

Effects of Surfactant and Viscoelasticity on Turbulent Bubbly Flows

by

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Dedicated to my kids M. Rafay and Urooj Fatima

ABSTRACT

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Interface-resolved direct numerical simulations are performed to examine the combined effects of soluble surfactant and viscoelasticity on the structure of a bubbly turbulent channel flow. The incompressible flow equations are solved fully coupled with the FENE-P viscoelastic model and the equations governing interfacial and bulk surfactant concentrations. The latter coupling is achieved through a non-linear equation of state which relates the surface tension to the surfactant concentration at the interface. The two-fluid Navier-Stokes equations are solved using a front-tracking method.

First, the effects of soluble surfactant on the lateral migration of a bubble in a pressure-driven channel flow are examined. Extensive computations are performed to investigate the bubble dynamics for a wide range of parameters. It is found that surfactant dramatically changes the bubble dynamics. In the clean case, the bubble position depends on its deformability, characterized by the Eötvös (Eo) and the capillary (Ca) numbers. The spherical bubble moves towards the wall, while the deformable one migrates away from it. On the other hand, in the presence of the surfactant, even the spherical bubble moves away from the wall. It is also found that the contaminated bubble stays away from the wall for $Eo \leq 0.1$ and $Eo \geq 1.5$ while it migrates towards the wall for $0.1 < Eo < 1.5$. Also, at high Eo , the onset of path instability is observed for both the clean and the contaminated cases. However, adding surfactant to the system triggers the path instability earlier and amplifies the oscillations afterwards.

Next, simulations are performed to examine the combined effects of soluble surfactant and viscoelasticity on the structure of a bubbly turbulent channel flow. It is found that, for the surfactant-free case, bubbles move toward the wall due to inertial lift force, resulting in formation of wall layers and a significant decrease in the flow

rate. Conversely, a high-enough concentration of surfactant changes the direction of lateral migration of bubbles, i.e., the contaminated bubbles move toward the core region and spread out across the channel. When viscoelasticity is considered, viscoelastic stresses counteract the Marangoni stresses, promoting formation of bubbly wall-layers and consequently strong decrease in the flow rate. The formation of bubble wall-layers for combined case depends on the interplay of the inertial and elastic, and Marangoni forces.

Further, effects of different types of surfactant are examined using the physical sorption kinetics. For Newtonian turbulent bubbly flow, effects of Triton X-100 and 1-Pentanol are examined. It is observed that the sorption kinetics highly affect the dynamics of bubbly flow. Minute amount of Triton X-100 is found to be sufficient to prevent the formation of bubble clusters. On the other hand, 100 times more of 1-Pentanol surfactant is not sufficient to prevent the formation of layers. For viscoelastic turbulent flow, it is found that, polymer drag reduction is completely lost for the surfactant-free case, and the addition of small amount of surfactant (Triton X-100) restores the polymer drag reduction for the viscoelastic turbulent bubbly flows.

Lastly, the polymer drag reduction of turbulent poly-dispersed bubbly flow is examined in the presence of soluble surfactant. It is found that the drag increases for the clean viscoelastic poly-dispersed bubbly flow but it is lower than the corresponding Newtonian flow due the lateral migration of large bubbles to the center of channel. In the presence of surfactant, the drag reduction for viscoelastic poly-dispersed bubbly flow is revived.

ÖZETÇE

Kabarcıklı Türbülanslı Akışlarda Yüzey Aktif Maddesi ve Viskoelastisitenin Etkileri

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Gaz-sıvı arayüzeyinin çözümlendiği doğrudan simülasyon yöntemi kullanılarak kabarcıklı ve türbülanslı kanal akışları üzerindeki çözülebilir yüzey aktif maddesi ve viskoelastisitenin ayrı ayrı ve kombine etkileri incelendi. Sıkıştırılmaz akış denklemleri FENE-P viskoelastik model denklemleri ve çözülebilir yüzey aktif maddesi evölüsyon bünye denklemleri ile birlikte sayısal olarak çözüldü. Ara-yüzeydeki yüzey aktif maddesinin yüzey gerilmesine etkisi doğrusal olmayan bir durum denklemi kullanılarak hesaba katıldı. Navier-Stokes denklemleri karışamayan iki-akışkanlı akışlar için ara-yüz izleme yöntemi kullanılarak çözüldü.

İlk olarak yüzey aktif maddesinin tek bir gaz kabarcığının basınç-tahrikli bir kanal-daki yanal hareketi üzerindeki etkileri incelendi. Kabarcık dinamiğini araştırmak amacıyla simülasyonlar büyük bir parametre aralığı için yapıldı. Yüzey aktif maddesinin akış dinamiğini dramatik olarak değiştirdiği tespit edildi. Yüzey aktif maddesinin bulunmadığı temiz ara-yüz durumunda kabarcığın kanal içindeki pozisyonunun Eotvos (Eo) sayısı ve kapilari sayısı (Ca) ile karakterize edilen kabarcığın deforme olabilmesine bağlı olduğu bulundu. Küresel kabarcık kanal duvarına doğru hareket ederken deforme olabilen kabarcık kanal merkezine doğru hareket etmektedir. Yüzey aktif maddesi eklenmesi durumunda ise küresel kabarcık bile kanal merkezine doğru hareket etmektedir. Buna ilave olarak $Eo \leq 0.1$ ve $Eo \geq 1.5$ durumunda kabarcık duvardan uzakta konumlanırken $0.1 < Eo < 1.5$ durumunda duvara doğru hareket etmektedir. Ayrıca büyük Eotvos sayısında hem temiz hem de kirlenmiş kabarcığın yörünge karasızlığına uğradığı gözlemlendi. Fakat yüzey aktif maddesi eklenmesi durumunda karasızlık daha önce başlamakta ve salınım genliği büyümektedir.

Daha sonra kabarcıklı ve türbülanslı kanal akışında yüzey aktif maddesi ve viskoelastisitenin ayarı ayrı ve kombine etkileri incelendi. Yüzey aktif maddesinin bulunduğu durumda aerodinamik kaldırma kuvveti etkisiyle kabarcıkların duvara doğru hareket edip orada kabarcık tabakası oluşturduğu ve bunun sonucu olarak ise akış oranının azaldığı bulundu. Yüzey aktif maddesi eklenmesi durumunda ise bunun tam tersi olarak kabarcıkların yön değiştirip kanal merkezine doğru hareket ettiği ve kanal kesitinde homojen olarak dağıldığı gözlemlendi. Viskoelastik etkilerin hesaba katıldığı durumda ise viskoelastik gerilmeler Marangoni gerilmesinin tersi yönde etki etmekte, duvardaki kabarcık tabakasının oluşmasına katkı sağlamakta ve bunun sonucu olarak akış debisi önemli ölçüde azalmaktadır.

Ayrıca değişik yüzey aktif maddelerinin etkileri de incelendi. Bu amaçla değişik sorpsiyon kinetik özelliklere sahip Triton X-100 ve 1-Pentanol yüzey aktif maddelerinin fiziksel özellikleri kullanılarak simülasyonlar yapıldı. Sorpsiyon kinetiğinin akış üzerinde çok büyük etkilerinin olduğu tespit edildi. Çok küçük miktardaki Triton X-100 maddesinin eklenmesiyle duvardaki kabarcık katmanının oluşumu tamamıyla engellenirken bunun 100 kat fazlası 1-Pentanol eklenmesinin bile önemli bir etkisinin olmadığı gözlemlendi. Viskoelastik türbülanslı akışlarda polimerin sürüklenme kuvvetini azaltan etkisinin nerede ise tamamıyla kaybolduğu ama yüzey aktif maddesi eklenmesiyle bu etkinin tekrar ortaya çıktığı tespit edildi.

Son olarak, yüzey aktif maddesiyle kirlenmiş polidispers kabarcıkların bulunduğu türbülanslı kanal akışında polimer kaynaklı sürüklenme kuvvetinin azalması incelendi. Yüzey aktif maddesinin olmadığı durumda kabarcıkların duvarda tabaka oluşturduğu ve Newtonsal duruma göre sürüklenme kuvveti azalsa da polimerlerin sürüklenme azaltma etkisinin büyük oranda ortadan kalktığı gözlemlendi. Yüzey aktif maddesi eklenmesi durumunda ise polimer kaynaklı sürüklenme kuvveti azalmasının tekrardan ortaya çıktığı bulundu.

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Chapter 1

INTRODUCTION

Multiphase/multi-fluid flows are ubiquitous in many natural processes and industrial applications. Understanding of such flows is very essential to predict the behavior of natural and industrial processes. A free-falling rain droplet in air, pyroclastic flows from volcanoes, sedimentation flows in river bed, and also different biological flows such as blood cells moving in vessel are few examples of natural processes. Multiphase flows are also frequently encountered in many industrial applications such as core annular flows for oil transportation in petroleum industries, atomization and sprays in painting coating and cooling, irrigation, and in many more applications.

Numerical analysis have become an essential tool for the medical and the industrial sector to help improve their products and system designs for maximum efficiency. Over decades, researchers have developed various numerical techniques to simulate multiphase flows. Simulating multiphase flows is a challenging task due to the sharp property gradients exist across the interface that continuously moves, deforms and even undergoes topological changes.

Bubbly flows are one of a type of multiphase flows. Bubbly flows are encountered in many industrial applications such as bubble column reactors [96] and pressurized water reactor (PWR) [8]. The dynamics of bubbly flow impact the efficiency and safety of these devices. Therefore it is fundamentally important to examine the behavior of bubbly flows. Surfactant/contamination is naturally present or synthetically added to manipulate the dynamics of bubbly flows. Surfactant molecules typically consist of a hydrophilic head and a hydrophobic tail. Detergents, wetting agents, emulsifiers, foaming agents, or dispersants may serve as surfactants.

Surfactant molecules have tendency to accumulate at fluid-fluid interface, create a buffer zone between two immiscible fluids, and thus reduce the interfacial tension. A non-uniform distribution of interfacial surfactant concentration results in Marangoni stresses which critically influence dynamics of multiphase flows. It is well known that addition of small amount of surfactant can alter the behavior of bubbly flows completely [108]. The long-chain surfactant molecules do not only modify the interfacial properties (e.g., reduce the surface tension) but they also make the host fluid viscoelastic [112]. Moreover, long-chain polymers are often added to turbulent liquid flows for the purpose of drag reduction (DR) known as Toms effect [125]. The drag-reducing polymer molecules also act as a surfactant in multiphase flows. It is therefore fundamentally important to understand the interactions and combined effects of the surfactant and viscoelasticity on turbulent multiphase flows from both the scientific and applications point of views.

1.0.1 Viscoelastic fluids

Non-Newtonian fluids may display various peculiar properties, such as shear-thinning, shear-thickening, elasticity and memory effects under different conditions. Shear-thinning and shear-thickening fluids show an apparent viscosity which decreases and increases with the applied shear rate. Elastic effects characterize the trend of the complex structures to relax back to their original configurations after being stretched by the flow. Memory effect has a close link to the fluid elasticity. The flow may remember the history of its past deformation over a duration specified by the relaxation time. The classification of these fluids is shown schematically in Fig. 1.1 where a typical shear stress response to the rate of strain is depicted for each class of fluid.

Numerous polymeric fluids are also referred as viscoelastic fluids for example molten polymers, shampoos, glues, eggs white, Bouncing Putty and offset printing inks. The viscoelastic fluids exhibits both viscous and elastic characteristics. The viscoelastic fluids not only have non-Newtonian response to the rate of strain but also have non-zero normal stress differences due to interaction of polymer molecules with

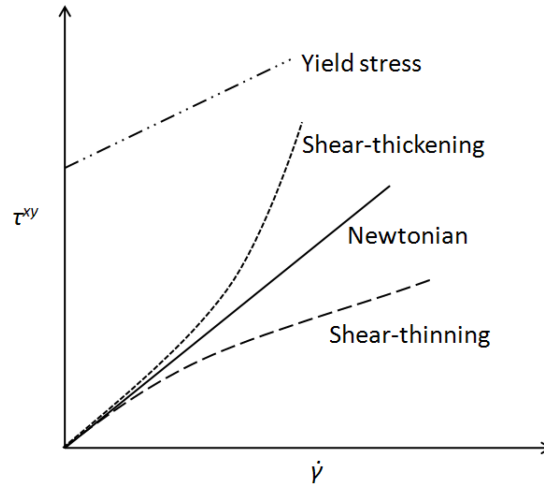


Figure 1.1: Classification of fluids.

the flow. In a shear flow, polymer molecules stretch along the streamlines and exert non-isotropic stress back on the fluid causing non-zero normal stress differences. Note that the normal stress differences are identically zero in Newtonian fluids. These normal stress differences are the main reason for many exotic phenomena observed in viscoelastic fluid flows such as reversal of direction in the secondary flow in a stirred beaker [47], the Weissenberg or rod climbing effect [38], die swell effect [113] and turbulence at low Reynolds number [40].

The works of Rivlin [88] and Oldroyd [78] are the earliest attempts for the development of constitutive relationships between stress and strain. For many decades, the development of rheological models have been an active research topic. The kinetic theory of dilute polymer solutions have been used to drive the differential constitutive models. In these models, polymer molecules are modeled as dumbbells having two beads connected by a mass-less spring as shown in Fig. 1.2. The interaction amongst the polymer molecules is ignored and only interaction between the polymer molecules and the Newtonian fluid is considered. The upper convected Maxwell model (UCM) and the Oldroyd-B model derived by Oldroyd [78] are the simplest models used for viscoelastic flows. The drawback of these models is that the the dumbbells stretch infinitely which leads to nonphysical singularity. To over-

come this issue, more sophisticated models have been developed, which restrict the extensibility of the polymer chains. Such models are commonly known as finitely extensible nonlinear elastic (FENE) type models. The FENE-P model of Peterlin [86] and FENE-CR model of Chilcott and Rallison [13] are examples of FENE type models. The FENE-P model captures the shear thinning effect. The Giesekus model [39] also restricts the extensibility of polymers and, in addition to shear-thinning effects, it can also predict the non-zero second normal stress differences. The governing equations for the general form of all these models are

$$\nabla \cdot \mathbf{u} = 0, \quad (1.1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mu_s (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \nabla \cdot \boldsymbol{\tau}, \quad (1.2)$$

$$\boldsymbol{\tau} + \lambda \left(\frac{\partial \boldsymbol{\tau}}{\partial t} + \nabla \cdot (\mathbf{u} \boldsymbol{\tau}) - (\nabla \mathbf{u})^T \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \nabla \mathbf{u} \right) + f(\boldsymbol{\tau}, D) = 2\mu_p D, \quad (1.3)$$

where $\mathbf{u}$, p , $\boldsymbol{\tau}$, μ_s , μ_p are the velocity vector, pressure fields, viscoelastic extra stress tensor, the solvent and polymeric viscosity, respectively. Function $f(\boldsymbol{\tau}, D)$ is specified for three types of models as follows:

$$f(\boldsymbol{\tau}, D) = \begin{cases} 0 & \text{Oldroyd-B and UCM models,} \\ \alpha \frac{\lambda}{\mu_p} \boldsymbol{\tau} & \text{Giesekus model,} \\ \epsilon \frac{\lambda}{\mu_p} \text{tr}(\boldsymbol{\tau}) \boldsymbol{\tau} + 2\eta \lambda (D \boldsymbol{\tau} + \boldsymbol{\tau} D) & \text{Phan-Thien Tanner (PTT) model,} \end{cases} \quad (1.4)$$

where α , ϵ , and η are the model parameters. The FENE-P model is used in this study. The FENE-P model is discussed in detail in next chapters. The interested reader is referred to Owens and Phillips [82] for the details of these models and other constitutive equations.

1.1 Front Tracking Method

As mentioned, simulating multiphase flows is a challenging task and researchers have developed various numerical methods over decades to overcome this difficult task. In

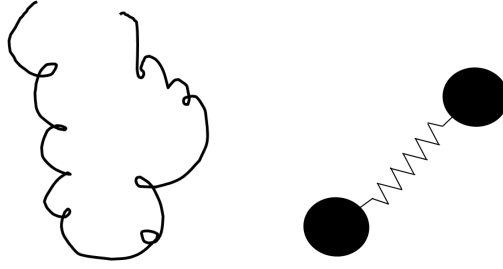


Figure 1.2: Modelling of polymer molecule (left) as a dumbbell (right).

the 1960s, the Marker and Cell (MAC) [43] method was developed to simulate free-surface and multiphase flows to examine interfacial instabilities, gravity currents, waves and droplet collisions with walls, and other problems. In this method, Lagrangian virtual particles are considered in the fluid region. These particles advance with the local fluid velocity on the Eulerian staggered grid and therefore defines the interface shape and location at current time.

Hirt and Nichols [48] introduced the volume of fluid method (VOF). It is a memory efficient-region scheme, in which the volume fraction of each fluid is tracked through every cell in the Eulerian grid. Multiphase simulations have also been performed by a level-set function [81, 104]. In this method, a level-set function is kept as a signed distance function throughout the simulation so that level-set function remains continuous and well resolved. Jacqmin [51] performed critical test cases to show the ability of the phase field method to simulate two phase flows. The above mentioned methods are known as interface capturing method. There also exist another method known as interface tracking method. In this method, interface is represented by a separate Lagrangian grid, whereas the governing equations are solved on the background Eulerian mesh. Tryggvason et al. [119, 120] devised a front-tracking method based on interface tracking method. For the present study, front-tracking method is used to track the interfaces.

In the front-tracking method (FTM), the boundary between the fluids (interface) is represented by the connected marker points that are move by local flow velocity interpolated from the fixed Eulerian grid as shown in Fig 1.3. This approach is

different than the one used for VOF method, in which a marker function identifying the different fluids directly, is advected. For FTM, two separate grids are used the Eulerian grid and Lagrangian grid. The equations governing the fluid flow are solved on the Eulerian grid and the Lagrangian grid is used to track the interface. We use *front* to refer to the complete set of computational objects used to represent the interface. Figure 1.4 shows the result of a simulation of a buoyant bubble at one instant. The langragian front grid is clearly visible with a cross-sectional plane of the regular structured fluid grid, where the velocity field is plotted. The front grid is used for the accurate advection of the fluid interface and the computations of surface tension.

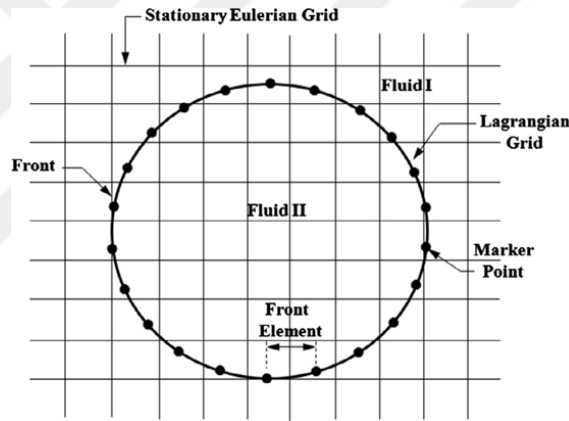


Figure 1.3: The Lagrangian and Eulerian grids used in front-tracking method. The flow equations are solved on the fixed Eulerian grid. The interface between different phases is represented by a Lagrangian grid consisting of connected marker points.

Three-dimensional fronts are represented by a triangular mesh shown in Fig 1.5. Three points are connected by a triangular element. The points only know their coordinates, but the elements know about their corner points and the elements that share their edges. The corners of each element and the edges are numbered counterclockwise (or clockwise). Figure 1.5 shows the key variables that are stored for a three-dimensional front. The front points are moved by interpolating the front point velocity from the fixed grid. By using first-order explicit Euler integration,

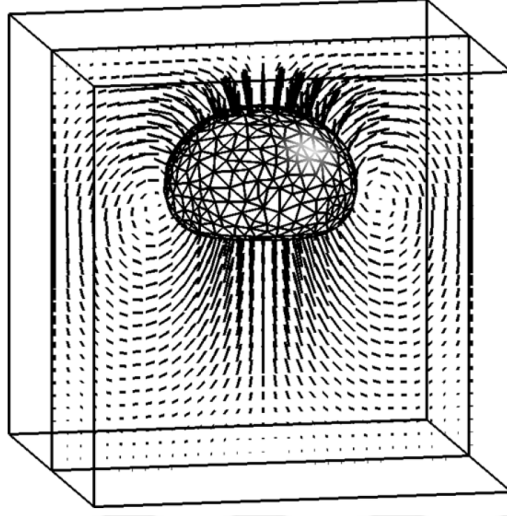


Figure 1.4: Front-tracking simulation of a buoyant bubble. The bubble surface is tracked by an unstructured triangular grid, but the flow equations are solved on a regular structured grid.

the new location of the points is given by

$$\mathbf{x}_f^{n+1} = \mathbf{x}_f^n + \mathbf{v}_f^n \Delta t, \quad (1.5)$$

where $\mathbf{x}_f$ is the front position, $\mathbf{v}_f$ is the front velocity, and Δt is the time step. Superscript n denotes the current time and $n + 1$ denotes the end of the time step. Then the material properties are evaluated based on the new locations of the marker points as

$$\rho^{n+1} = \rho(\mathbf{x}_f^{n+1}), \quad \mu^{n+1} = \mu(\mathbf{x}_f^{n+1}). \quad (1.6)$$

After the front is moved/advected, it is essential to perform the restructuring of the front as it will stretch and deform as a result of the fluid motion. Stretching and compression causes long and short separation distance between the marker points, respectively. Thus, it is important to add or delete the front element to resolve the front adequately. Figure 1.6 shows a restructuring approach based on splitting an edge of an element to refine the front and collapsing an edge to coarsen it. The splitting of an edge results in the addition of one new front point and two new front elements and the collapse of an edge removes one point and two elements from the

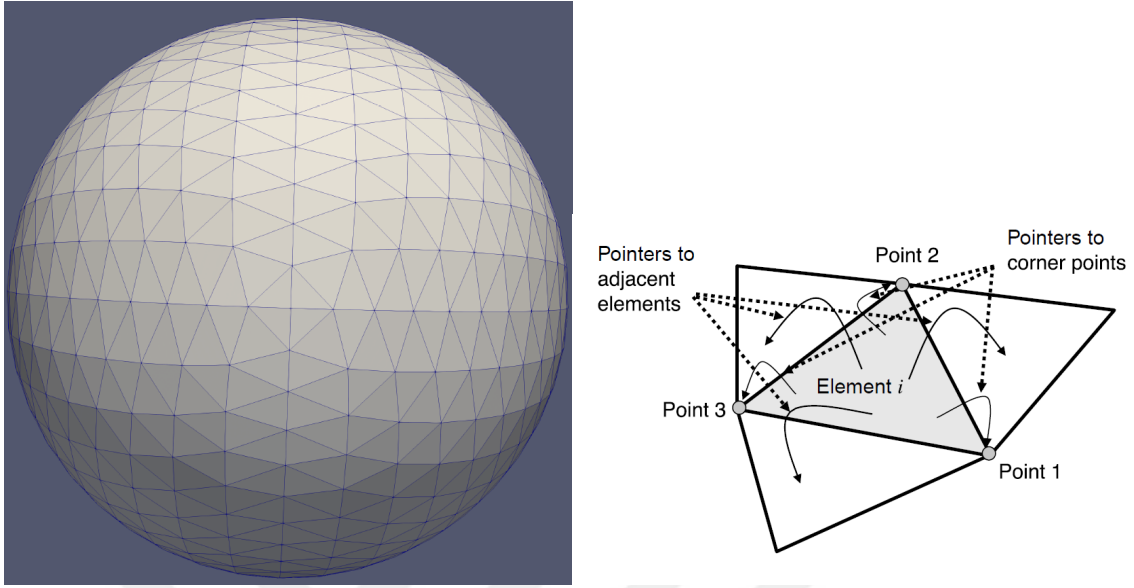


Figure 1.5: The structure of a three-dimensional front. The points only “know” their coordinates. The elements, on the other hand, carry all information about the structure of the front, including pointers to the corner points and to the adjacent elements.

front. The decision for the addition and deletion of an element is based on the the size of each element, the length of its edges, or its shape. The shape is monitored by aspect ratio and is compared with that of an equilateral triangle. Thus, the restructuring is controlled by the length of the edges and aspect ratio of an element. The preset values used are based on the corresponding fixed grid size i.e., shortest edge ($a_{min} = h/3$, where h is the Eulerian grid spacing), longest edge ($a_{max} = h$) and aspect ratio of an element ($asp_{max} = \text{aspect ratio of an equilateral triangle}$). Generally, $asp_{max} = 1.41$ gives better results. The longest edge is split and two new elements are added, if the longest edge is longer than a_{max} . The shortest edge is collapsed and two elements are deleted if the shortest edge is smaller than a_{min} . If the aspect ratio of an element is larger than asp_{max} and its shortest edge is larger than a_{min} , two elements are also added. The restructuring of front is schematically shown in Fig 1.6.

