of interfacial capillary, Weber, Froude and Reynolds numbers, and consistency with models for gravity dominated flows (Charnock, 1955; Wu, 1980) was demonstrated.

Small interfacial fluctuations in the non-entraining regime were studied in the current work, and we tested a small amplitude version of our roughness scale model against direct numerical simulations. The small amplitude version implies a more suitable geometrical model for small fluctuations, than the original large amplitude version of the model in the entraining regime. The numerical simulations provide information on the interfacial dynamics and structure, and the turbulence length scales and energies near the interface. This may offer an advantage over laboratory measurements where this detailed information may not always be available. The lattice Boltzmann simulation model we have developed (e.g., Furtado and Skartlien, 2010, and references therein; Skartlien et al., 2011) also includes surfactant, such that we were able to explore how the roughness scale depends on the surfactant dynamics on the interface in terms of Marangoni stresses.

Direct numerical simulations of *naturally developed* turbulence with interfaces in two-phase flow is computationally expensive due to the required domain size that is needed to obtain sufficiently large Reynolds numbers (e.g., Ménard et al., 2007; Guo and Shen, 2010). In contrast, *forced turbulence* in volumes near the interface allows one to drastically reduce the size of the computational domain while still obtaining sufficiently vigorous turbulence in the interfacial region. However, this offers only an approximate and qualitative way of studying the response and dynamics of the interface to turbulence, since one does not necessarily capture all aspects of the turbulence structures (morphology and size distribution of the vortex structures) that is found in naturally driven two-phase flows. Furthermore, the natural feedback on the turbulence from the interface is not necessarily captured.

The forcing scheme of ten Cate et al. (2006) for lattice Boltzmann simulations was implemented in our model. To prevent direct forcing of the interface and allow for a naturally developed flow near the interface, we invoked "forcing windows" that were tapered to zero well outside the interfacial region. The width of the interfacial region, in terms of the difference between the maximum and minimum heights of the interfacial fluctuations, depends on the forcing energy. The extent of the forcing windows (above and below the interfacial region) were chosen so that the largest energy input rate to the forcing did not cause interfacial fluctuations that overlapped with the forcing windows.

Surfactant lowers the interfacial tension on the average, so that the associated interfacial energy is reduced and the interface may be less stable with larger fluctuation amplitudes, if we assume the same forcing conditions. However, advection of surfactant on the interface in response to the external turbulent flow introduces surfactant density gradients when the interfacial flow is locally divergent/convergent (expanding/contracting). The associated interfacial tension gradients induces tangential Marangoni stresses that oppose the tangential velocities adjacent to the interface (e.g., Sarpkaya, 1996), and this provides a feedback effect that reduces the liquid turbulent kinetic energy near gas/liquid interfaces (e.g., Tsai, 1996; Lee and Saylor, 2010). Much focus has been put on this phenomenon in the context of suppressed surface renewal rates and gas transfer rates over the interface (with emphasis on CO_2 transfer from the atmosphere to the ocean). Tsai (1996) used numerical simulations to study the effect on the turbulent shear layer under the air–sea interface. The horizontal fluctuations were suppressed, and the vertical fluctuations were also attenuated, in the presence of insoluble surfactant. Lee and Saylor (2010) performed experiments in a wind/water tunnel with a surfactant monolayer, and confirmed that surfactant reduced both the subsurface turbulent fluctuations, and the gas mass transfer rate over the interface.

It must be noted that surfactant may also introduce viscous effects in the interface in addition to elasticity and Marangoni stresses. A more viscous interface acts stabilizing and may suppress capillary waves (the well known "oil-on-water effect"), while lowered interfacial tension, elasticity and Marangoni effects may act destabilizing on propagating waves (Blyth and Pozrikidis, 2004).

First, we develop a small amplitude version for the interfacial energy model, and this constitutes the main ingredient in the roughness scale model that we use in the current work. A discussion of the roughness scale model in terms of closure relations in turbulence models, follows thereafter. The 3D simulation setup with the oil/water/surfactant lattice Boltzmann model with forced turbulence is then summarized, before we discuss the roughness scale model in the context of the simulation results.

Model for the interfacial energy and roughness scale

An interfacial energy was derived in Skartlien et al. (2014), where we considered interfacial deformations with horizontal scale L (comparable to the turbulent length scale in the fluids parallel to the interface), and height scale δ (the vertical displacement relative to the unperturbed interface in the absence of turbulent kinetic energy). It was assumed that the characteristic fluctuation