The accurate computation of the surface tension is perhaps one of the most critical aspects of any method designed to simulate multiphase flows. For the front-

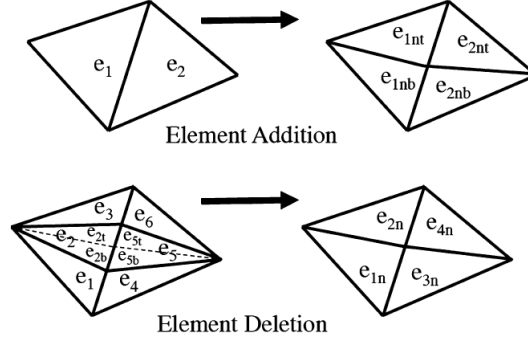


Figure 1.6: The restructuring of the front elements. The long edge of an element is split into two daughter elements (top) and the short edge of two elements are collapsed to delete two elements (bottom).

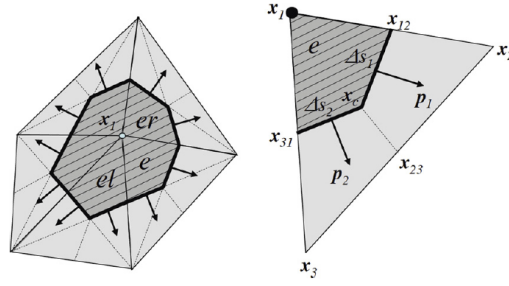


Figure 1.7: Computations of surface gradient, surface Laplacian and surface tension force of the 3D front. The surface gradient and surface tension forces are computed at the nodes by adding up contributions from the adjacent elements. The surface Laplacian is computed at cell centers

tracking method, the surface tension force is determined on the Lagrangian grid and distributed onto the Eulerian grid. The surface tension on a surface segment is given by

$$\delta f_e = \oint_{\Delta C} \sigma(\Gamma) \mathbf{p} dl \quad (1.7)$$

where $\sigma(\Gamma)$ is surface tension coefficient evaluated as a function of interfacial surfactant concentration (Γ) using the equation of state

$$\sigma = \sigma_s \left[1 + \beta_s \ln \left(1 - \frac{\Gamma}{\Gamma_\infty} \right) \right], \quad (1.8)$$

where $\beta_s = \frac{RT\Gamma_\infty}{\sigma_s}$ is the elasticity number. The surface segment can be selected

in different ways and here we select a surface segment consisting of a third of all the elements connected to a given point. The surface segment for the point with coordinates $\mathbf{x}_1$ is the cross-hatched area, bounded by a thick line, in the left side of Fig. 1.7. Focusing now on the one of the elements, denoted by e , in more detail (right-hand side of Fig. 1.7). The area contributing to each point is found by identifying the centroid of the element and drawing lines from the centroid to the midpoints of the edges of the element that connect to the point in the middle. The centroid of element e is at

$$\mathbf{x}_c = \frac{1}{3}(\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3). \quad (1.9)$$

The midpoints of the sides are

$$\mathbf{x}_{12} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2), \quad \mathbf{x}_{23} = \frac{1}{2}(\mathbf{x}_2 + \mathbf{x}_3), \quad \mathbf{x}_{13} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_3). \quad (1.10)$$

The normal to the element is found by

$$\mathbf{n}_e = \frac{\Delta \mathbf{x}_{12} \times \Delta \mathbf{x}_{13}}{|\Delta \mathbf{x}_{12} \times \Delta \mathbf{x}_{13}|} \quad (1.11)$$

where $\Delta \mathbf{x}_{12} = (\mathbf{x}_1 - \mathbf{x}_2)$ and so on. Since the force on the side connecting $\mathbf{x}_1$ and $\mathbf{x}_{12}$ is canceled by the force from the other element bordering that side, and the same is true for the side connecting $\mathbf{x}_1$ and $\mathbf{x}_{31}$, we only need to consider the lines connecting $\mathbf{x}_{12}$ to $\mathbf{x}_c$ and $\mathbf{x}_c$ to $\mathbf{x}_{31}$. The integral over the first line segment is

$$\oint_{\Delta C} \sigma(\Gamma) \mathbf{p} dl \approx \sigma(\Gamma_1) \mathbf{p}_1 \Delta s_1 = \sigma(\Gamma_1) \mathbf{n}_e \times \frac{\mathbf{x}_c - \mathbf{x}_{12}}{\Delta s_1} \Delta s_1 = \sigma(\Gamma_1) \mathbf{n}_e \times (\mathbf{x}_c - \mathbf{x}_{12}) \quad (1.12)$$

The net contribution to the force on the area segment surrounding point 1, from element e , is the integral over both line segments. Thus, we can write

$$\delta f_{1e} = \oint_{\Delta C_e} \sigma(\Gamma) \mathbf{p} dl \approx \sigma(\Gamma_1) \mathbf{p}_1 \Delta s_1 + \sigma(\Gamma_2) \mathbf{p}_2 \Delta s_2 \quad (1.13)$$

where $\Gamma_1 = (\Gamma_e + \Gamma_{er})/2$ and $\Gamma_2 = (\Gamma_e + \Gamma_{e1})/2$. The contributions from the other elements sharing node 1 are computed in a similar fashion and summed up to find the net force. The surface tension forces computed at the nodes as described above are then distributed onto neighboring Eulerian grid points as a body force in a

conservative manner using Peskin's distribution. Details of the distribution can be found in Tryggvason et al.[119].

In the presence of surfactant, during refining of the front as discussed above, special attention is paid to conserve the total surfactant mass. For instance, in Fig. 1.6 after splitting element e_1 , the interfacial surfactant concentration in the daughter cells is set equal to

$$\Gamma_{e1nb} = \Gamma_{e1nt} = \frac{\Delta A_{e1}}{\Delta A_{e1nb} + \Delta A_{e1nt}} \Gamma_{e1} \quad (1.14)$$

where ΔA_{e1nb} and ΔA_{e1nt} are the area of the bottom and top daughter cells, respectively. The total mass is also strictly conserved in deleting elements. For instance, the interfacial surfactant concentration of e_{1n} in the bottom sketch of Fig. 1.6 is set to

$$\Gamma_{e1n} = \frac{\Delta A_{e1} \Gamma_{e1} + \Delta A_{e2b} \Gamma_{e2}}{\Delta A_{e1n}} \quad (1.15)$$

where ΔA_{e2b} is the area of the lower piece of the element e_2 that becomes part of the element e_{1n} after the deletion.

1.2 Outline and Contribution of the Thesis

Extensive simulations are performed to examine the sole and combined effects of surfactant and viscoelasticity on turbulent bubbly flows using front-tracking method. This dissertation is organized as follows:

In Chapter 2¹, the effects of soluble surfactant on the lateral migration of a bubble in a pressure-driven channel flow are examined by interface-resolved numerical simulations. Extensive computations are performed to investigate the bubble dynamics for a wide range of parameters. It is found that surfactant dramatically changes the bubble dynamics. The onset of path instability is observed for both the clean and the contaminated cases.

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In Chapter 3², interface-resolved direct numerical simulations are performed to examine the combined effects of soluble surfactant and viscoelasticity on the structure of a bubbly turbulent channel flow. The incompressible flow equations are solved fully coupled with the FENE-P viscoelastic model and the equations governing interfacial and bulk surfactant concentrations. The latter coupling is achieved through a non-linear equation of state which relates the surface tension to the surfactant concentration at the interface. The two-fluid Navier-Stokes equations are solved using a front-tracking method, augmented with a very efficient FFT-based pressure projection method that allows for massively parallel simulations of turbulent flows.

In chapter 4³, effects of different types of surfactant are examined using the physical sorption kinetics. For Newtonian turbulent bubbly flows, effects of Triton X-100 and 1-Pentanol are examined. It is observed that the sorption kinetics highly affect the dynamics of bubbly flow. Minute amount of Triton X-100 is found to be sufficient to prevent the formation of bubble clusters. On the other hand, 100 times more of 1-Pentanol surfactant is not sufficient to prevent the formation of layers. For viscoelastic turbulent flow, it is found that, polymer drag reduction is completely lost for the surfactant-free case, and the addition of small amount of surfactant (Triton X-100) restores the polymer drag reduction for the viscoelastic turbulent bubbly flows.

Finally, conclusions are drawn in Chapter 5.

We have also examined the effects of surfactant and viscoelasticity on poly-dispersed turbulent bubbly flow ($Re_\tau = 250$). The results of this study are discussed in Appendix A because these simulations are not complete yet. These simulations are very expensive and were performed at JUWELS HPC, Germany under PRACE project. We had received 18 Mcore hours under PRACE project for the durrantion of 1 year. There was sudden shutdown of JUWELS HPC in summer of 2020 due to dangerous cyber attacks and because of this we lost two months of computational time. Thus, simulations are still incomplete. The simulations will be completed at

²Published as a paper under the same chapter title in *Computers & Fluids* page 104717, (2020)

³To be submitted as a paper under the same chapter title

BESKOW HPC, Sweden.



Chapter 2

EFFECTS OF SOLUBLE SURFACTANT ON LATERAL MIGRATION OF A BUBBLE IN A PRESSURE DRIVEN CHANNEL FLOW

2.1 Introduction

Surfactants are often naturally present or externally added into an interfacial system [61, 103]. It has been shown that even a small amount of surfactant can lead to dramatic structural changes of a bubbly flow, i.e., changes in bubble rise velocity, lateral migration, bubble-bubble interactions and mass transfer [110]. These structural changes can be utilized to perform useful functions in different applications such as microfluidics [97, 105, 5], medicine [41] and industrial processes [108]. For instance, surfactants play a pivotal role in the safety and efficiency of the equipment in nuclear reactors and bubble columns. It is thus of significant importance to understand the effects of surfactants on the movement of a bubble.

The relevance to natural and many industrial applications has made the dynamics of an air bubble rising in a stagnant and flowing liquid an active research area. It is well known that surfactant causes a reduction in the rising velocity of a bubble [15], which is explained by the so-called Marangoni effect [36]. A fully contaminated spherical bubble behaves as a rigid sphere in water, as the drag coefficient of a spherical bubble approaches that of a rigid sphere when a sufficient amount of surfactant is present. This phenomenological explanation was first given by Frumkin and Levich [36]. Cuenot et al. [17] has provided a comprehensive review regarding this subject until 1996. Later, Takemura and Yabe [111] used the stagnant cap model to explain the mechanism of the transient process where the bubble behavior changes from that of a fluid sphere to that of a solid particle. Almatroushi

and Borhan [4] examined the effects of surfactant on the buoyancy-driven motion of bubbles and drops in a vertical tube experimentally. They observed the surfactant retardation effect for the cases of small air bubbles and viscous drops. Tasoglu et al. [115] numerically examined the effect of soluble surfactants on the unsteady motion and deformation of a bubble rising in an otherwise quiescent liquid contained in an axisymmetric tube by using a finite-difference/front-tracking method. They considered nearly spherical, ellipsoidal, and dimpled ellipsoidal-cap regimes of bubble motion. They have shown that the surfactants generally reduce the terminal velocity of the bubble, especially in the nearly spherical regime where bubble behaves similar to a solid sphere and its terminal velocity approaches that of an equivalent solid sphere. [117] examined the motion of a buoyancy-driven bubble in a so-called ‘self-wetting fluid’. They showed that the motion of a spherical bubble in the Stokes flow limit can be arrested in a self-wetting liquid due to thermocapillary Marangoni stresses.

Recent studies on bubble motion show that the presence of surfactant has drastic effect not only on the vertical motion but also on the lateral migration of a bubble [37]. Fukuta et al. [37] examined the behavior of the lift force acting on a contaminated bubble in a linear shear flow. They showed that the lift force acting on a spherical bubble decreases from the value of a clean bubble to near zero with an increase of Langmuir number. Takagi et al. [109] showed that addition of surfactant drastically alters the behavior of an upward bubbly flow. They performed experiments to investigate the effects of species and concentration of surfactant on the flow structure. They found that in the absence of surfactant, some bubbles coalesced during the rising process and thus formed bubbles of larger size (deformable bubbles) which then moved toward the channel center instead of the channel wall. An addition of a small amount of 3-Pentanol surfactant prevented the bubble coalescence and bubbles remained nearly spherical, thus bubbles moved toward the wall mainly due to aerodynamic lift force. However, as the amount of 3-Pentanol surfactant is increased, nearly spherical bubbles moved toward the center of channel due to the Marangoni stresses. Muradoglu and Tryggvason [77] developed a front-tracking

method for simulation of soluble surfactant in 3D multiphase flows. They studied the effects of soluble surfactants on the motion of buoyancy-driven bubbles in a straight square channel in undeformable (spherical) and deformable (ellipsoidal) regimes. They also simulated a few cases of lateral migration of bubbles in a pressure-driven channel flow with a soluble surfactant and found that the contaminated bubble drifts away from the channel wall and stabilizes at the center of the channel when the surfactant-induced Marangoni stresses are sufficiently large. However, their focus was on the numerical method rather than the flow physics. More recently, Lu et al. [64] examined the effect of insoluble surfactant on the structure of turbulent bubbly upflow in a vertical channel by direct numerical simulations (DNS). They showed that, in the presence of surfactant, contaminated bubbles migrate to the center, whereas clean bubbles move towards the wall. Hayashi and Tomiyama [44] investigated numerically the effect of surfactant on lift coefficients of bubbles in linear shear flows by using the interface tracking method. They showed that the lift coefficient of a bubble decreases as the Langmuir number increases. Therefore, surfactant decreases the critical values of Eo and Re at which the coefficient changes its sign.

The effects of surfactant on lateral migration of a droplet and a bubble have been also studied in the creeping flow regime. Pak et al. [83] used a reciprocal theorem to examine the effects of insoluble surfactant on lateral migration of a spherical droplet in an unbounded Poiseuille flow in the limit of vanishing Reynolds and surface Peclet numbers. They showed that surfactant-induced Marangoni stresses cause cross-streamline migration of the droplet towards the centre of the Poiseuille flow and the magnitude of the lateral migration depends linearly on the distance of the drop from the centre of the Poiseuille flow. Das et al. [20] studied analytically the combined effect of bulk-insoluble surfactant and a varying temperature on the motion of a viscous droplet in a shear flow. Neglecting the fluid inertia, they found that the droplet speed and direction of motion are strongly influenced by the interfacial transport of surfactant. Das and Chakraborty [19] performed a numerical and analytical study to examine the effect of surface viscosity on the motion of a

surfactant-laden droplet in a non-isothermal Poiseuille flow. Neglecting the fluid inertia, they found that the droplet migration velocity is notably affected by the dilatational viscosity, whereas the effects of the shear viscosity are negligible.

It is well known that the path of a rising bubble in a bulk liquid experiences a path instability, i.e., bubble motion changes from straight to zigzag/spiral when bubble size exceeds a critical value [42]. Kelley and Wu [56] showed that the path of circular air bubble rising in a viscous fluid of a Hele-Shaw cell changes from a straight path to a zigzag one when the Reynolds number of the bubble exceeds a critical value. They observed that this path instability is a consequence of the vortex shedding behind the bubble. Zenit and Magnaudet [129] experimentally studied the conditions for which the paths of freely rising bubbles become oscillatory. They argued that the dominant parameter to trigger the instability is the bubble shape rather than Reynolds number of the bubble and that the path instability is a direct consequence of the wake instability. Tripathi et al. [118] performed numerical simulations on a spherical bubble rising in a quiescent fluid. They observed five distinct regimes (namely, axisymmetric, skirted, zigzagging/spiralling, peripheral breakup, and central breakup) with sharply defined boundaries in the Galilei number (Ga)-Eötvös number (Eu) phase plot. Sharaf et al. [94] performed extensive experiments over the entire range of Ga and Eu reported by Tripathi et al. [118] and provided a similar phase plot in the $Ga - Eu$ plane. However, they found one major difference, that is, unlike five different regions of bubble behavior in the numerical phase plot, only four regions were identified experimentally while a central breakup (region V) was not observed. Balla et al. [6] have also observed path instability for a non-isothermal rising bubble in a so-called ‘self-wetting’ fluid.

Surfactant affects the path instability of a rising bubble. Tagawa et al. [107] experimentally examined the effect of surfactant on the path instability of a rising bubble. They categorized the bubble motion as straight/helical/zigzag on the basis of bubble Reynolds number and the normalized drag coefficient. Recently, Pesci et al. [85] studied the effects of soluble surfactant on dynamics of a single bubble rising in a large spherical domain. They found that the bubble path depends both on the

initial surface and bulk contamination. Another observation was that a quasi-steady state velocity of a bubble can be attained without reaching an equilibrium between ad- and desorption of surfactants.

In the present study, extensive numerical simulations are performed to examine the effects of surfactant on the lateral migration and the path instability of a bubble in a pressure driven flow at a finite Reynolds number. We consider both the soluble and insoluble surfactant cases. Simulations are performed to investigate drop dynamics for a wide range of parameters including the capillary number (Ca), the elasticity number (β_s), the bulk surfactant concentration (C_∞) and the Eötvös number (EO).

2.2 Formulation and Numerical Method

Following Ref. [77], a single set of equations can be written for the entire computational domain provided that the jumps in the material properties such as density, viscosity and molecular diffusion coefficient are correctly treated and the effects of surface tension are included properly in the momentum equations. In the one-field formulation, the Navier-Stokes equations for the whole domain can be written as follows:

$$\begin{aligned} \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \mathbf{g} \Delta \rho \\ &+ \int_A [\sigma(\Gamma) \kappa \mathbf{n} + \nabla_s \sigma(\Gamma)] \delta(\mathbf{x} - \mathbf{x}_f) dA, \end{aligned} \quad (2.1)$$

where $\mathbf{u}$, p are the velocity vector and pressure fields, respectively, $\mathbf{g}$ is the gravitational acceleration vector and ρ and μ are the discontinuous density and viscosity fields, respectively. The effects of surface tension are included as a body force in the last term on the right hand side, where σ is the surface tension coefficient that is function of the surfactant concentration Γ at the interface, κ is twice the mean curvature, and $\mathbf{n}$ is a unit vector normal to the interface. $\nabla_s \sigma(\Gamma)$ represents the surfactant-induced Marangoni stresses where the surface gradient is defined as

$$\nabla_s = \nabla - \mathbf{n}(\mathbf{n} \cdot \nabla). \quad (2.2)$$

The surface tension acts only on the interface as indicated by the three-dimensional delta function δ whose arguments $\mathbf{x}$ and $\mathbf{x}_f$ are the point at which the equation is evaluated and a point at the interface, respectively. The Navier-Stokes equations are supplemented by the incompressibility condition

$$\nabla \cdot \mathbf{u} = 0. \quad (2.3)$$

We also assume that the material properties remain constant following a fluid particle, i.e.,

$$\frac{D\rho}{Dt} = 0; \quad \frac{D\mu}{Dt} = 0, \quad (2.4)$$

where $\frac{D}{Dt}$ is the material derivative. The density and viscosity vary discontinuously across the fluid interface and are given by

$$\rho = \rho_o I(\mathbf{x}, t) + \rho_i (1 - I(\mathbf{x}, t)), \quad (2.5)$$

$$\mu = \mu_o I(\mathbf{x}, t) + \mu_i (1 - I(\mathbf{x}, t)), \quad (2.6)$$

where the subscripts “ i ” and “ o ” denote the properties of the drop and bulk fluid, respectively, and I is the indicator function defined as

$$I(\mathbf{x}, t) = \begin{cases} 1 & \text{in bulk fluid,} \\ 0 & \text{in bubble fluid.} \end{cases} \quad (2.7)$$

The surface tension is a function of the surfactant concentration and determined by the Langmuir equation of state

$$\sigma = \sigma_s \left[1 + \beta_s \ln \left(1 - \frac{\Gamma}{\Gamma_\infty} \right) \right], \quad (2.8)$$

where $\beta_s = \frac{RT\Gamma_\infty}{\sigma_s}$ is the elasticity number. Equation (3.8) is slightly modified to avoid negative values of the surface tension [76, 77]

$$\sigma = \sigma_s \left[\max \left(\epsilon_\sigma, 1 + \beta_s \ln \left(1 - \frac{\Gamma}{\Gamma_\infty} \right) \right) \right], \quad (2.9)$$

where ϵ_σ is taken as 0.05 in the present study. The evolution equation for the interfacial surfactant concentration was derived by Stone [102]. Following Ref. [77] the interfacial surfactant is solved on the Lagrangian grid and can be expressed as

$$\frac{D\Gamma A}{Dt} = AD_s \nabla_s^2 \Gamma + A\dot{S}_\Gamma, \quad (2.10)$$

where A is the surface area of an element of the interface, D_s is the diffusion coefficient along the interface and $\dot{S}_\Gamma$ is the source term given by

$$\dot{S}_\Gamma = k_a C_s (\Gamma_\infty - \Gamma) - k_d \Gamma, \quad (2.11)$$

where k_a and k_d are adsorption and desorption coefficients, respectively, and C_s is the concentration of the surfactant in the bulk fluid immediately adjacent to the interface. The bulk surfactant concentration is governed by the advection-diffusion equation in the form

$$\frac{\partial C}{\partial t} + \nabla \cdot (C \mathbf{u}) = \nabla \cdot (D_{co} \nabla C), \quad (2.12)$$

where the coefficient D_{co} is related to the molecular diffusion coefficient D_c and the indicator function I as

$$D_{co} = D_c I(\mathbf{x}, t). \quad (2.13)$$

The source term in Eq. (3.10) is related to the bulk concentration by [27]

$$\dot{S}_\Gamma = -D_{co}(\mathbf{n} \cdot \nabla C|_{interface}). \quad (2.14)$$

The boundary condition at the interface given by Eq. (3.13) is first converted into a source term for the bulk surfactant evolution equation. In this approach it is assumed that all the mass transfer between the interface and the bulk takes place in a thin adsorption layer adjacent to the interface. Thus, the total amount of mass adsorbed on the interface is distributed over the adsorption layer and added to the bulk concentration evolution equation as a negative source term in a conservative manner. Equation (3.11) thus takes the form as

$$\frac{\partial C}{\partial t} + \nabla \cdot (C \mathbf{u}) = \nabla \cdot (D_{co} \nabla C) + \dot{S}_c, \quad (2.15)$$

where $\dot{S}_c$ is the source term evaluated at the interface and distributed onto the adsorption layer in a conservative manner. The details of this treatment can be found in Muradoglu and Tryggvason [77, 76].

The flow equations (4.3) and (2.3) are solved fully coupled with the bulk (2.15) and interfacial (3.9) surfactant concentration evolution equations using the finite-difference/front-tracking method [77, 119, 120, 122]. The momentum and the continuity equations are solved on a stationary staggered Eulerian grid and are discretized by second-order central difference approximations for the spatial derivatives except for the convective terms in the momentum and the bulk surfactant concentration equations that are discretized using the QUICK and the fifth order WENO-Z schemes, respectively. Time integration is done by a second order predictor-corrector method [77]. The incompressibility condition leads to a non-separable Poisson equation for pressure which is solved using the parallel semi-coarsening multigrid (PFMG) solver in the HYPRE library [32]. Detailed description of the numerical method can be found in Muradoglu and Tryggvason [77, 76].

2.3 Problem Statement and Computational Setup

Figure. 2.3 schematically depicts the lateral migration of the contaminated bubble in a pressure driven flow and Fig. 2.3 shows the computational setup. As shown in Fig. 2.3, a spherical bubble of diameter d_b is placed instantly near the left wall with the center initially located at $(x_c, y_c, z_c) = (2.615d_b, 1.29d_b, 1.38d_b)$. The interfacial surfactant concentration is initialized as clean ($\Gamma = 0$) or contaminated ($\Gamma = \Gamma_{eq}$) for soluble and insoluble surfactants, respectively, whereas the bulk concentration uniform at $C = C_\infty$. The flow is initialized assuming a pressure driven fully developed laminar channel flow with the average channel velocity given by

$$V_o = \frac{1}{12\mu_o} \left(-\frac{dp}{dz} \right) H^2, \quad (2.16)$$

where H is the channel width and $(-\frac{dp}{dz})$ is an applied constant pressure gradient. The computational domain is rectangular, bounded by two vertical walls at which the no-slip boundary conditions are applied. The periodic boundary conditions are used in the spanwise (x) and the streamwise directions (z). The domain size is $5.236d_b \times 6.667d_b \times 10.472d_b$ and is resolved by a $128 \times 192 \times 256$ grid in the spanwise (x), wall-normal (y) and streamwise (z) direction, respectively. The grid is slightly

stretched near the walls in the wall-normal (y) direction. The average distance y_w , also called the separation distance, is defined as the distance between the wall and the bubble center. The Reynolds numbers based on the bubble diameter and channel width are set to $Re_b = \frac{\rho_o V_o d_b}{\mu_o} = 150$ and $Re_c = \frac{\rho_o V_o H}{\mu_o} = 1000$, respectively. For all the simulations the density ($\frac{\rho_o}{\rho_i}$) and viscosity ($\frac{\mu_o}{\mu_i}$) ratios are set to 10. Note that a typical liquid-air system has an order of magnitude larger density and viscosity ratios than used here. However, it has been previously demonstrated [114, 75, 79] that higher property ratios do not affect the results significantly. Therefore, the property ratios are kept small in order to enhance the numerical stability, relax the time-step restrictions and thus to reduce the computational cost.

In the present study, all simulations are performed using dimensional quantities but the results are expressed in terms of relevant non-dimensional quantities. The diameter of bubble d_b and average channel velocity V_o are used as length and velocity scales, respectively, and $\mathcal{T} = d_b/V_o$ as the time scale to define various governing non-dimensional numbers as summarized below:

$$\begin{aligned} Re_b &= \frac{\rho_o V_o d_b}{\mu_o}; \quad Re_c = \frac{\rho_o V_o H}{\mu_o}; \quad Ca = \frac{\mu_o V_o}{\sigma_s}; \quad Eo = \frac{g \Delta \rho d_b^2}{\sigma_s}; \quad M = g \mu_o^4 / \rho_o \sigma^3; \\ Ga &= \rho_o g^{1/2} R^{3/2} / \mu_o; \quad Pe_c = \frac{V_o d_b}{D_c}; \quad Pe_s = \frac{V_o d_b}{D_s}; \quad Bi = \frac{k_d d_b}{V_o}; \\ Da &= \frac{\Gamma_\infty}{d_b C_\infty}; \quad \beta_s = \frac{\mathcal{R} T \Gamma_\infty}{\sigma_s}, \end{aligned} \quad (2.17)$$

where Re_b , Re_c , Ca , Eo , M , Ga , Pe_c , Pe_s , Bi , Da , k and β_s are the Reynolds number based on the bubble diameter, the Reynolds number based on channel width, the capillary number, the Eötvös number, the Morton number, the Galilei number, the Peclet number based on bulk surfactant diffusivity, the Peclet number based on interface surfactant diffusivity, the Biot number, the Damkohler number, the dimensionless adsorption depth and the elasticity number, respectively.

Following Bunner and Tryggvason [11], the bubble deformation is quantified by the deformation parameter defined as square root of the ratio of the largest and the smallest eigenvalue of the second moment of inertia tensor, i.e.,

$$deformation = \sqrt{I_{max}/I_{min}}, \quad (2.18)$$

where I_{max} and I_{min} are the maximum and minimum eigenvalues of the second moment of inertia tensor, given by

$$I_{ij} = \frac{1}{\mathcal{V}_b} \int_{Vol} (x_i - x_{io})(x_j - x_{jo})dV, \quad (2.19)$$

where $\mathcal{V}_b$ is the volume of the bubble and x_{io} and x_{jo} are the coordinates of the bubble's centroid in the i -th and j -th directions, respectively. Bunner and Tryggvason [11] have shown that deformation quantification by this method is approximately equal to the ratio of the smallest to the longest axis for modestly deformed ellipsoids. For more complex bubble shapes, deformation quantification used here is a more general definition of the bubble deformation than the ratios of the longest and the shortest axis and eliminates any uncertainty in identifying those axis.

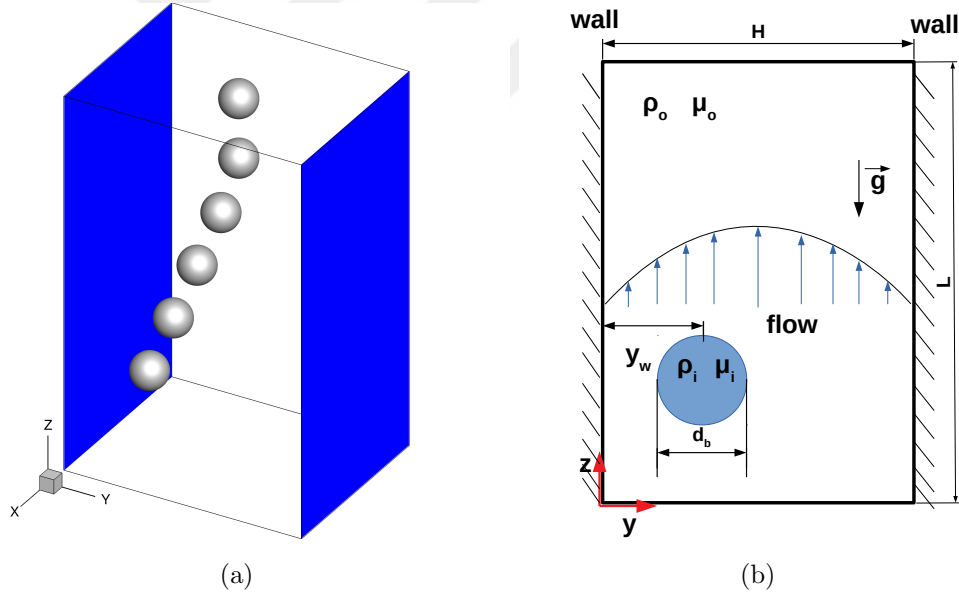


Figure 2.1: (a) Depiction of lateral migration of a contaminated bubble in a pressure driven flow. (b) Computational setup.

2.4 Results and Discussion

Simulations are performed to investigate the effects of soluble surfactant on the lateral migration of a bubble by using fully parallelized three-dimensional front-tracking method [33]. Each simulation is performed by using 24 and 8 cores for

the domain and front, respectively. Muradoglu and Tryggvason [77] performed an extensive grid convergence study of the present numerical method for a similar setting, therefore it is not repeated here. Following Ref. [77], the base line parameters are chosen as $Re_c = 1000$, $Eo = 0$, $\beta_s = 0.5$, $Pe_s = Pe_c = 200$, $k = 0.125$, $Bi = 1.2$, and $Da = 6.667$. The parameters are fixed to the base line values unless indicated otherwise. The results are first presented for the non-buoyant case to separate effects of gravity and surfactants. Then the results are presented for the buoyant case. We note that the Morton number is $M = 1.85 \times 10^{-7}$ for $Eo = 1.5$ in the buoyant case which is higher than the Morton number of $M = 2.52 \times 10^{-11}$ for an air bubble in water at 20°C but could be matched by using a water-glycerin (W-G) solution [59]. For this water-glycerin solution, $Eo = 1.5$ used here corresponds to a bubble with diameter of 0.9 mm. The channel width is $6.6 \times d_b$ or 6 mm and our channel Reynolds number corresponds to a bulk velocity of 2.7 m/s.

2.4.1 Non-buoyant case ($Eo = 0$).

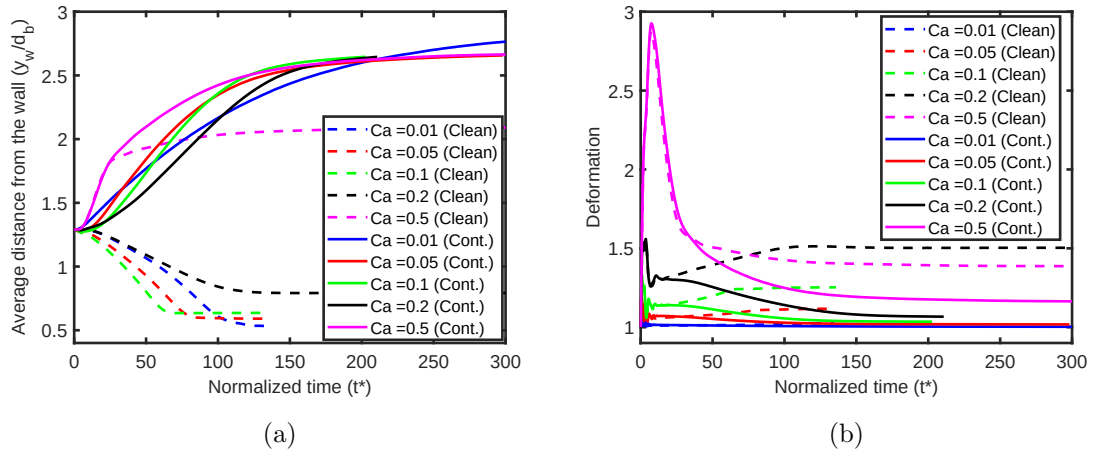


Figure 2.2: Effect of capillary Number (Ca) on the average distance from the wall (left) and the bubble deformation (right). $Re_c = 1000$, $\beta_s = 0.5$, $Pe_s = Pe_c = 200$, $k = 0.125$, $Bi = 1.2$, $Da = 6.667$

Initially, simulations are performed to investigate the effects of the capillary number on the dynamics of a clean and a contaminated bubble (soluble surfactant)

by varying Ca between $0.01 \leq Ca \leq 0.5$, while keeping all other parameters fixed at their values in the base line case. The non-dimensional average distance from the wall (y_w/d_b) and the bubble deformation are shown in Fig. 2.2 against the dimensionless time (t^*).

A clean spherical bubble experiences a lift force in a direction perpendicular to both the direction of motion and the rotation axis. As shown in Fig. 2.1, the non-uniform fluid flow causes the bubble to rotate, resulting in a force in the negative y direction, i.e., towards the left wall. The resulting lift force on the bubble, also known as the Magnus effect, causes the lateral migration of the spherical bubble towards the left wall. Indeed, Fig. 2.4.1 shows that the bubble moves towards the wall for $Ca \leq 0.2$, while it moves towards the channel center for $Ca = 0.5$. The lateral migration of the bubble towards the wall is mainly due to the aerodynamic lift force. As the bubble becomes more deformable for $Ca = 0.5$, the non axisymmetric shape of the bubble changes the direction of rotation of the bubble [29] and thus the bubble moves away from the wall in the direction of lift force maintaining higher separation distance. This steady separation distance is the function of the capillary number which in turn is a measure of the bubble deformation: the larger Ca , the more the bubble deforms and the longer is the steady separation distance. Ervin and Tryggvason[29] also supported our observation by reporting that the lift coefficient of a bubble becomes negative when the bubble deforms strongly. Similar observations have been also made recently by Alghalibi et al. [3] for hyperelastic fluid particles. Now we move on to consider the contaminated case, depicted by solid lines in Fig. 2.4.1. For the contaminated bubble, the presence of the surfactant changes the dynamics of the bubble completely. The non-uniform distribution of interfacial surfactant concentration leads to a variation of surface tension along the bubble surface, which causes tangential shear stress on the surface, known as Marangoni stresses. This Marangoni stresses counteract and dominate over the aerodynamic lift force for all Ca considered in this work. As a result, the contaminated bubble moves towards the channel center for all Ca .

The bubble deformation against time is shown in Fig. 2.4.1. As expected, the

bubble deformation increases with Ca at all times for both clean and contaminated cases, except for the highest capillary number ($Ca = 0.5$) in the clean case. For all bubbles, the deformation first sharply increases due to high shear stresses near the wall, then relaxes to its steady state values. After the initial spike, the deformation of the contaminated bubble decreases with time due to the fact that the bubble moves towards the channel center, where the shear force is reduced. On the other hand, the clean bubble for $Ca \leq 0.2$ drifts towards the wall, where the higher shear forces deform it more until a steady state separation distance is achieved. At $Ca = 0.5$ however, the clean bubble moves towards the centerline and hence the deformation decreases with t^* , similarly to the contaminated case.

Next, simulations are performed to examine combined effects of the solubility of the surfactant and the capillary number. The interfacial surfactant concentration is initially set to the equilibrium concentration, $\Gamma_{eq} = \frac{k}{1+k}\Gamma_\infty$, for the insoluble case while the bubble is initially clean in the soluble case. In the insoluble case, the source term is also switched off to avoid mass exchange by setting the adsorption (k_a) and the desorption (k_d) coefficients to zero in the source term given in Eq. (3.10). The evolution of the non-dimensional separation distance (y_w/d_b) and the bubble deformation are depicted against the normalized time (t^*) for both soluble and insoluble cases as shown in Fig. 2.3. Note that, although not shown in Fig. 2.3, simulations are also performed for the soluble cases with the interfacial surfactant concentration initialized uniformly at Γ_{eq} and the results are found to be essentially the same as the initially clean cases except for the very early transient period of time, i.e., approximately for $t^* < 20$. As can be seen in Fig. 2.3, the bubble moves towards the channel center for both cases, but the separation distance in the case of insoluble surfactant is larger. The difference in the separation distance is negligible at $Ca = 0.01$ and $Ca = 0.05$, while it increases at higher Ca . We observe that the time evolution of the deformation parameter remains very similar for both soluble and insoluble cases. To explain the differences in wall separation, the evolution of interfacial insoluble and soluble surfactant concentration for the most deformable bubble ($Ca = 0.5$) is shown in Fig. 2.4. Snapshots are taken at the non-dimensional

times of $t^* = 0.0, 16.6, 66.6$ and 116.6 . Initially at $t^* = 0$, the interfacial surfactant concentration is uniformly distributed over the surface of the bubble for the insoluble case, whereas, for the soluble one, the bubble surface is either clean (the second row) or uniform at Γ_{eq} (the third row). At $t^* = 16.6$, the contaminated bubble strongly deforms for all the cases as it moves away from the wall. It can be seen that the amount of surfactant advected to the nose of the bubble is higher for the insoluble case. This leads to larger Marangoni stresses and thus faster transient lateral migration for the insoluble case at intermediate times, leading to a larger wall separation distance. As the bubble approaches an equilibrium condition at later times, the interfacial surfactant concentration distribution becomes similar for both insoluble and soluble cases. Figure 2.4 shows that the initial interfacial surfactant concentration in the soluble case has a negligible effect on the surfactant distribution at the interface and thus on the lateral migration of the bubble except for the very early transient period of approximately $t^* < 20$.

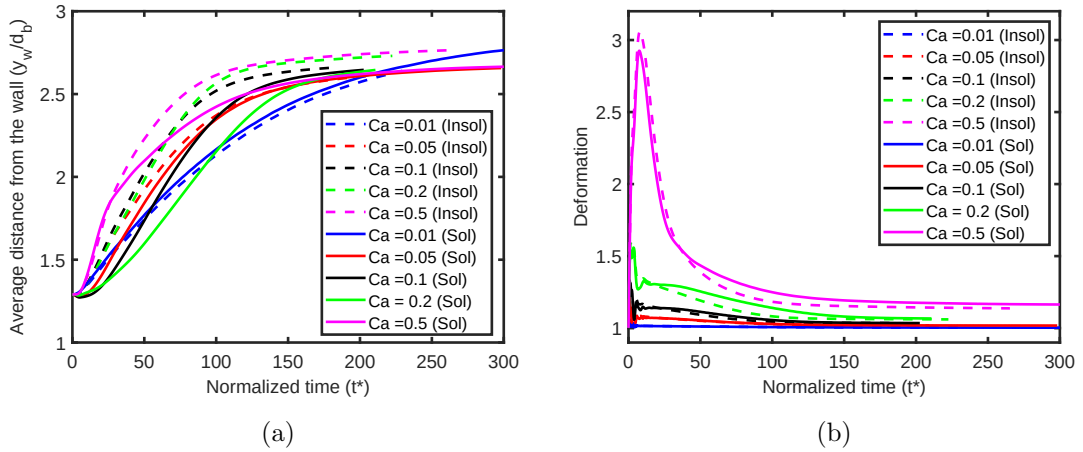


Figure 2.3: Effect of the soluble and insoluble surfactant on the average distance from the wall. $Re_c = 1000, \beta_s = 0.5, Pe_s = Pe_c = 200, k = 0.125, Bi = 1.2, Da = 6.667$

Then, the effect of the elasticity number β_s on the bubble dynamics is examined for a nearly spherical bubble ($Ca = 0.05$) as shown in Fig. 2.5. The physico-chemical parameter β_s determines the sensitivity of interfacial tension to variations in surfactant concentration, i.e., the larger β_s , the stronger the surfactant. Figure 2.5

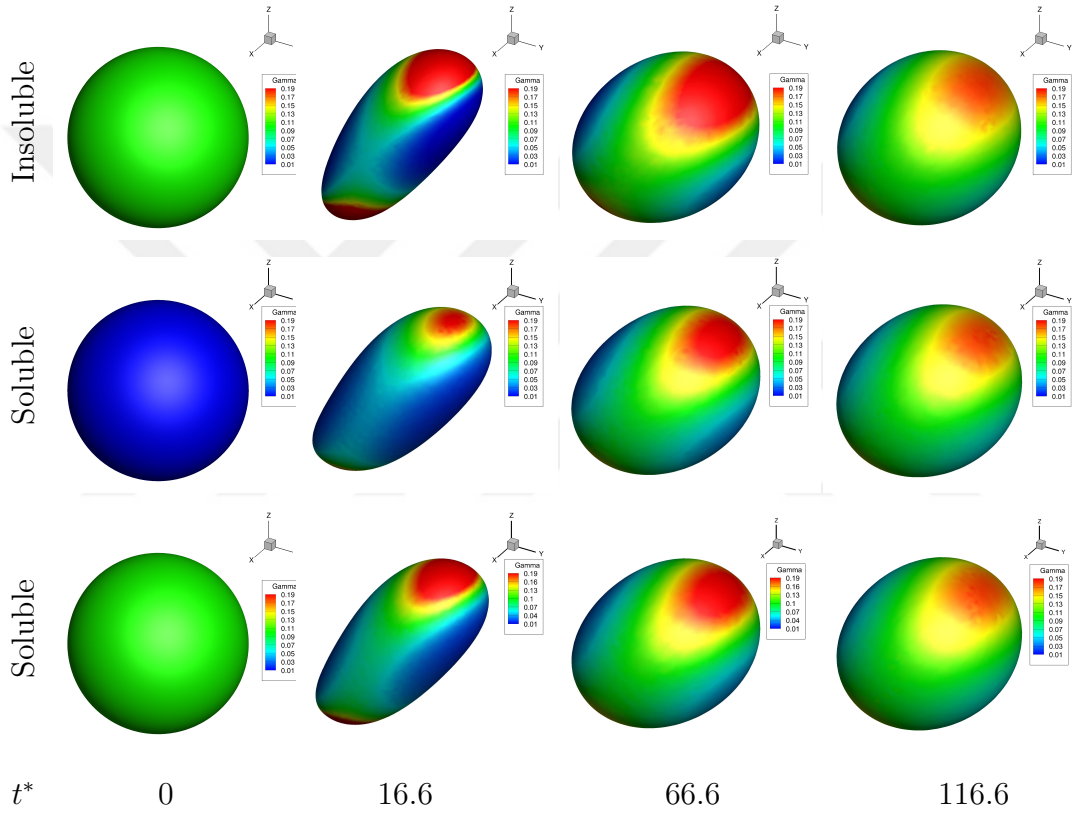


Figure 2.4: Evolution of contaminated bubble in the pressure-driven flow for $Ca = 0.5$: The insoluble surfactant case (top row) and the soluble surfactant cases with the initially clean ($\Gamma_{initial} = 0$) (middle row) and initially uniform at the equilibrium ($\Gamma_{initial} = \Gamma_{eq}$) (bottom row) distributions. $Re_c = 1000, \beta_s = 0.5, Pe_s = Pe_c = 200, k = 0.0, Bi = 0.0, Da = 6.667$.

shows that for $\beta_s = 0$ (clean), the bubble moves towards the channel wall and maintains a certain steady separation distance. Increasing the elasticity number to $\beta_s = 0.1$ triggers a change in bubble dynamics. At early times, the bubble maintains the same separation distance, but eventually migrates to the center of the channel. Increasing further the elasticity number to $\beta_s = 0.25$, the direction of lateral migration completely changes at initial times and the bubble migrates away from the wall. For $\beta_s > 0.25$, we observe similar results. The contours of the interfacial surfactant for $\beta_s = 0.1$ and $\beta_s = 0.25$ are also shown in the inset of Fig. 2.5 at $t^* = 50$. It can be seen that the interfacial surfactant distribution at $\beta_s = 0.25$ is more uniform than the $\beta_s = 0.1$. This is due to the rigidifying effect of surfactant, that is, increasing β_s , increases the Marangoni stresses which causes the reduction in surface mobility of the bubble. A similar trend is observed for the deformation of the bubble. For the clean bubble ($\beta_s = 0.0$), the deformation increases due to higher shear stresses at the wall. At $\beta_s = 0.1$, the deformation is initially nearly constant in time, until the bubble starts drifting to the channel center, where the deformation decreases. Further increasing the elasticity number ($\beta_s \geq 0.25$), the deformation of the contaminated bubble first oscillates and then decreases, as the bubble moves towards the channel center.

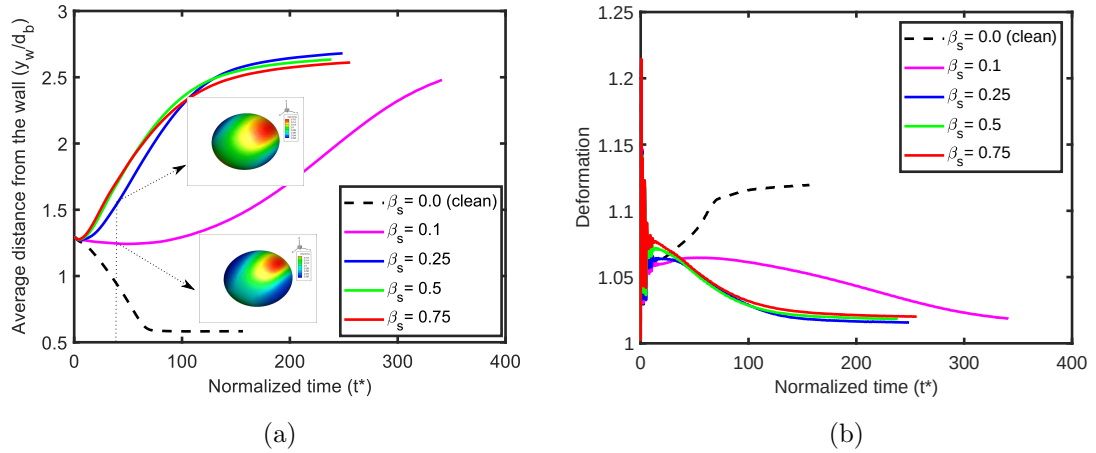


Figure 2.5: Effect of the elasticity number (β_s): The time evolution of the average distance from the wall (left) and the bubble deformation (right). $Re_c = 1000$, $Ca = 0.05$, $Pe_s = Pe_c = 200$, $k = 0.125$, $Bi = 1.2$, $Da = 6.667$

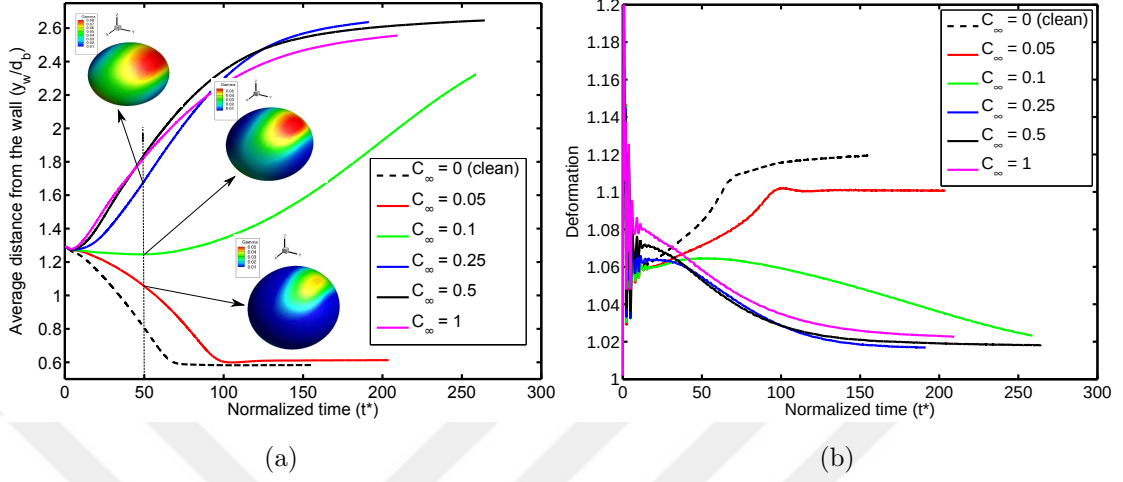


Figure 2.6: Effect of the bulk surfactant concentration (C_∞): The time evolution of the average distance from the wall (left) and bubble deformation (right). $Re_c = 1000$, $\beta_s = 0.5$, $Pe_s = Pe_c = 200$, $Bi = 1.2$,

Additionally, the effect of the bulk surfactant concentration in the range of $0 \leq C_\infty \leq 1$ is examined for a nearly spherical bubble ($Ca = 0.05$ and $\beta_s = 0.5$), as shown in Fig. 2.6. In the clean case ($C_\infty = 0$), the bubble moves towards the wall in agreement with the earlier observations. It is worth noting that at $C_\infty = 0.05$, the direction of the migration remains the same, although the final separation distance is larger and consequently it takes longer to reach the steady state. At $C_\infty = 0.1$, the bubble maintains nearly the same separation distance until $t^* < 70$ while it starts drifting to the channel center at later times. Further increasing the concentration to $C_\infty \geq 0.25$, the contaminated bubble moves towards the channel center and maintains a certain steady separation distance. To gain further insight, the bubble with the interfacial surfactant concentration contours are plotted in the inset of Fig. 2.6 for three values of $C_\infty = 0.05, 0.1$ and 0.25 at $t^* = 50$. In the case of $C_\infty = 0.05$, the amount of the surfactant adsorbed on the surface is negligible thus the aerodynamic lift force dominates over the Marangoni stresses. As a result, the direction of the migration is the same as the clean bubble. For $C_\infty = 0.1$, the surface is more contaminated leading to larger Marangoni stresses which grow in time. The contaminated bubble maintains the same separation distance at early times and

then eventually, migrates to the center of the channel at later times. Furthermore, in the presence of sufficient amount of the surfactant at $C_\infty = 0.25$, the surface of the bubble is contaminated significantly, and the Marangoni force dominates the aerodynamic lift force; hence, the contaminated bubble drifts away from the wall. These results are consistent with the experimental findings of Takagi et al.[109] on the effect of surfactants on the bubbly flow. Evolution of the deformation in the range of $0 \leq C_\infty \leq 1$ is also shown in Fig. 2.6 (right). The deformation initially oscillates at high shear stresses near the wall, then increases for $C_\infty \leq 0.05$ and decreases for $C_\infty \geq 0.1$ before reaching a steady value. The deformation decreases with C_∞ , as the bubble migrates towards the region of low shear stresses with C_∞ .

2.4.2 Buoyant case ($Eo \neq 0$).

Here, the effect of the *Eötvös* number is examined for clean and contaminated bubbles. Simulations are performed for Eo ranging from 0 to 3, as shown in Fig. 2.7. For the clean case, it is observed that the bubble moves towards the wall for all Eo , except for the lightest (most deformable) bubble at $Eo = 3$, as shown in Fig. 2.4.2. It is interesting to observe that the effect of the Eo on the steady separation distance is less than effect of Ca . At $Eo = 3$, the aerodynamic lift force reverses its direction and thus, bubble migrates towards the center of the channel. It starts oscillating (path instability)[85] as it approaches to the center of the channel, which will be discussed in more detail below. On the other hand, the effect of Eo is more significant on the contaminated case as shown in Fig. 2.4.2. At $Eo = 0$, the contaminated bubble migrates towards the centerline. However, the behavior of the contaminated bubble changes completely with an increase of Eo . For $Eo \leq 1$, the bubble migrates towards the wall, maintaining a slightly larger separation distance than in the corresponding clean case. This is due to the buoyancy-induced increase in the velocity of the bubble that results in a higher aerodynamic lift force. At $Eo = 1.5$, the contaminated bubble initially moves towards the wall but then eventually migrates to the center of the channel, where it starts oscillating. At $Eo = 2.0$, the direction of the lateral migration is reversed and hence the bubble migrates towards the center

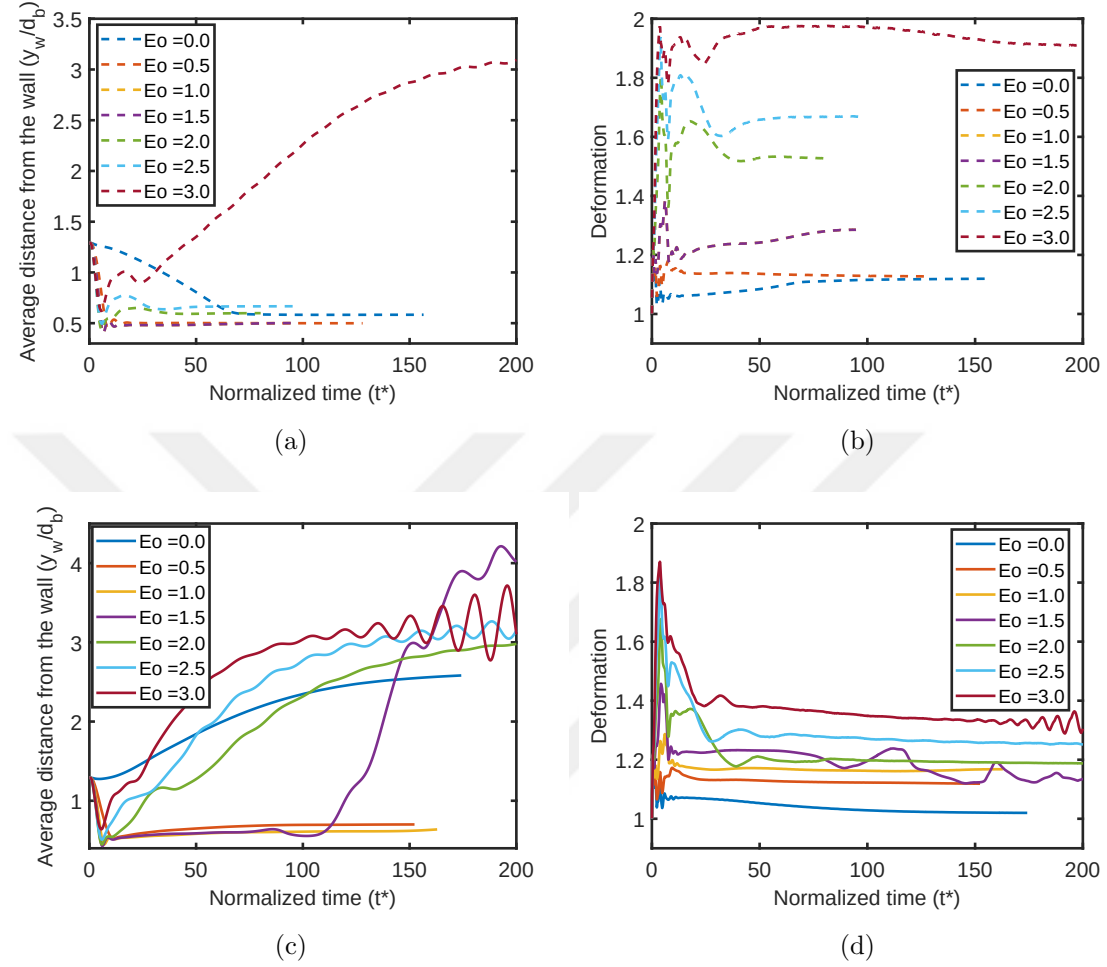


Figure 2.7: Effect of the *Eötvös* number (Eo): (a) Average distance from the wall (clean case) (b) deformation of the bubbles (clean case) (c) average distance from the wall (contaminated case) and (d) deformation for contaminated bubbles. $Re_c = 1000$, $Ca = 0.05$, $\beta_s = 0.5$, $Pe_s = Pe_c = 200$, $k = 0.125$, $Bi = 1.2$, $Da = 6.667$

and maintains a certain steady separation distance. Path instability is observed for the cases of $Eo = 2.5$ and $Eo = 3.0$ as the bubble approaches the center of the channel as seen in Fig. 2.4.2. Deformation of the clean and the contaminated bubbles is shown in Fig. 2.4.2 and Fig. 2.4.2, respectively. As expected, the deformation increases with Eo for both cases. Also, it can be seen that the deformation of the contaminated bubbles is lower than the clean bubbles irrespective of their average distance from the wall. This is attributed to the rigidifying effect of surfactant on the contaminated bubbles.

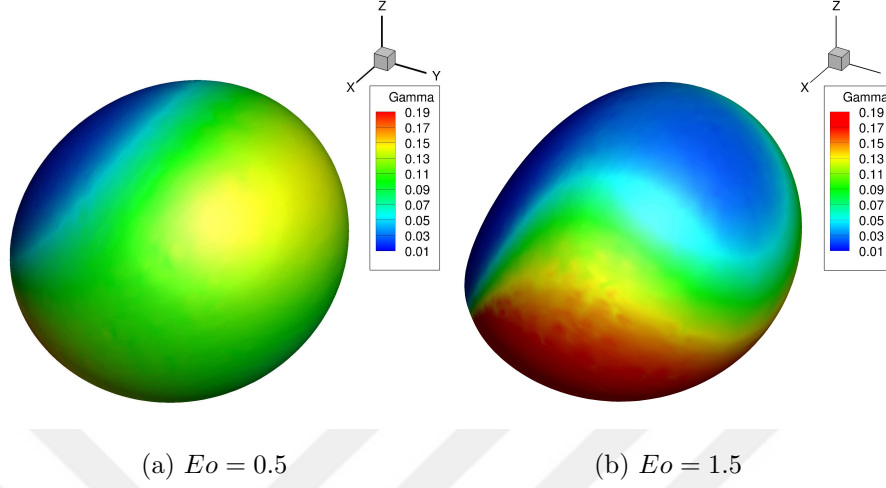


Figure 2.8: Surfactant concentration for (a) $Eo = 0.5$ (moves towards the wall) and (b) $Eo = 1.5$ (moves away from the wall) at $t^* = 100$. $Re_c = 1000$, $\beta_s = 0.5$, $Pe_s = Pe_c = 200$, $k = 0.125$, $Bi = 1.2$, $Da = 6.667$

To understand the distinct behavior of two contaminated bubbles at $Eo = 0.5$ and 1.5 , bubbles with contours of interfacial surfactant are plotted in Fig. 2.8 at $t^* = 100$. Note that the bubble dynamics is critical beyond this time as shown in Fig. 2.4.2. Indeed, as can be seen in Fig. 2.8a, the contaminated bubble at $Eo = 0.5$ is nearly spherical and the surfactant concentration is almost uniform leading to small Marangoni stresses. The aerodynamic lift force dominates the force due to surfactants-induced Marangoni force, as a result the bubble maintains the same separation distance in time. On the other hand at $Eo = 1.5$, for the contaminated bubble the surfactant concentration is more non-uniform, that is, more surfactant is advected to the rear end leading to larger Marangoni stresses. Thus, the Marangoni stresses overcome the lift force and contaminated bubble migrates to the channel center as the time progresses. To give more insight on the effects of Eo , bubbles at $Eo = 0, 1, 2$ and 3 with constant contours of interfacial surfactant concentration are shown in Fig. 2.9 at initial, intermediate and later times (at approximate steady state). Initially at $t^* = 8.3$, the adsorption of surfactant at $Eo = 0$ is much higher than the other cases, therefore the contaminated bubble instantly migrates towards the center unlike in other cases where it first migrates towards the wall. At inter-

mediate time, the bubble at $Eu = 0$ and $t^* = 83.3$ stays spherical but with high concentration at the front, drifting the bubble away from the wall. On the other hand, the bubble at $Eu = 1$ and $t^* = 83.3$ is deformable and the distribution of surfactant concentration is almost uniform, maintaining the bubble close to the wall. On the contrary, for the bubbles at $Eu = 2$ ($t^* = 89.4$) and $Eu = 3$ ($t^* = 75$), the surfactant has accumulated at the bottom of the bubbles due to strong convection, and approaches an axisymmetric distribution as the contaminated bubbles migrate to the center of channel. Note that the bubble behaves similarly at later times. The contaminated bubble at $Eu = 0$ also migrates to the center but the interfacial surfactant concentration is different than the $Eu = 2$ and $Eu = 3$ cases, that is, surfactant is advected to the nose of the bubble rather than the bottom of the bubble.

Finally, the effects of the *Eötvös* number on the path instability of the clean and the contaminated bubbles are studied. The three-dimensional trajectory of the bubble for $0 < Eu \leq 3$ is shown in Fig. 2.10. Note that for the clean case, the path instability is only observed at highest *Eötvös* number considered in this work, i.e., at $Eu = 3$. As can be seen, after the clean bubble reaches the center of the channel, its motion changes from straight to zigzag path. Zenit and Magnaudet [129] experimentally studied the conditions for which the path of freely rising bubble becomes oscillatory. They found that the criteria of path instability of a bubble with a free-slip surface is not the Reynolds number but the aspect ratio $\mathcal{A} > 2.0$ of the bubble shape. It is interesting to observe that the deformation parameter for $Eu = 3$ is less than $Eu = 2$ as shown in Fig. 2.4.2. There are several possible reasons for this discrepancy. Firstly, the present work considers a rising bubble in a pressure driven flow rather than the freely rising bubble considered by Ref. [129]. Secondly, there is a clear difference in the definition of the deformation parameter (see Eq. 2.19). Tripathi et al. [118] and Sharaf et al. [94] performed numerical and experimental studies, respectively, to generate a phase plot in the Galilei and *Eötvös* numbers plane, which separates distinct regimes in terms of bubble behavior. According to their phase plots, the clean case at $Eu = 3$ also lies in the oscillatory

regime (region III). In the presence of surfactant, the critical *Eötvös* number (Eo_{cr}) at which the path instability is triggered is affected significantly. In the current work, addition of surfactant leads to decrease in the critical *Eötvös* number from $Eo_{cr} \approx 3$ for the clean case to $Eo_{cr} \approx 1.5$ for the contaminated case. Another difference is that the contaminated bubble at $Eo = 1.5$ is in a spiral motion rather than the zigzag motion observed for the clean case. Further increasing the *Eötvös* number to $Eo = 2.0$ and $Eo = 2.5$, leads to a zigzag path instability. Finally at $Eo = 3$, the path initially changes from straight to zigzag and later to helical/spiral. Note that, this zigzag-helical transition is also observed for freely rising clean bubbles in the experimental study of Shew et al. [95] and numerical study of Mougin and Magnaudet [73]. The terminal velocity at $Eo = 3$ for both clean and contaminated bubbles along the rising direction z and $x - y$ plane is shown in the Fig. 2.11. As can be seen, the quasi-steady state terminal velocity of the contaminated bubble along rising z direction is lower than that of the clean bubble due to the Marangoni stresses which increase the drag force of the rising bubble. On the contrary, the terminal velocity of contaminated bubble along $x - y$ plane is much higher than the clean bubble due to the Marangoni stresses. Thus, the increase in the magnitude of oscillation and reduction of the critical parameters at which path instability is triggered can be attributed to the effect of Marangoni stresses. Figure 2.12 shows the vortical structures for the clean ($Eo = 3$) and the contaminated ($Eo = 2.5$ and $Eo = 3$) cases, at different time instants. As can be seen, for the zigzag motion of the bubbles the wake structure consists of two counter-rotating vortices with a symmetry plane and at each cycle (from one peak of y_w to another) the two vortices interchange their signs. Note that the zigzag motion is observed for both cases ($Eo = 2.5$ and $Eo = 3$) at all time instances, except for $t^* \geq 489.4$ at $Eo = 3$ where the contaminated bubble follows helical trajectory. For the clean case at $Eo = 3$, the vortical structures decay with time and almost vanish at $t^* = 381.2$, as the bubble stabilizes at later times. On the other hand, for the contaminated case at $Eo = 2.5$, the vortical structures do not vanish with time, as the bubble continues to oscillate indefinitely. For the contaminated bubble ($Eo = 3$), the vortical structure

changes when its motion changes from zigzag to helical at non-dimensional time $t^* = 489.4$. For the helical motion, two counter-rotating vortices of opposite sign are formed that wrap around each other as shown in Fig. 2.12. Figure 2.13 shows the interfacial surfactant concentration and orientation of the contaminated bubble at the same non-dimensional times at which the vortical structures are shown. As can be seen the orientation of the bubbles is tilted towards the direction of motion for zigzag motion and at such instants the Marangoni-induced force would act in the same direction resulting in the enhancement of horizontal oscillation magnitude as observed in Fig. 2.5.

2.5 Conclusions

A finite-difference/front-tracking (FD/FT) method is used to examine the effects of soluble surfactant on the lateral migration of nearly spherical and deformable bubbles in a pressure-driven channel flow. It is found that a small amount of surfactant can alter direction of lateral migration of a bubble. The clean bubble moves toward the wall and maintains a steady separation distance depending on the deformability (Ca) of the bubble. On the contrary, the contaminated bubble migrates toward the center of the channel and its steady separation distance is nearly independent of the deformability (Ca) of the bubble. By comparing soluble and insoluble surfactant cases for different capillary numbers, it is observed that the lateral migration of the bubble is faster in case of insoluble surfactant than the soluble surfactant during the transient period and this difference in both cases increases with the capillary number.

The effects of the bulk surfactant concentration (C_∞) and the elasticity number (β_s) on the lateral migration of the bubble are examined by extensive simulations. It is found that in both cases, the bubble migrates toward the center of channel after a critical value of $C_\infty = 0.25$ and $\beta_s = 0.25$.

Finally the effect of *Eötvös* number on the lateral migration is examined. For the clean case, the bubble moves away from the wall only at high $Eu = 3$, whereas it migrates towards it at smaller values. In the presence of surfactant, the bubble

reverses the direction of lateral migration for $Eo = 0$ and $Eo \geq 1.5$, while it moves towards the wall in the values in between. Path instability is observed for rising bubbles in both clean and contaminated cases. It is observed that the surfactant reduces the critical values at which a path instability is triggered.

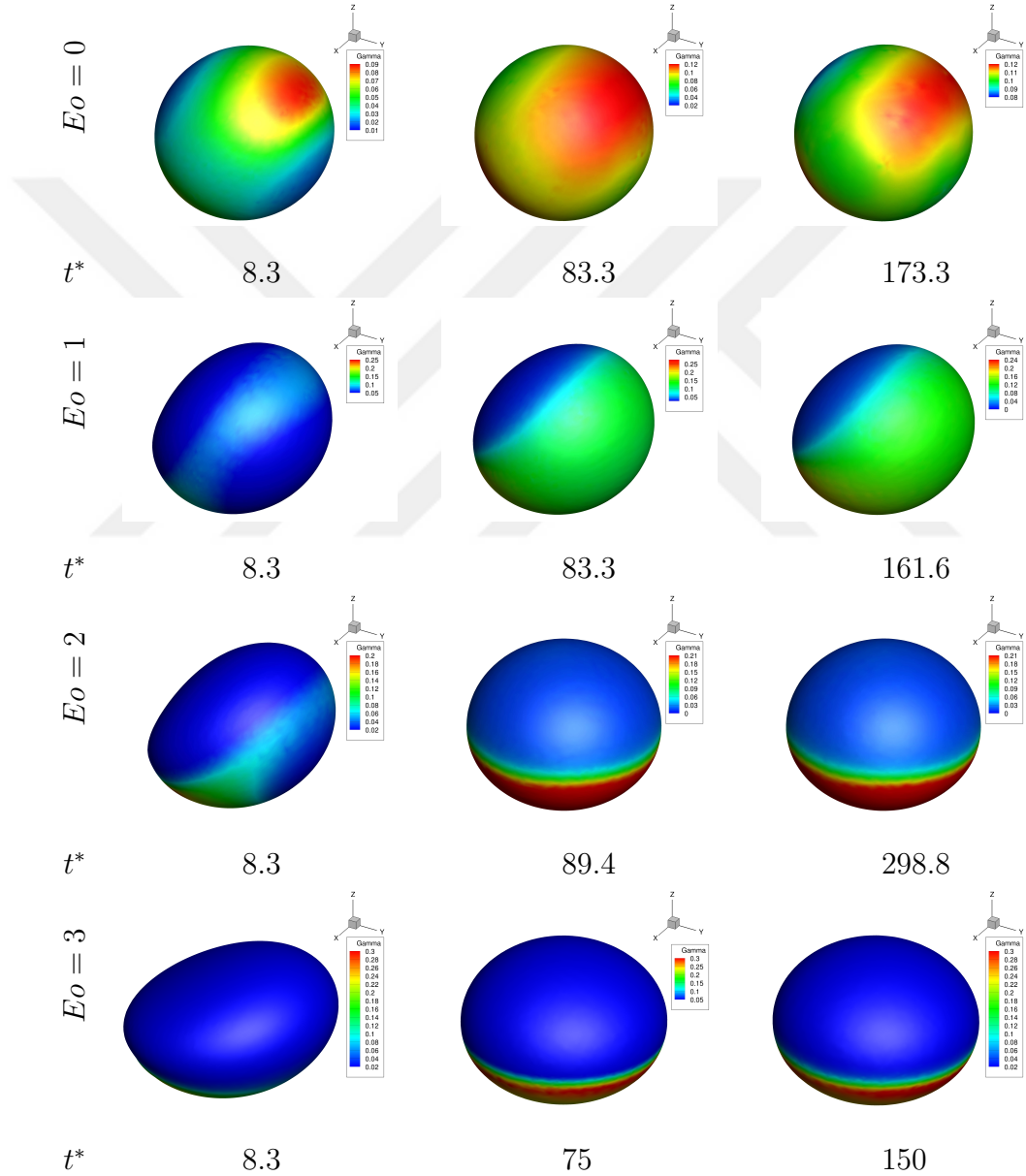


Figure 2.9: Surfactant concentration at various times for $Eo = 0, 1, 2$ and 3 . $Re_c = 1000, Ca = 0.05, \beta_s = 0.5, Pe_s = Pe_c = 200, k = 0.125, Bi = 1.2, Da = 6.667$

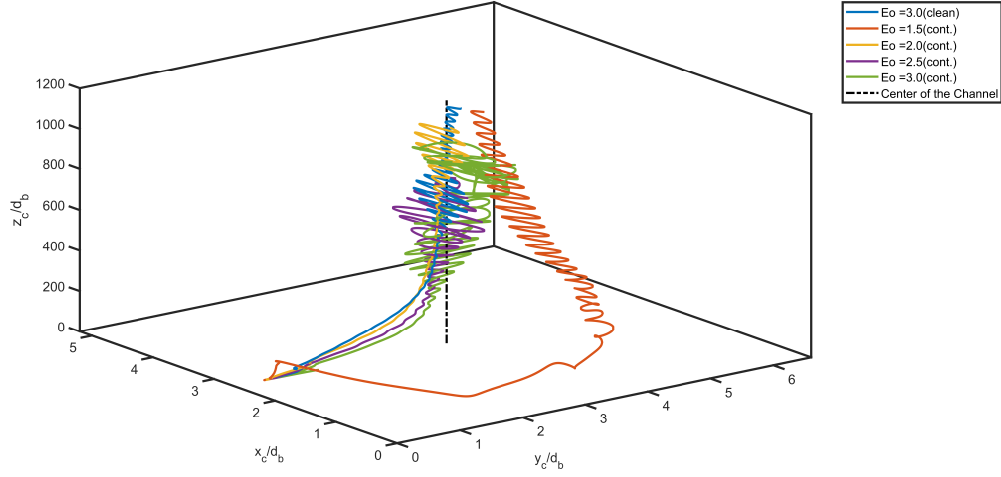


Figure 2.10: The three-dimensional trajectories of the rising bubbles. $Re_c = 1000, Ca = 0.05, \beta_s = 0.5, Pe_s = Pe_c = 200, k = 0.125, Bi = 1.2, Da = 6.667$

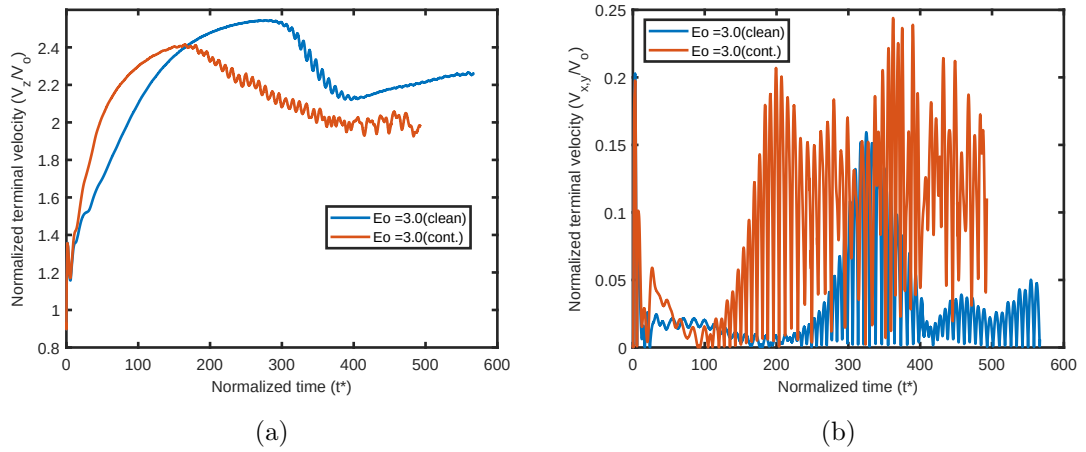


Figure 2.11: The terminal velocity of the clean and contaminated bubbles: The components of the terminal velocity (a) along the rising z direction (V_z) and (b) along the $x - y$ plane (lateral) defined as $V_{x,y} = \sqrt{V_x^2 + V_y^2}$. $Re_c = 1000, Ca = 0.05, \beta_s = 0.5, Pe_s = Pe_c = 200, k = 0.125, Bi = 1.2, Da = 6.667$

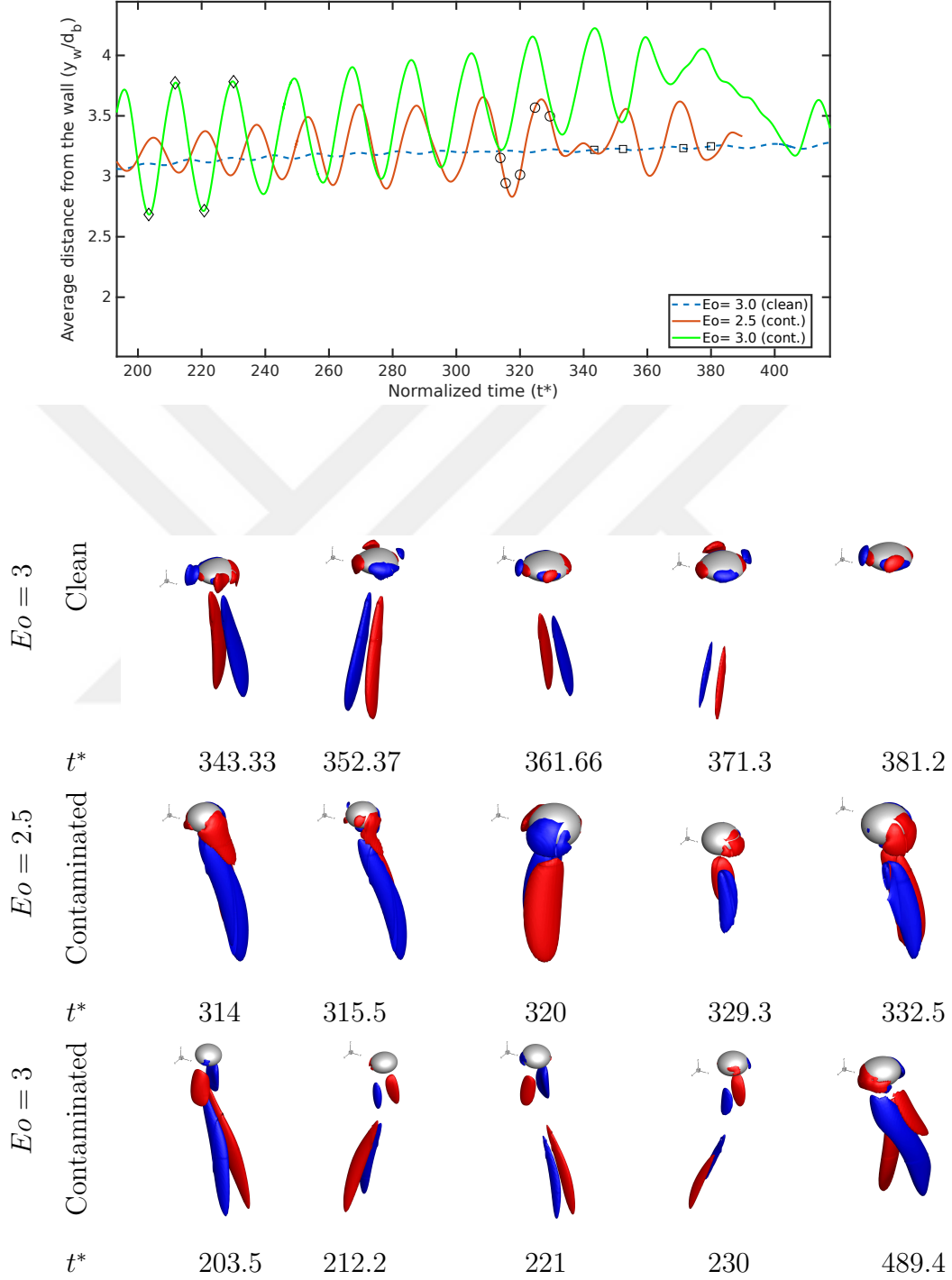


Figure 2.12: (Color online) Non-dimensional vorticity contour plots. (Lower panel) The first row shows the vorticity ($\omega_z^* = \pm 0.42$) contour plot for clean bubble $Eo = 3.0$. Second row shows the vorticity ($\omega_z^* = \pm 0.3$) contour plot for contaminated bubble $Eo = 2.5$. Third row shows the vorticity ($\omega_z^* = \pm 0.54$) contour plot for contaminated bubble $Eo = 3.0$. The top plot show the variation of average distance of bubble from the wall where the symbols indicate the times at which the vorticity contour plots are shown in the lower panel.

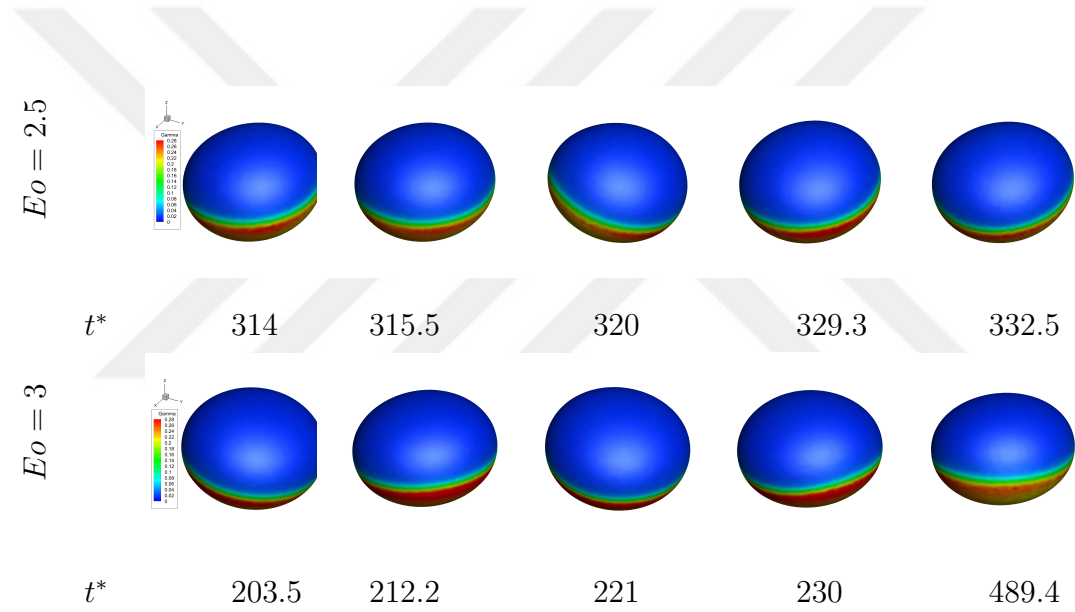


Figure 2.13: Interfacial surfactant concentration and orientation of the contaminated bubble for $Eo = 2.5$ (first row) and $Eo = 3$ (second row).

Chapter 3

TURBULENT BUBBLY CHANNEL FLOWS: EFFECTS OF SOLUBLE SURFACTANT AND VISCOELASTICITY

3.1 Introduction

Complex fluids containing polymer additives exhibit viscoelastic behavior and surfactant is often added to manipulate multiphase flows. The viscoelasticity and surfactant coexist in many multiphase flow systems of practical interest such as household products, the oil and gas industry, and heating and cooling processes. In many cases the flow can be turbulent, exhibiting chaotic and multi-scale dynamics, and thus making the flow extremely complex. Polymer additives exhibit various exotic behaviors that can be exploited to perform useful functions. For instance, addition of a very small volume fraction of polymer particles in a suspending fluid can lead up to 80% drag reduction in turbulent wall-bounded transport [125]. This phenomenon is very sophisticated and its full understanding remains elusive, see e.g. [125]. Even the flow instabilities leading to the onset of turbulence are greatly modified by the presence of polymers [7]. Introducing a second gaseous phase with surfactant contamination into this problem results in even more complex and exciting dynamics, as the two-fluid interface dynamics is tightly coupled with the elastic turbulence and the local surfactant concentration.

Numerous studies have analysed the effect of solid particles and drops or bubbles under gravity in an otherwise quiescent non-Newtonian fluid, see e.g., Zenit et al. [128] for a recent review. Other studies have focused on the rheology of such suspensions in highly laminar low Reynolds number shear flows [21]. Cross-stream migration of particles is of particular interest as it plays a critical role in many engineering and biological flows [58]. Studies on the effect of viscoelasticity on the lateral

migration of a droplet suggest various opposing scenarios of migration towards wall or center of a channel. Chan et al. [12] performed an analysis based on the small perturbations using a second order fluid model and found that the viscoelasticity contained in either phase promotes migration away from the wall. Mukherjee et al. [74] examined the motion of a Newtonian droplet in a viscoelastic medium using a front-tracking method at a low Reynolds number and proposed a semi-analytic theory to explain the observed behavior based on the numerical simulations. In contrast with findings of Chan et al. [12], they found that there is a net viscoelastic lift force acting on the droplet stemming from the normal stress differences, which drives a droplet towards the wall. More recently, Hazra et al. [45] experimentally examined the cross-stream motion of a viscoelastic drop in a viscoelastic medium in the Stokes flow regime. They proposed a presence of a viscoelasticity-induced lift force in the droplet-phase driving a droplet towards center of a channel. D'Avino et al. [22] and Yuan et al. [127] have provided detailed reviews on the migration of a particle in a viscoelastic fluid. The detailed numerical simulations by Mukherjee et al. [74] provide an explanation for the conflicting results about the cross-stream migration of a droplet in a viscoelastic continuous phase. They pointed out the importance of drop inclination (i.e., its alignment with the flow) as well as drop deformation. They showed that viscoelasticity reduces drop inclination and deformation varies non-monotonically, and the subtle competition between these two effects determines the net effect of matrix viscoelasticity on cross-stream migration of droplet. Their careful numerical and theoretical analysis reveals that the matrix viscoelasticity acts to drive the droplet towards the channel wall due to larger effect of non-Newtonian contribution to the difference of first and second normal non-Newtonian stresses. Their study clearly demonstrates importance of detailed numerical simulations for understanding of subtle effects of viscoelasticity on multiphase flows even in the absence of inertia at very low Reynolds numbers. Strong non-linear interactions of viscoelasticity and inertia make the problem much harder and severely limit predictive capability of perturbative analysis, and thus require detailed direct numerical simulations.

Direct numerical simulations (DNS) have been performed to examine behavior of bubbly channel flows for both cases of nearly spherical and deformable bubbles in the absence of viscoelasticity and surfactant. In the case of nearly spherical bubbles, Lu et al. [62] found that the clean (i.e., surfactant-free) bubbles tend to form a layer at the wall for upflow, while bubble-free wall layers are formed for downflow in vertical laminar flows. Lu et al. [66] have also examined the bubbly flows in the turbulent regime using a similar computational setup. They showed that, for nearly spherical bubbles, the formation of wall layers results in a reduction of the liquid flow rate, and the layered bubbles form horizontal clusters, whereas more deformable bubbles, instead, move toward the channel center. Later, Lu et al. [67] performed simulations for a larger system containing over hundred bubbles at a larger Reynolds number. The overall structure of the bubbly flow has been found to be similar to that of the smaller system. They also observed the formation of bubble clusters similar to the experimental observations of Takagi et al. [110] for weakly-contaminated bubbly flows. Numerous other studies of DNS of turbulent bubbly flows can be found in the recent review by Elgobashi [28].

Surfactant has a drastic effect on the behavior of bubbly flows [115, 80, 110]. Takagi et al. [110] performed experiments to investigate the effects of different surfactants on the structure of upward turbulent bubbly flows in a vertical channel. In the surfactant-free case, they found that nearly spherical bubbles tend to form layers at the wall, where they merge during the rising process, and subsequently become deformable and move toward the channel center. When a small amount of surfactant, just enough to prevent coalescence, is added to the bulk fluid, the bubbles remain spherical, tend to move toward the wall and form bubble clusters. Conversely, with a significant surfactant concentration, the bubbles do not tend to move toward the channel wall but spread out across the channel. Motivated by this experimental study, Muradoglu et al. [77] and Ahmed et al. [2] studied the effects of soluble surfactants on lateral migration of a single bubble in a pressure-driven channel flow. They both found that surfactant-induced Marangoni stresses act to move the bubble away from the wall and bubble stabilizes at the channel centerline in

the presence of sufficiently strong surfactant contamination. Lu et al. [64] examined the effect of insoluble surfactants on the structure of turbulent bubbly upflow in a vertical channel by DNS. They showed that surfactant contamination prevents the formation of bubble-rich wall layers and bubbles are uniformly distributed across the channel cross-section. Pesci et al. [85] computationally examined the dynamics of single rising bubbles influenced by soluble surfactant. They observed that the quasi steady state of the rise velocity is reached without ad- and desorption being necessarily in equilibrium. Soligo et al. [99, 98] developed a modified phase field method (PFM) for simulations of turbulent flows with large and deformable surfactant-laden droplets. They have used this method to examine breakage/coalescence rates and size distribution of surfactant-laden droplets in turbulent flow.

Even though effects of polymers and surfactant have been studied separately, their interactions and combined effects on pressure-driven turbulent bubbly channel flows remain a challenging problem that has not been explored experimentally or computationally. Only a few numerical studies [116, 84, 52] have been recently done to examine the effect of surfactant and viscoelasticity on the deformation and shape of a buoyancy-driven droplet. In this regard, the three-dimensional interface-resolved numerical simulations can provide significant insight about this highly complex phenomenon. In the present study, we report the results of the first direct numerical simulations where the combined effects of viscoelasticity and surfactant on turbulent bubbly flows are investigated.

3.2 Computational setup and numerical method

We consider vertical turbulent channel flow as shown in Fig. 3.1. The flow is periodic in the spanwise (x) and streamwise (z) directions, while no-slip/no-penetration boundary conditions are applied at the walls (y direction). The flow is driven upward by an imposed constant pressure gradient $\frac{dp^*}{dz^*}$. Note that dimensional quantities are denoted by the superscript $*$ in the present study, e.g., p^* and p represent the dimensional and non-dimensional pressure, respectively. At a statistically steady state, the average wall shear stress τ_w^* is related to the pressure gradient and the weight of the

bubble/liquid mixture by a streamwise momentum balance:

$$\tau_w^* = - \left(\frac{dp^*}{dz^*} + \rho_{av}^* g^* \right) h^* = -\mathcal{B}^* h^*, \quad (3.1)$$

where ρ_{av}^* is the average density in the mixture and h^* is the channel half-width. Note that the value of $\mathcal{B}^*$ dictates the bulk flow direction, i.e., upflow ($\mathcal{B}^* < 0$) and downflow ($\mathcal{B}^* > 0$). In all the cases, spherical bubbles are placed randomly in a vertical channel in an initially single-phase fully developed turbulent flow, with a friction Reynolds number of $Re_\tau = w_\tau h / \nu_o = 127.3$. Here, the friction velocity is $w_\tau^* = \sqrt{\tau_w^* / \rho_o^*}$, where ρ_o^* and ν_o^* are the density and kinematic viscosity of the liquid respectively. Before the addition of the bubbles, the channel Reynolds number, based on the average bulk velocity and full channel width, is about $Re_{bulk} \approx 3786$. The single-phase turbulent channel flow is generated by initializing the flow field with a streamwise-aligned vortex pair [46], which effectively triggers transition to turbulence. The physical parameters governing the flow are listed in Table 4.1 where subscripts “i” and “o” denote the properties of the inner (dispersed) and the outer (continuous) fluids, respectively, and λ^* is the polymer relaxation time. The Morton number ($M = g^* \mu_o^{*4} / \rho_o^* \sigma_s^{*3}$) used here is $M = 6.17 \times 10^{-10}$ which is higher than the Morton number of $M = 2.52 \times 10^{-11}$ for an air bubble in water at 20°C but could be matched by using an aqueous solution of sugar [101].

The incompressible flow equations for a viscoelastic fluid are discretized using a second-order finite-difference/front-tracking (FD/FT) method [119]. Following [119], [77] and [49], a single set of governing equations can be written for the entire computational domain provided the jumps in the material properties are taken into account and the effects of the interfacial surface tension are treated appropriately. The governing equations are non-dimensionalized using a length scale $\mathcal{L}^*$, a velocity scale $\mathcal{U}^*$ and a time scale $\mathcal{T}^* = \frac{\mathcal{L}^*}{\mathcal{U}^*}$. The length and velocity scales are taken as $\mathcal{L}^* = 2h^*$ and $\mathcal{U}^* = W_b^*$ where W_b^* is the average axial velocity of the corresponding single phase flow. The density and viscosity are non-dimensionalized using the density ρ_o^* and total viscosity μ_o^* of the continuous phase while the surface tension is normalized by the surface tension of the surfactant-free gas-liquid interface σ_s^* . The non-dimensional momentum equation, accounting for interphase coupling, is than

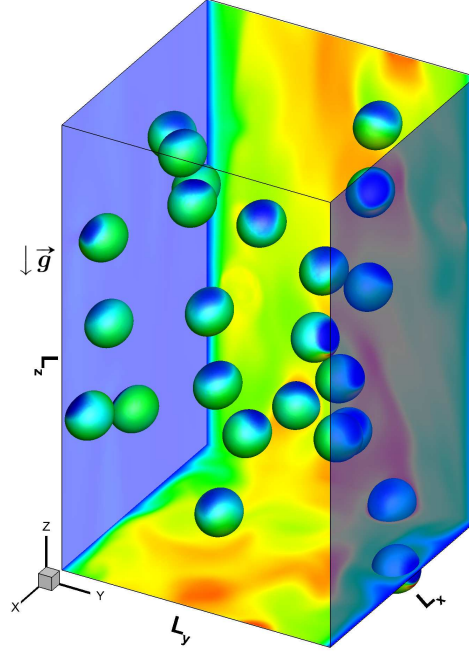


Figure 3.1: Schematic representation of the computational setup considered in the present work. The contours on the plane represent streamwise velocity with the scale ranging from $0.15W_b^*$ (blue) to $1.1W_b^*$ (red) where W_b^* is the average bulk velocity in the single-phase case. The contours on the bubble surface represent interfacial surfactant concentration (Γ) with the scale ranging from 0 (blue) to 0.15 (red).

given by

$$\begin{aligned} \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \frac{(\rho - \rho_{av}) \mathbf{g}}{Fr^2} + \nabla \cdot \boldsymbol{\tau} + \frac{1}{Re} \nabla \cdot \mu_s (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \\ &+ \frac{1}{We} \int_A [\sigma(\Gamma) \kappa \mathbf{n} + \nabla_s \sigma(\Gamma)] \delta(\mathbf{x} - \mathbf{x}_f) dA, \end{aligned} \quad (3.2)$$

where ρ , $\mathbf{u}$, p , $\boldsymbol{\tau}$, μ_s and σ are the non-dimensional density, the velocity vector, the pressure, the polymer stress tensor, the solvent viscosity and the surface tension coefficient, respectively. The unit vector $\mathbf{g}$ points in the direction of the gravitational acceleration. In Eq. (4.3), the last term on the right hand side represents the surface tension where A is the surface area, κ is twice the mean curvature, $\mathbf{n}$ is the unit normal vector and ∇_s is the gradient operator along the interface defined as

$$\nabla_s = \nabla - \mathbf{n}(\mathbf{n} \cdot \nabla). \quad (3.3)$$

We emphasize that the surface tension is a function of the interfacial surfactant concentration Γ and $\nabla_s \sigma(\Gamma)$ represents the surfactant-induced Marangoni stress. The non-dimensional numbers in Eq. (4.3) are Reynolds number ($Re = \rho_o^* \mathcal{U}^* \mathcal{L}^* / \mu_o^*$), Froude number ($Fr = \frac{\mathcal{U}^*}{\sqrt{g^* \mathcal{L}^*}}$), with g^* being the magnitude of the gravitational acceleration and the Weber number ($We = \frac{\rho_o^* \mathcal{U}^{*2} \mathcal{L}^*}{\sigma_s^*}$).

The fluid properties remain constant along material lines, i.e.,

$$\frac{D\rho}{Dt} = 0, \quad \frac{D\mu_s}{Dt} = 0, \quad \frac{D\mu_p}{Dt} = 0, \quad \frac{D\lambda}{Dt} = 0, \quad (3.4)$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$ is the material derivative. The indicator function is used to set the material properties in each phase and is defined as

$$I(\mathbf{x}, t) = \begin{cases} 1 & \text{in bulk fluid,} \\ 0 & \text{in bubble domain.} \end{cases} \quad (3.5)$$

Then a material property, ϕ , is specified as

$$\phi = \phi_o I(\mathbf{x}, t) + \phi_i (1 - I(\mathbf{x}, t)), \quad (3.6)$$

where the subscripts “ i ” and “ o ” denote the properties of the bubble and bulk fluid, respectively.

The present soluble surfactant methodology is same as that developed by Muradoglu et al [76, 77], and is described below for completeness. The C_∞ ($= \frac{C_\infty^*}{C_{ref}^*}$) represents the non-dimensional initial bulk surfactant concentration and Γ ($= \frac{\Gamma^*}{\Gamma_{max}^*}$) represents the non-dimensional interfacial surfactant concentration, where C_{ref}^* and Γ_{max}^* denote the reference bulk surfactant concentration taken as the critical micelle concentration (CMC) and the maximum packing concentration, respectively. The surface tension coefficient is made dimensionless with σ_s^* . The local value of the surface tension coefficient is related to the local surfactant concentration through the Langmuir equation of state [61]

$$\sigma = 1 + \beta_s \ln(1 - \Gamma), \quad (3.7)$$

where β_s is the elasticity number. Equation (3.8) is bounded to prevent nonphysical (negative) values of the surface tension:

$$\sigma = \max(\epsilon_\sigma, 1 + \beta_s \ln(1 - \Gamma)), \quad (3.8)$$

Table 3.1: Physical and computational parameters governing the flow.

Friction Reynolds number	Re_τ	127.3
Domain size	$L_x \times L_y \times L_z$	$\pi/2 \times 2 \times \pi$
Resolution	$N_x \times N_y \times N_z$	$128 \times 192 \times 256$
Inner-scaled resolution	$\Delta x^+ = \Delta z^+$	1.56
Inner-scaled resolution	$\Delta y^+ \text{ min/max}$	0.76/1.72
Channel half-width	h^*	1.0
Bubble diameter	d_b^*	0.3
Void fraction	Φ	3.44%
Density and viscosity ratio	$\rho_i^*/\rho_o^*, \mu_i^*/\mu_o^*$	0.05, 0.1
Total pressure gradient	$\mathcal{B}^* = \frac{dp^*}{dz^*} + \rho_{av}^* g^*$	-0.0018
Surface tension	σ_s^*	0.01
Gravitational acceleration	g^*	0.05
Single-phase average bulk velocity	W_b^*	0.63
Eötvös Number	$Eo = \rho_o^* g^* d_b^{*2} / \sigma_s^*$	0.45
Morton Number	$M = g^* \mu_o^{*4} / \rho_o^* \sigma_s^{*3}$	6.17×10^{-10}
Peclet number	$Pe_c = Pe_s = 2h^* W_b^* / D_c^*$	1680
Biot Number	$Bi = 2h^* k_d^* / W_b^*$	6.33
Damkohler Number	$Da = \Gamma_{max}^* / 2h^* C_\infty^*$	2.0/1.0/0.5
Langmuir number	$La = k_a^* C_\infty^* / k_d^*$	0.0625/0.125/0.25
Elasticity Number	$\beta_s = R^* T^* \Gamma_\infty^* / \sigma_s^*$	0.5
Weissenberg Number	$Wi = \lambda^* W_b^* / 2h^*$	0/5/10
Solvent viscosity ratio	$\beta = \mu_s^* / \mu_o^*$	0.9
Extensibility parameter	L	60

where ϵ_σ is taken as 0.05 in the present study. Note that ϵ_σ is typically larger than this value in the common physical systems (e.g., $\epsilon_\sigma \sim 0.2 - 0.3$) but it does not have any influence on the present results since the interfacial surfactant concentration remains much lower than the maximum packing concentration in all the cases

considered here. The evolution equation for the interfacial surfactant concentration was derived by Stone [102] and can be expressed in the non-dimensional form as

$$\frac{1}{A} \frac{D\Gamma A}{Dt} = \frac{1}{Pe_s} \nabla_s^2 \Gamma + Bi \dot{S}_\Gamma, \quad (3.9)$$

where A is the surface area of an element of the interface and $Pe_s = \frac{u^* \mathcal{L}^*}{D_s^*}$ is the interfacial Peclet number with D_s^* being the diffusion coefficient along the interface. The Biot number is defined as $Bi = \frac{k_d^* \mathcal{L}^*}{u^*}$, where k_d^* is the desorption coefficient. The non-dimensional source term $\dot{S}_\Gamma$ is given by

$$\dot{S}_\Gamma = La C_s (1 - \Gamma) - \Gamma, \quad (3.10)$$

where C_s is the bulk surfactant concentration near the interface and La is the Langmuir number defined as $La = \frac{k_a^* C_{ref}^*}{k_d^*}$ with k_a^* being the adsorption coefficient. The bulk surfactant concentration is governed by an advection-diffusion equation of the form

$$\frac{\partial C}{\partial t} + \nabla \cdot (C \mathbf{u}) = \frac{1}{Pe_c} \nabla \cdot (D_{co} \nabla C), \quad (3.11)$$

where $Pe_c = \frac{u^* \mathcal{L}^*}{D_c^*}$ is the Peclet number based on bulk surfactant diffusivity. The coefficient D_{co}^* is related to the molecular diffusion coefficient D_c^* and the phase indicator function I as

$$D_{co}^* = D_c^* I(\mathbf{x}, t). \quad (3.12)$$

The source term in Eq. (3.10) is related to the bulk concentration by

$$\dot{S}_\Gamma = -\frac{1}{Pe_c Da} (\mathbf{n} \cdot \nabla C_{\text{interface}}). \quad (3.13)$$

where $Da = \frac{\Gamma_{max}^*}{\mathcal{L}^* C_{ref}^*}$ is the Damköhler number. Following Muradoglu et al. [77], the boundary condition at the interface given by Eq. (3.13) is first converted into a source term for the bulk surfactant evolution equation. In this approach it is assumed that all the mass transfer between the interface and bulk takes place in a thin adsorption layer adjacent to the interface. Thus, the total amount of mass adsorbed on the interface is distributed over the adsorption layer, and added to the

bulk concentration evolution equation as a negative source term. Equation (3.11) thus takes the following form:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\mathbf{u}) = \frac{1}{Pe_c} \nabla \cdot (D_{co} \nabla C) + \dot{S}_c, \quad (3.14)$$

where $\dot{S}_c$ is the source term evaluated at the interface and distributed onto the adsorption layer in a conservative manner. The details of this treatment can be found in [77].

The FENE-P model is adopted as the constitutive equation for the polymeric stress tensor $\boldsymbol{\tau}$. This constitutive equation and its numerical solution are described in details in [49, 50]. The model can be written as

$$\begin{aligned} \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{B}) - (\nabla \mathbf{u})^T \cdot \mathbf{B} - \mathbf{B} \cdot \nabla \mathbf{u} &= -\frac{1}{Wi} (F\mathbf{B} - \mathbf{I}), \\ F &= \frac{L^2}{L^2 - \text{trace}(\mathbf{B})}, \end{aligned} \quad (3.15)$$

where $\mathbf{B}$, Wi , L , and $\mathbf{I}$ are the conformation tensor, the Weissenberg number defined as $Wi = \frac{\lambda^* U^*}{L^*}$ with λ^* being the polymer relaxation time, the maximum polymer extensibility, and the identity tensor, respectively. Once the conformation tensor is obtained from Eq. (3.15), the polymeric stress tensor is computed as

$$\boldsymbol{\tau} = \frac{1}{ReWi} (1 - \beta) (F\mathbf{B} - \mathbf{I}), \quad (3.16)$$

where $\beta = \mu_s^*/\mu_o^*$ is the solvent viscosity ratio.

The viscoelastic constitutive equations are highly non-linear and become extremely stiff at high Weissenberg numbers. Thus, their numerical solution is generally a formidable task and is notoriously difficult especially at high Weissenberg numbers [49, 50]. To overcome the so-called high Weissenberg number problem, the log-conformation method is employed [34] in the present simulations. In this approach, Eq. (3.15) is rewritten in terms of the logarithm of the conformation tensor through eigendecomposition, i.e., $\boldsymbol{\Psi} = \log \mathbf{B}$, which ensures the positive definiteness of the conformation tensor. The core feature of the formulation is the decomposition of the gradient of the divergence free velocity field $\nabla \mathbf{u}^T$ into two anti-symmetric tensors denoted by $\boldsymbol{\Omega}$ (pure rotation) and $\mathbf{N}$, and a symmetric tensor denoted by $\mathbf{D}$

which commutes with the conformation tensor [34], i.e.,

$$\nabla \mathbf{u}^T = \mathbf{\Omega} + \mathbf{D} + \mathbf{N}\mathbf{B}^{-1}. \quad (3.17)$$

Inserting Eq. (3.17) into Eq. (3.15) and replacing the conformation tensor with the new variable $\mathbf{\Psi}$, the transformed constitutive equations can be written as

$$\frac{\partial \mathbf{\Psi}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{\Psi}) - (\mathbf{\Omega}\mathbf{\Psi} - \mathbf{\Psi}\mathbf{\Omega}) - 2\mathbf{D} = \frac{F}{Wi}(e^{-\mathbf{\Psi}} - \mathbf{I}). \quad (3.18)$$

Once Eq. (3.18) is solved for $\mathbf{\Psi}$, the conformation tensor is then obtained using the inverse transformation as $\mathbf{B} = e^{\mathbf{\Psi}}$.

3.2.1 Flow Solver

The flow equations (Eq. (4.3)) are solved fully coupled with the FENE-P model (Eq. (3.18)) and the interfacial and bulk surfactant concentration evolution equations (Eqs. (3.9) and (3.14)) using a front-tracking/finite-difference (FD/FT) method [119, 77, 49]. All the field equations are solved on a fixed Eulerian grid with a staggered arrangement where the velocity nodes are located at the cell faces while the material properties, the pressure, the bulk surfactant concentration and the extra stresses are all located at the cell centers[49]. The interfacial surfactant concentration evolution equation is solved on a separate Lagrangian grid [77]. The spatial derivatives are discretized with second-order central differences for the diffusive terms, while the convective terms are discretized using a QUICK scheme [60] in the momentum equation, and a fifth-order WENO-Z [10] scheme in the viscoelastic and the bulk surfactant concentration equations. The equations are integrated in time with a second-order predictor-corrector method in which the first-order solution (Euler method) serves as a predictor that is then corrected by the trapezoidal rule [119].

The details of the front-tracking method can be found in the review paper by Tryggvason et al. [119] and in the recent book by Tryggvason et al. [120]. The numerical methods for the treatment of soluble surfactant and viscoelasticity have been fully discussed by Muradoglu et al. [77] and Izbassarov et al. [49], respectively.

The new ingredient of the numerical method in the present study is the FFT-based pressure solver which is briefly described here. Since the projection method requires solution of a variable-density Poisson equation in the multiphase flows, FFT-based solvers cannot be used directly. To overcome this difficulty, the pressure-splitting technique presented in [24] and [23] is adopted, allowing for a direct and fast solution of a constant-coefficients Poisson equation using the same FFT-based solver. Regarding the FFT-based pressure solver, the overall procedure to advance time from time step n to the first-order predicted solution at time step $n + 1$ is provided below:

$$\frac{\rho^{n+1}\mathbf{u}^t - \rho^n\mathbf{u}^n}{\Delta t} = \left[-\nabla_h \cdot (\rho\mathbf{u}\mathbf{u}) + \frac{1}{Re}\nabla_h \cdot (\mu_s(\nabla_h\mathbf{u} + \nabla_h^T\mathbf{u})) + \frac{(\rho - \rho_{av})\mathbf{g}}{Fr^2} \right. \\ \left. + \nabla \cdot \boldsymbol{\tau} + \frac{1}{We} \int_A [\sigma(\Gamma)\kappa\mathbf{n} + \nabla_s\sigma(\Gamma)]\delta(\mathbf{x} - \mathbf{x}_f)dA \right]^n, \quad (3.19)$$

$$\nabla^2 p^{n+1} = \nabla \cdot \left[\left(1 - \frac{\rho_0}{\rho^{n+1}} \right) \nabla (2p^n - p^{n-1}) \right] + \frac{\rho_0}{\Delta t} \nabla \cdot \mathbf{u}^t, \quad (3.20)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^t - \Delta t \left[\frac{1}{\rho_0} \nabla p^{n+1} + \left(\frac{1}{\rho^{n+1}} - \frac{1}{\rho_0} \right) \nabla (2p^n - p^{n-1}) \right], \quad (3.21)$$

$$\boldsymbol{\Psi}^{n+1} = \boldsymbol{\Psi}^n + \Delta t \left(-\nabla \cdot (\mathbf{u}\boldsymbol{\Psi}) + (\boldsymbol{\Omega}\boldsymbol{\Psi} - \boldsymbol{\Psi}\boldsymbol{\Omega}) + 2\mathbf{D} + \frac{F}{Wi}(e^{-\boldsymbol{\Psi}} - \mathbf{I}) \right)^n, \quad (3.22)$$

where ∇_h is the discrete version of the nabla operator, $\rho_0 = \min(\rho_i, \rho_o)$ and $\mathbf{u}^t$ is the unprojected (temporary) velocity. The solution at this stage provides an estimate at the new time level and is used to compute the solution at the time level $n + 2$. Then solutions at time levels n and $n + 2$ are averaged to obtain a second order solution at the new time level $n + 1$ as described by Tryggvason et al. [119]. Note that the overall time-integration scheme is equivalent to the trapezoidal rule for the linear problem.

3.2.2 Parallelization

The parallelization method developed by Farooqi et al. [33] is slightly modified for the FFT-based pressure solver in the present study. First, the previous iterative

Table 3.2: Wall clock time per time step in seconds, and corresponding speedup of the DNS solver when a FFT-based Poisson solver is used instead of the iterative solver of HYPRE (PFMG).

Multigrid tolerance	HYPRE	FFT	Speedup
$ \nabla_h \cdot \mathbf{u} _{max} < 10^{-5}$	4.7	2.1	2.2
$ \nabla_h \cdot \mathbf{u} _{max} < 10^{-10}$	16.3	2.1	7.8

multigrid Poisson solver in the HYPRE library [32], the most demanding part of the numerical method, has been replaced with a versatile and efficient FFT-based direct solver for a constant-coefficients Poisson equation of the DNS code *CaNS*; see [16] for more details. The extension of the solver for the phase indicator function with this approach is trivial. To determine the overall speed up of the numerical algorithm, simulations are performed for a fully developed laminar flow using the domain size of $2 \times 2 \times 2$ discretized by 512^3 and 64 randomly distributed bubbles. Number of cores for the domain and fronts are 256 and 64, respectively. The results are summarized in Table 3.2. The FFT solver satisfies the divergence-free constraint on the velocity field to near the machine precision at every grid point (i.e., $|\nabla_h \cdot \mathbf{u}|_{max} < 10^{-14}$) whereas, the HYPRE (PFMG) reduces the residuals below a prespecified tolerance value i.e., $|\nabla_h \cdot \mathbf{u}|_{max} < \mathcal{E}_{tol}$. As can be seen, the present numerical algorithm with the FFT solver gets 2 and 8 times speed up for the error tolerances $\mathcal{E}_{tol} = 10^{-5}$ and $\mathcal{E}_{tol} = 10^{-10}$, respectively. Note that $\mathcal{E}_{tol} = 10^{-5}$ is sufficient to achieve a desired overall numerical accuracy for the kind of simulations presented here.

Next, the new parallelization strategy for the Lagrangian grid is implemented for the present computational setup, namely Particles-Per-Front (PPF), where *Fronts* denote to the processes computing on the Lagrangian grid. The PPF is compared with our previous strategy, namely Redundantly-All-Compute (RAC) [33]. The Redundantly-All-Compute algorithm is based on domain decomposition method similar to the Eulerian grid parallelization, where each subdomain can be assigned to one MPI-process and bubbles are distributed among the parallel *Fronts*. The *Front* containing the center of a bubble becomes the *owner* of that bubble. An

example where 16 randomly distributed bubbles are assigned to 2 *Fronts* is shown in the left panel of Fig. 3.2. As can be seen, the load on 2 *Fronts* is different due to the location of bubbles in the physical domain and this can continuously happen as bubbles move in the physical domain. To prevent this scenario, we parallelize the Lagrangian grid in a way that bubbles are assigned directly to the *Fronts* independent of their location in the physical domain. In this approach, the load on each *Front* will remain constant throughout the simulation. A typical example of this strategy where 16 randomly distributed bubbles are assigned to 2 *Fronts* (8 per *Front*) is shown in the right panel of Fig. 3.2.

The parallelization of the 3D front-tracking method leads to three types of communication, namely: (1) *Domain* to *Domain*, (2) *Front* to *Front* and (3) *Front* to *Domain*. The Particles-Per-Front (PPF) parallelization strategy does not affect the *Domain* to *Domain* communication, and therefore remains the same as described by Farooqi et al. [33]. The *Front* to *Front* communication is completely eliminated for the (PPF) strategy as the ownership of the bubbles does not change with location of bubbles in the physical domain. The total message size between a *Front* and all its *Domains* in a single time-step is

$$M_{f2d} = M_{send} + M_{recv} \quad (3.23)$$

$$M_{send} = 9 \times \sum_{i=1}^{np} P_i + 5 \times \sum_{i=1}^{ne} E_i, \quad M_{recv} = 3 \times \sum_{i=1}^{np} P_i + \sum_{i=1}^{ne} E_i \quad (3.24)$$

where P_i and E_i are the total number of points and the total number of elements for the i^{th} bubble, respectively. M_{send} is the data sent and M_{recv} is the data received by the *Front*. For each point there are point coordinates in the x , y , and z directions and every point coordinate has a corresponding surface tension force and normal vector to the edge of the element. For each element there are center coordinates of element, corresponding value of Γ and the element area. A total of 14 double precision data should be sent to a *Domain* while only updated point coordinates and $\dot{S}_\Gamma$ are received from a *Domain*. Let d_x , d_y , and d_z be the dimensions of the MPI partitions for the *Domains*. The number of messages sent and received by the *Front* in a single time-step would be $2d^3$ (Assuming $d = d_x = d_y = d_z$) because all

point coordinates destined to a single *Domain* could be packed in a single message. If there are f *Fronts* and an approximately equal number of *Domains* are assigned to each *Front*, then for the RAC strategy, the number of messages and message size per *Front* are reduced by a factor of f ; each *Front* exchanges $2d^3/f$ messages with size of M_{f2d}/f . However, the actual message size per *Front* can vary based on how bubbles are distributed in the physical domain. For the PPF strategy the number of messages and message size per *Front* will remain same. Thus, the PPF strategy works better for the modest domain and grid size and RAC works better for large scale simulations.

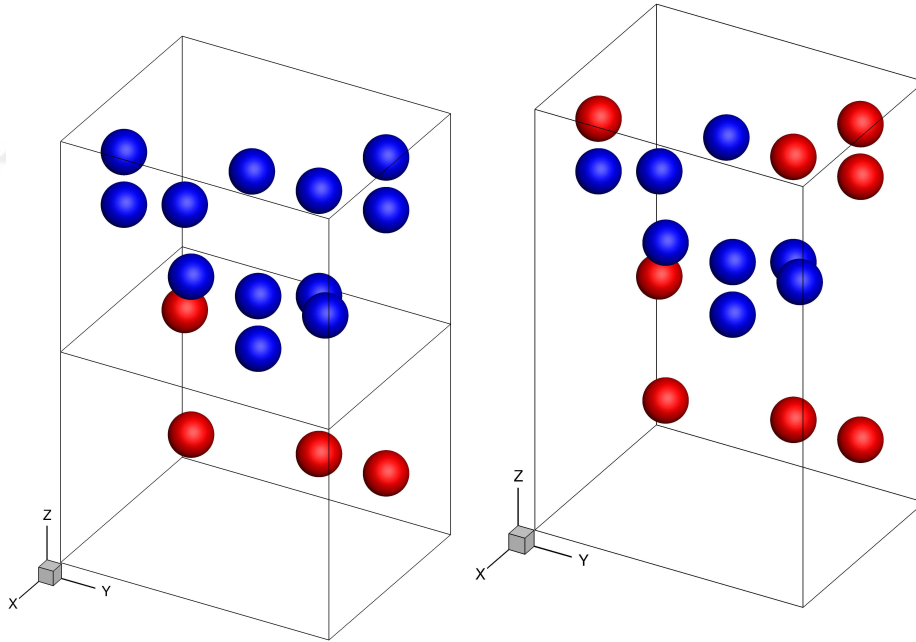


Figure 3.2: (Left) Computational load distribution under Redundantly-All-Compute (RAC) scheme, in contrast to that of the Particle-Per-Front (PPF) scheme (right) where the load distribution is decoupled from the domain decomposition. Blue and red colors denote load on Rank 1 and Rank 2, respectively.

3.3 Results and Discussion

The numerical method was first validated against the DNS results of turbulent bubbly channel flow in the absence of viscoelasticity and surfactant by Lu et al. [64]. Figure 3.3 shows the time history of the liquid flow rate (panel (a)) and the profile of the mean turbulent kinetic energy (panel (b)) for the turbulent multiphase flow in a statistically steady state, compared to the DNS results by Lu et al. [64]. The present results are in excellent agreement with the results of Lu et al. [64] showing the accuracy of the present simulations. The size of the computational domain is $\pi/2 \times 2 \times \pi$ and it is resolved by $128 \times 192 \times 256$ grid points in the spanwise (x), wall-normal (y) and streamwise (z) directions, respectively. This configuration has also been used in various previous turbulent bubbly flow studies [63, 65, 66, 64] using the same numerical method, i.e., finite-difference/front-tracking (FD/FT) method and essentially the same code. This is the so-called “minimal flow unit” first studied numerically in detail by Jimenez and Moin [54] and by many others since then. The number of bubbles, 24, used in the present setup is relatively a modest number. Lu and Tryggvason [67] studied the behavior of turbulent bubbly flows at much higher Reynolds number ($Re_\tau = 250$) and used 140 bubbles. They have also used the same domain size $\pi/2 \times 2 \times \pi$ resolved by a $256 \times 384 \times 512$ grid. Thus the grid resolution used in the present simulations ensures the grid convergence.

The objective of the present study is to investigate the sole and combined effects of soluble surfactant and viscoelasticity on the turbulent bubbly flows. The deformation of the bubbles has a significant effect on the structure and dynamics of bubbly flows [66]. To minimize the effects of deformability of the bubbles, initially, spherical bubbles are included/added to the turbulent flow. The deformation of the bubbles can be characterized by two non-dimensional numbers for the present setup, i.e., the Capillary ($Ca = \mu_o^* W_b^* / \sigma_s^*$) and Eötvös ($Eo = \rho_o^* g^* d_b^{*2} / \sigma_s^*$) numbers. Both of these non-dimensional numbers are kept constant at low values, so that the bubbles remain nearly spherical for all the cases considered in this study. The governing parameters related to the surfactant other than C_∞ are also kept constant. Our

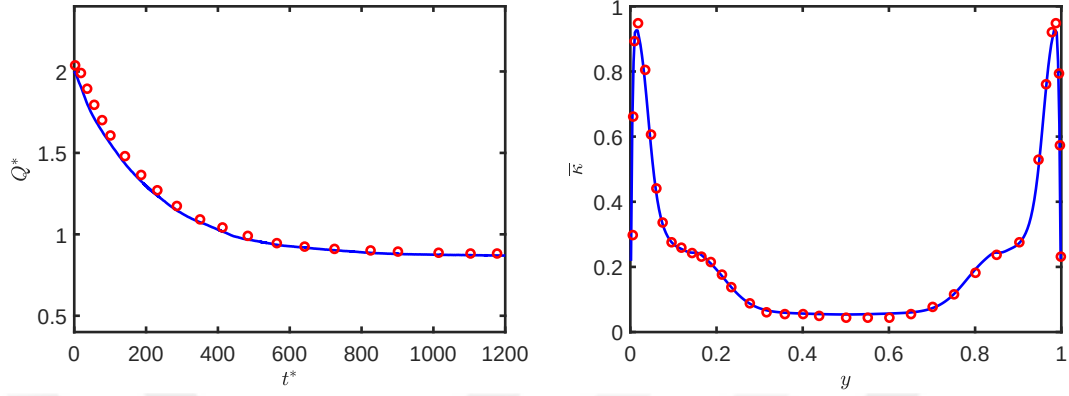


Figure 3.3: The turbulent multiphase flow: (left) The evolution of the flow rate and (right) the turbulent kinetic energy at $Re_\tau = 127.3$. The solid lines represent the current results and the symbols are the DNS data by Lu et al. [64]. The turbulent kinetic energy is scaled by w_τ^{*2}

previous study about the effects of surfactant [2] on the dynamics of single bubble has demonstrated that the elasticity number ($\beta_s = R^* T^* \Gamma_\infty^* / \sigma_s^*$) that signifies the strength of surfactant and the bulk surfactant concentration have very similar effects. In addition, other parameters related to surfactant such as bulk and interfacial Peclet numbers, the Biot number and the Damköhler number have only secondary effect on bubbly flows in statistically stationary state [2]. Therefore, it is deemed to be sufficient to only vary C_∞ to show the effects of surfactant in the present study. We also note that it is easy to vary C_∞ by simply adding more surfactant into the bulk fluid in an experimental study. The surfactant parameters used here are based on our previous studies [2, 77]. For the non-Newtonian flow cases, the Weissenberg number (Wi) quantifies the dynamic significance of the viscoelasticity. The other parameter related to the viscoelasticity is the solvent viscosity ratio (β) that essentially controls the magnitude of viscoelastic stresses as can be seen in Eq. (3.16). Thus only Wi is varied to characterize the effects of viscoelasticity.

First, extensive simulations are performed to investigate the effects of surfactant and viscoelasticity separately. Then their combined effects are investigated. For this purpose, first computations are carried out for a range of bulk surfactant concentra-

tions C_∞ to examine the effects of surfactant on bubbly flows without viscoelasticity in section (3.3.1). Then the simulations are repeated for three different Weissenberg numbers, quantifying the dynamic significance of the viscoelasticity, i.e., $Wi = 0, 5$ and 10 , in the absence of surfactant to determine the sole effects of viscoelasticity in section (3.3.2). Finally, the combined effects of surfactants and viscoelasticity are investigated in section (3.3.3).

3.3.1 Effects of soluble surfactant

Simulations are first performed to examine the sole effects of soluble surfactant on the bubbly channel flow. For this purpose, the both phases are set to be Newtonian and the bulk surfactant concentration is varied in the range of $C_\infty = 0$ (clean) and $C_\infty = 1$ (highly contaminated). Figure 3.3.1 & 3.3.1 presents the evolution of the liquid flow rate and the liquid velocity profiles at approximately statistically steady state for the clean and contaminated cases respectively. It can be seen that the presence of surfactant has a drastic effect on the dynamics of the turbulent bubbly flow. The addition of spherical bubbles to a statistically steady state turbulent single phase flow causes a significant increase in the drag and thus the flow rate decreases in comparison to the corresponding single phase flow. The addition of surfactant in the bubbly flows prevents this reduction of the flow rate. The maximum prevention occurs for the $C_\infty = 0.5$ case, for which the flow rate approaches that of the single phase flow rate in the fully developed regime.

Figure 3.5 shows the vortical structure of the bubbly flow for the bulk surfactant concentrations of $C_\infty = 0, 0.25$ and 0.5 . The vortical structures are identified using the Q -criterion [53] (see also the figure caption). Clearly, the presence of contamination exhibits a drastic effect on the flow. For a clean suspending phase, the dispersed bubbles migrate toward the wall and seem to relaminarize the flow – the only regions of high vorticity are associated with the footprint of the bubble wakes. With an increasing surfactant concentration, the bubbles appear to be more homogeneously distributed, and the flow is clearly in a turbulent state. The constant contours of the interfacial surfactant concentration and distribution of bubbles in

the streamwise-wall-normal and streamwise-spanwise plane are shown in Fig. 3.6. For the clean case, the bubbles migrate toward the channel wall mainly due to the hydrodynamic lift force [62]. When surfactant is added, the Marangoni stresses counteract this lift force and eventually reverse the direction of the lateral migration of the bubbles when C_∞ exceeds a critical value. As C_∞ is increased from 0 to 0.25, the number of bubbles in the core region is increased, though we still can see the wall-layer. In this case, the amount of surfactant adsorbed on the surface of the bubbles is significant, but not large enough to completely overcome the hydrodynamic lift that is responsible for the bubble wall layering. With a further increase of C_∞ , a larger portion of the area of the bubbles is contaminated. As a result, all bubbles detach from the wall, migrate toward the core region and spread out the channel cross-section, drastically changing the dynamics and the entire structure of the bubbly flows, as seen in Figs. 3.3.1 and 3.6.

To quantify the effects of surfactants on the flow, the transient and time-averaged quantities are shown in Fig. 3.7. The time-averaged quantities are obtained by averaging over a period of 200 computational time units once the flow reaches a statistically steady state. Note that the time unit is defined as h^*/W_b^* . The results show that the bubbly wall layer formation in the clean case has thickness of a bubble diameter as seen in the evolution of the number of bubbles in the wall layer (i.e., the number of bubbles with a centroid position lower than one bubble diameter). It is interesting to note that, for the clean bubbly flows, the formation of bubble-rich wall-layer with a thickness of about a bubble diameter is also observed in the laminar [62], weakly turbulent [64] and also for highly turbulent flows [67]. For the contaminated cases, as C_∞ increases, the bubbles move toward the core region. The void fraction peaks are less pronounced and located further away from the walls. For the highest concentration of $C_\infty = 1$, wall-layers again emerge similar to the case with $C_\infty = 0.25$. This interesting behavior is attributed to the fact that the bubble surface is nearly uniformly covered by the surfactant at the equilibrium concentration, resulting in a nearly uniform reduction in surface tension without much Marangoni stresses in the case of excessive surfactant concentrations. As regards

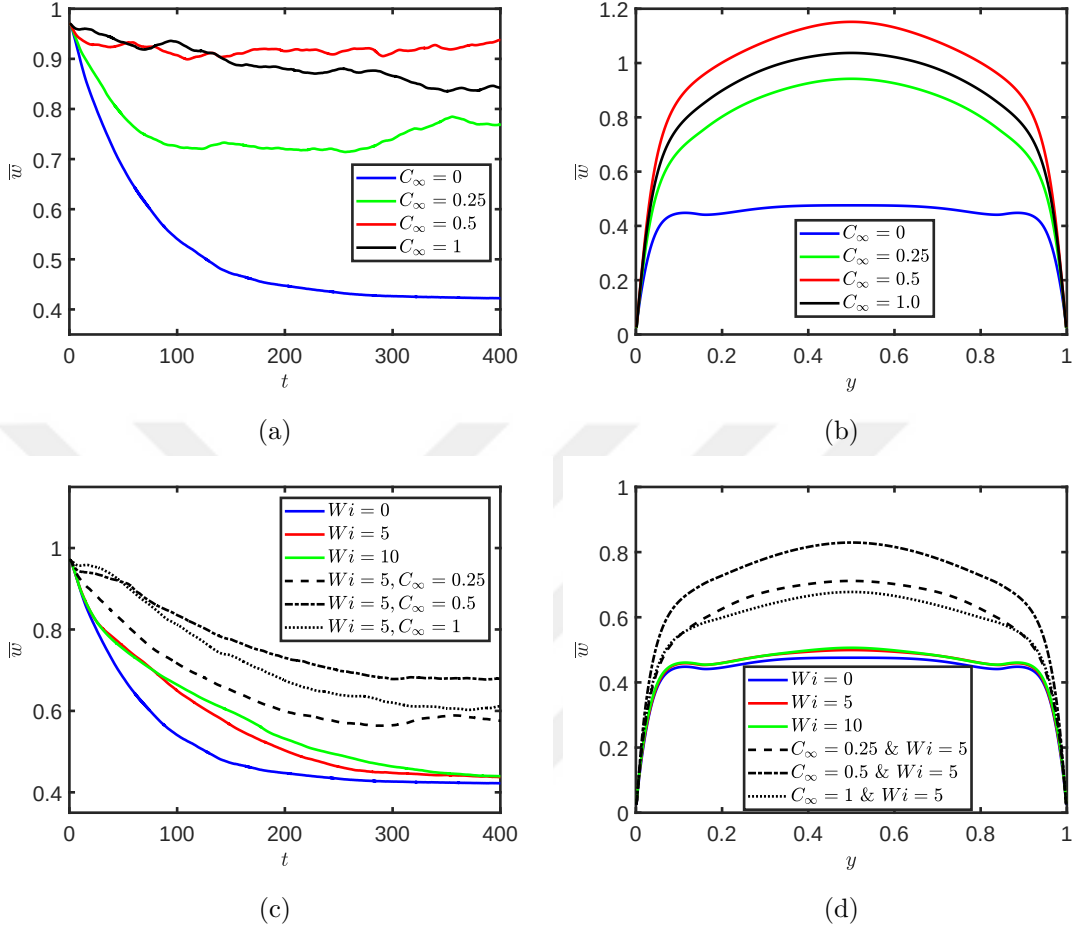


Figure 3.4: Newtonian flow (First row): (a) time evolution of the liquid flow rate for varying surfactant concentration, and (b) the averaged liquid velocity versus the wall-normal coordinate, after the flow reaches an approximate steady state. Non-Newtonian flow (second row): (c) time evolution of the liquid flow rate for a clean fluid and varying Weissenberg number, and for a fixed Weissenberg number and varying surfactant concentration (d) the averaged liquid velocity versus the wall-normal coordinate, after the flow reaches an approximate steady state. ($\bar{w} = \bar{w}^*/W_b^*$)

the Reynolds stresses, they increase from almost zero in the bulk of the channel for the clean case to the almost linear profile resembling the characteristic of a single-phase turbulent flow for the contaminated cases. As C_∞ increases, the Reynolds stress profile becomes closer and eventually matches that of the single-phase turbulent flow. It can be seen that, for the clean case, the turbulent kinetic energy level is low, which is consistent with the observation that the flow relaminarizes for the clean case. But the values of the kinetic energy are increased with C_∞ , except for

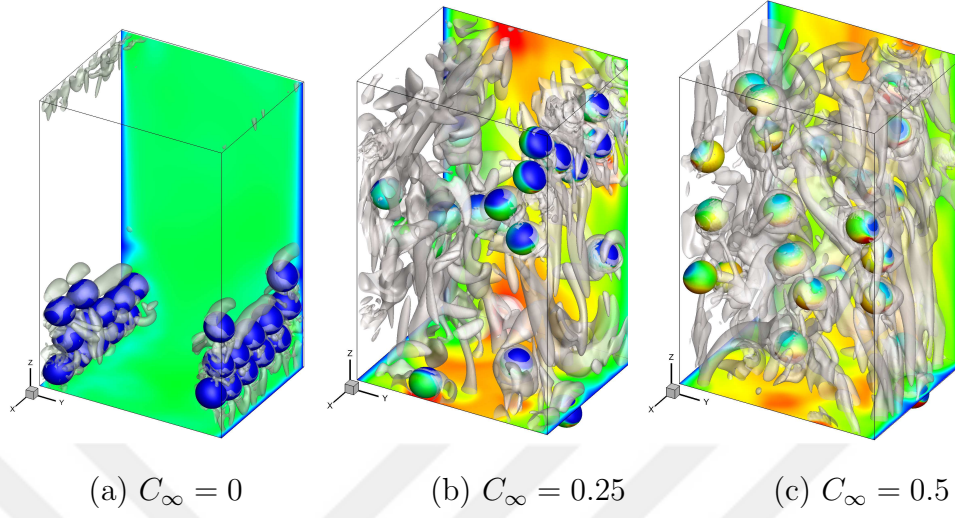


Figure 3.5: Sole effects of surfactant on the vortical structures in the fully-developed regime. The vortical structures are visualized using Q -criterion, i.e., the iso-contours of the normalized second invariant of the velocity-gradient tensor, $Q^*/(W_b^*/(2h^*))^2 = 1$, are plotted. The contours on the plane represent instantaneous streamwise velocity with the scale ranging from $0.15W_b^*$ (blue) to $1.1W_b^*$ (red). The contours on the bubble surface represent interfacial surfactant concentration (Γ) with the scale ranging from 0 (blue) to 0.15 (red).

the case of $C_\infty = 1$. Lu et al. [64] proposed that increase in the kinetic energy could be due to enhanced vorticity generation created by surfactant-induced rigidification of interfaces. The decrease in the Reynolds stress and turbulent kinetic energy are related to the increase in the bubble clustering near the wall.

3.3.2 Effects of viscoelasticity

We next examine the effects of viscoelasticity on the turbulent bubbly channel flows. For this purpose, simulations are first performed for the Weissenberg numbers of $Wi = 0$ (Newtonian), $Wi = 5$ (moderately viscoelastic) and $Wi = 10$ (highly viscoelastic) in the absence of surfactant to demonstrate the sole effects of the viscoelasticity. Simulations are then performed to examine the combined effects of surfactant and viscoelasticity for $Wi = 5$ in the presence of surfactant with the bulk concentrations of $C_\infty = 0.25, 0.5$ and 1.0 . The results are shown in Fig. 3.3.1 & 3.3.1.

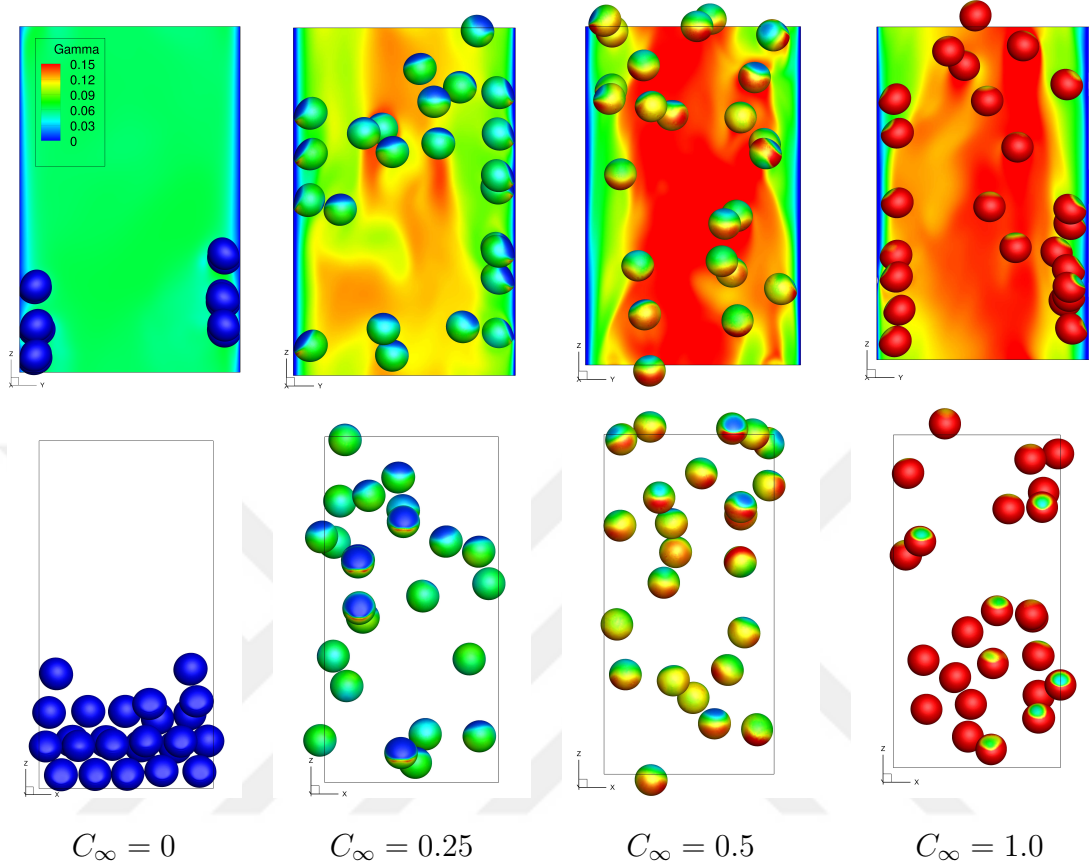


Figure 3.6: Sole effects of surfactant on the structure of Newtonian turbulent bubbly flow: bubble distribution on the streamwise-wall-normal plane (first row) and on the streamwise-spanwise plane (second row) when the flow has reached a statistically steady state. The contours on the plane represent instantaneous streamwise velocity with the scale ranging from $0.15W_b^*$ (blue) to $1.1W_b^*$ (red).

As can be seen, for the clean viscoelastic case, the effect of polymers on the structure of the bubbly channel flow is opposite to that of surfactant. Increasing the Weissenberg number (Wi) promotes the formation of bubbly wall-layers and consequently reduction in the flow rate as shown in Fig. 3.8 and Fig. 3.3.1, respectively. This interesting result is in fact consistent with the detailed numerical simulations of Mukherjee et al. [74] who showed that the matrix viscoelasticity induces a net force on the droplet pushing it towards the channel wall. As can be seen, at the initial stage ($t < 30 \approx 2\lambda_{Wi=5}$), the viscoelastic cases follow the Newtonian case. This can be attributed to the fact that polymers react to the flow at a finite timescale

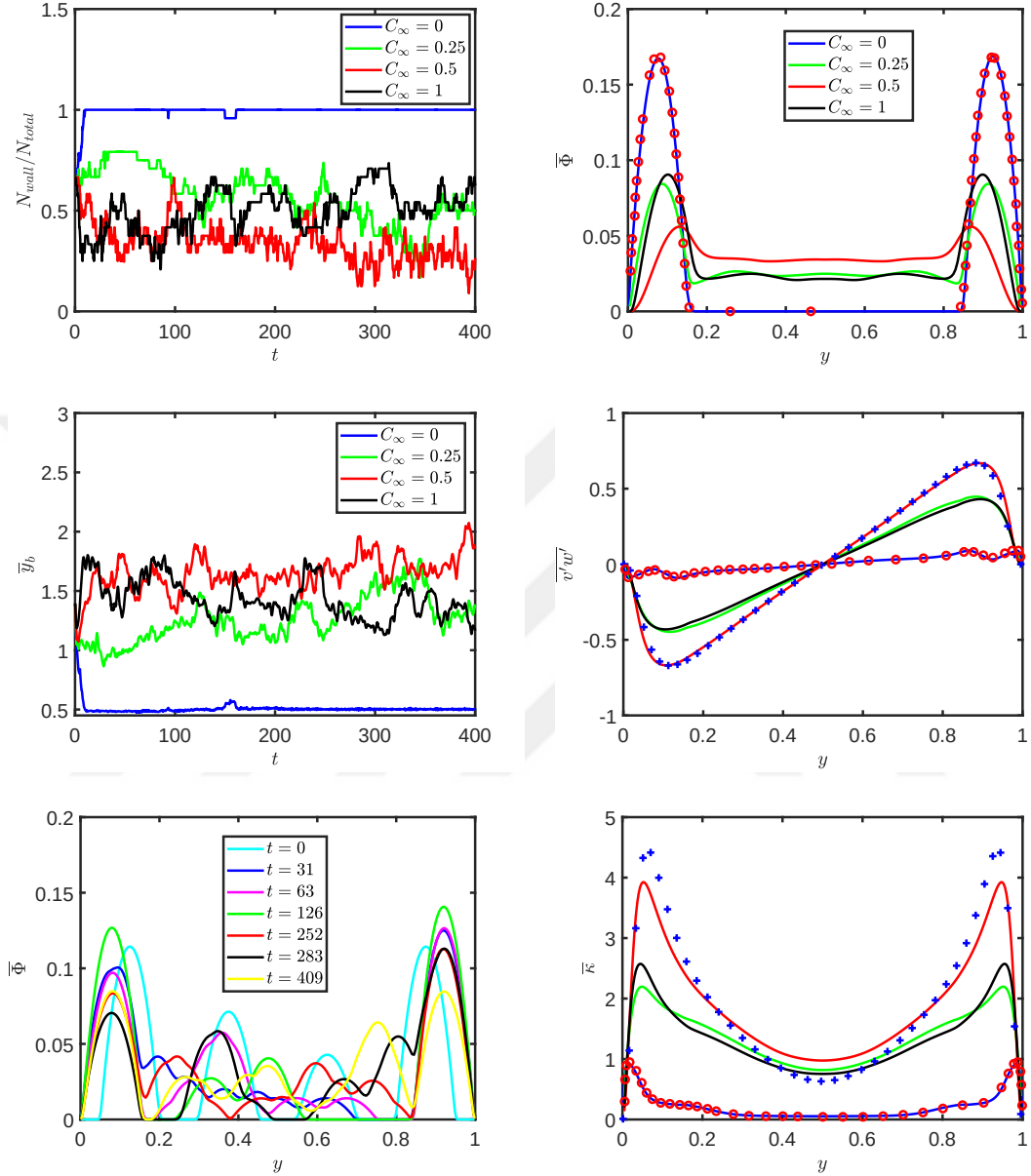


Figure 3.7: Sole effects of surfactant. The first and second columns show the transient and statistically stationary results, respectively. In the left column, the evolution of the number of bubbles in the wall layer (top), the average distance of the bubbles from the wall ($\bar{y}_b = \bar{y}_b^*/d_b^*$) (middle) and the average void fraction at various times for $C_\infty = 0.25$ (bottom). In the right column, statistically steady state results of the void fraction (top), the Reynolds stresses scaled by w_τ^{*2} (middle) and the turbulent kinetic energy scaled by w_τ^{*2} (bottom).

($\sim \lambda$). Initially, the polymer stresses are low, since there is not enough time for them to stretch. Eventually, the polymers fully stretch and the polymer stresses

become significant. At about $t = 60 \approx 2\lambda_{Wi=10}$, the time evolution of the flow rate starts to diverge from the Newtonian one, but still follows its trend, i.e., decreases monotonically. For time $t > 60$, two viscoelastic curves also separate due to different polymer stretching. It is well known that an addition of polymers results in drag reduction in single-phase flow [125], however its effects are more complex in multiphase flows. The drag is determined by the interplay between the viscoelastic effects (drag reduction) and the formation of bubbly wall-layers (drag promotion). In viscoelastic multiphase flows, the elastic lift is induced due to non-uniform normal stress difference [74]. This elastic lift force move the bubbles toward the channel wall. Figure 3.8 shows the bubble distribution and normalized first normal stress difference (N_1) for $Wi = 5$. As can be seen, the normal stress difference is larger on the wall side supporting the idea that the bubbles are forced to move towards the wall by the viscoelastic stresses. It is also seen that, for the clean case, the bubbles are accumulated at the walls forming horizontal bubble clusters. Bubble wall-layers are formed for all the Weissenberg numbers considered in this study. The formation of these wall-layers significantly diminishes the drag reduction effect of viscoelasticity observed for single-phase flows.

3.3.3 Combined effects of viscoelasticity and surfactant

To examine the dynamics of turbulent bubbly flow in presence of polymers and surfactant, the simulations are performed for range of bulk surfactant concentration ($C_\infty = 0.25, 0.5, 1.0$) while keeping the Weissenberg number ($Wi = 5$) constant. The results are shown in Fig. 3.3.1 & 3.3.1. As can be seen, the presence of surfactant does not show as dramatic effect as that in the case of Newtonian flow. The flow rate decreases for all combined cases compared to the corresponding single phase flow. The amount of surfactant does not seem to be sufficient to prevent this reduction in the flow rate. The minimum reduction in the flow rate occurs for $C_\infty = 0.5$ case, similar to the Newtonian flow, but the reduction in the flow rate is much higher for the combined case. To gain more insights on bubbly flow dynamics, bubble distribution is shown on streamwise-wall-normal ($z - y$) and streamwise-spanwise

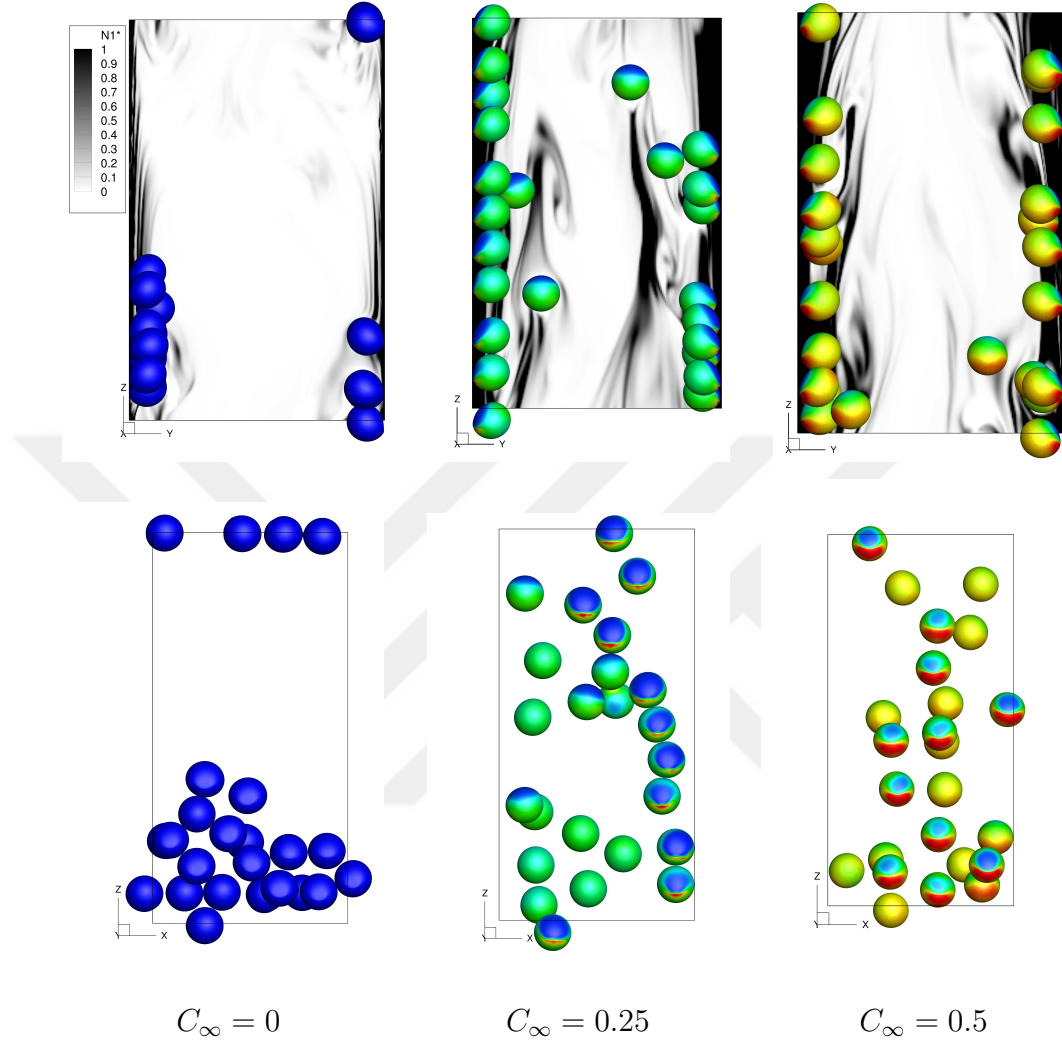


Figure 3.8: Effects of surfactant and viscoelasticity on the structure of turbulent bubbly flow. The first row shows the bubble distribution on streamwise-wall-normal plane, and the second row shows streamwise-spanwise plane. The plane contours represent normalized first normal stress difference defined as ($N_1 = \frac{\tau_{zz}^* - \tau_{yy}^*}{\tau_{wall}^*}$). The contours on the bubble surface represent the interfacial surfactant concentration (Γ) with the scale ranging from 0 (blue) to 0.15 (red).

($z - x$) planes in Fig. 3.8. As can be seen, for all the three combined cases, that is, clean and contaminated, bubbles accumulate at the channel walls forming bubble clusters which results in reduction of liquid flow rate. Although the surfactant concentration does not seem to be sufficient to alter the direction of migration of the bubbles, it has clearly affected the wall-layer structure. The bubbles in the

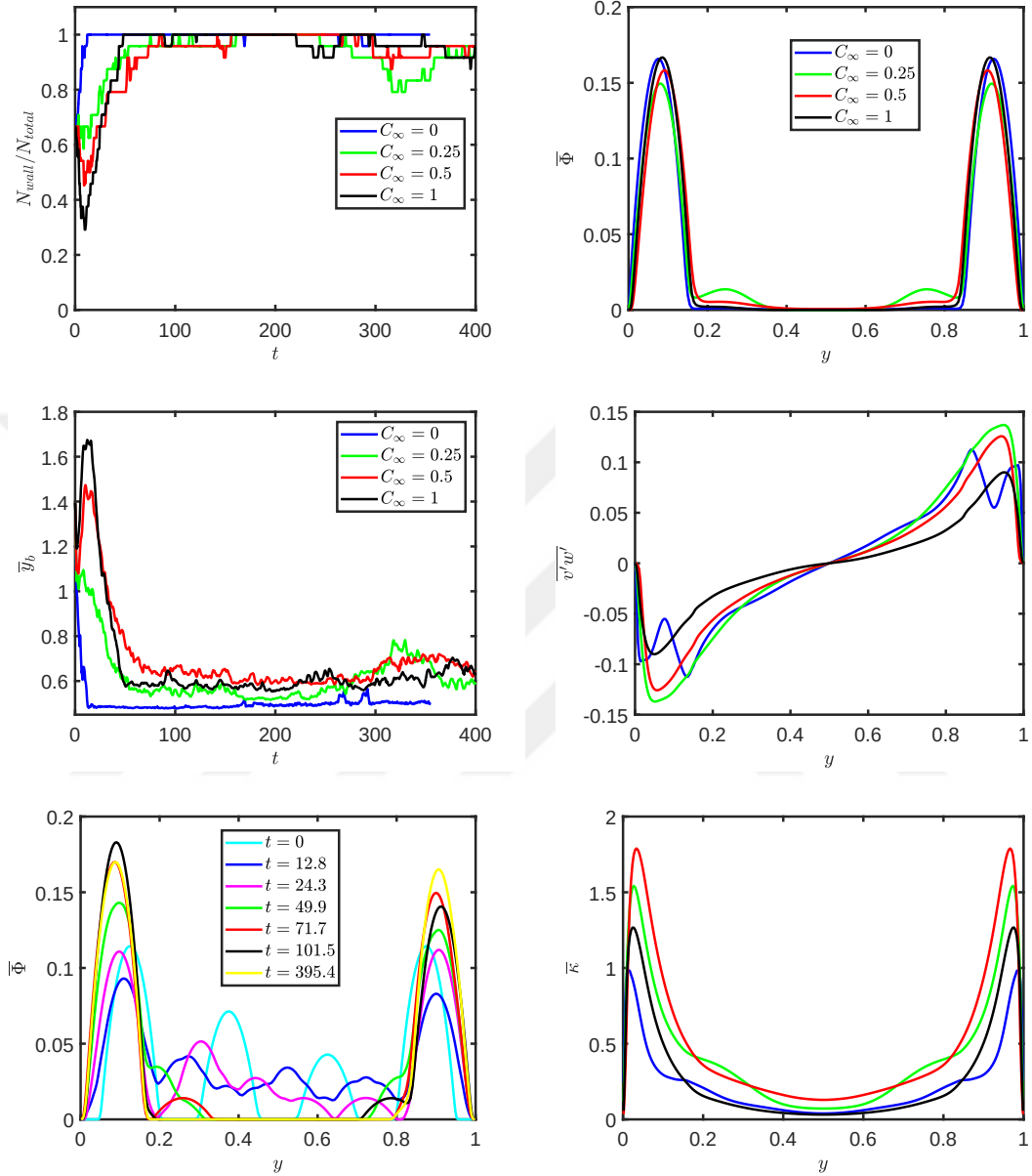


Figure 3.9: Effects of surfactant and viscoelasticity: First column (transient results): (top) Evolution of the number of bubbles in the wall layer, (middle) the average distance of the bubbles from the wall ($\bar{y}_b = \bar{y}_b^*/d_b^*$) and (bottom) the average void fraction for $C_\infty = 0.5$. Second column (statistically steady state results): (top) average void fraction (middle) Reynolds stresses scaled by w_τ^{*2} (bottom) turbulent kinetic energy scaled by w_τ^{*2} .

horizontal clusters for the contaminated cases are not as tightly packed as observed for the clean case. Instead, they are more randomly distributed in the streamwise-spanwise ($z - x$) plane. The contours of the first normal stress (N_1) are also shown

in Fig. 3.8. As can be seen, the elastic force increases with C_∞ mainly due to the increase in the bulk velocity of the liquid.

The combined effects of surfactant and viscoelasticity on the flow quantities are shown in Fig. 3.9. The transient results show that the surfactant effect is prominent during the initial times until the polymers fully stretch. Thus, initially bubbles move away from the wall as the Marangoni force overcome inertial lift force. Later, the inertial and elastic lift force overcome the Marangoni forces and change the direction of migration of the bubbles towards the channel wall. Thus, wall-layers are formed for all the C_∞ values unlike to the Newtonian case. The interaction between the wall-layer and core region for the $C_\infty = 0$ is marginal but as C_∞ increases, it can be seen that a few bubbles are moving in/out of the wall-layer continuously. As regards the Reynolds stresses, clear footprints of the bubble wall-layer can be seen near the wall. It can be also seen that the presence of surfactant has slightly improved the turbulent kinetic energy but overall it is low for all the cases due to the formation of bubble wall-layers.

3.4 Conclusions

An efficient fully parallelized finite-difference/front-tracking method has been used to examine the effects of soluble surfactant and viscoelasticity on turbulent bubbly channel flows. For the clean case, the earlier findings are verified: The clean bubbles move towards the wall due to hydrodynamic lift force and form a bubble-rich wall layer. It is found that addition of surfactant has significant influence on the overall flow structure of turbulent bubbly channel flow. Surfactant-induced Marangoni stresses counteract the hydrodynamic lift force and push the bubbles away from the wall region. At a high enough surfactant concentration $C_\infty = 0.5$, the formation of bubble wall layer is completely prevented resulting in a uniform void fraction distribution across the channel cross-section. The present results are in agreement with the earlier experimental [110] and the numerical [77, 64] studies, i.e., the addition of surfactant prevents the formation of the wall-layers. For $C_\infty = 1$, the trend reversal is also observed i.e., reforming of bubble clusters due to a more uniform interfacial

surfactant concentration. For the clean viscoelastic case, bubbles move toward the channel wall, similarly to the Newtonian case. The elastic force promotes the formation of the bubble wall-layer resulting in the reduction of the flow rate, which is consistent with the computational results of Mukherjee et al. [74]. Thus, the drag reduction effect of viscoelasticity observed for the single-phase flows diminishes due to the formation of bubble wall-layers. Finally, in the presence of combined effects of surfactant and viscoelasticity, similar wall-layer formation is observed, but the bubbles in the horizontal clusters show a more sparse distribution compared to the clean case.

Chapter 4

EFFECTS OF SURFACTANT ON POLYMER DRAG REDUCTION FOR VISCOELASTIC TURBULENT BUBBLY FLOWS

4.1 Introduction

Addition of polymers to single-phase turbulent flows leads to a significant drag reduction. Since its discovery by Toms (1948), the drag reducing property of polymer additives has been extensively studied for single-phase flows. This phenomenon is very sophisticated and its full understanding remains elusive [125]. Earlier explanations for the drag reduction can be classified into two schools of thought. The first one focuses on the viscous effects [71, 70, 90] and the other one the elastic effects [55, 106]. Even though both theories have found experimental support, they have not achieved unequivocal conclusions. The drag reduction is further categorized into two distinct regimes known as low drag reduction (LDR) and high drag reduction (HDR) [124]. Zhu et al. [130] have shown that the polymer-induced drag reduction follows different mechanisms for these different regimes. For the LDR regime ($DR \leq 40\%$), near-wall vortices are suppressed and streamwise velocity fluctuations are enhanced [26, 25]. However, the statistical trends are similar to Newtonian flow, i.e., the mean velocity profile follows a similar log-law slope with similar velocity fluctuation profiles. On the other hand, for HDR ($40\% < DR \leq 60\%$), streamwise velocity fluctuations almost vanish, Reynolds shear stress becomes significantly smaller and the slope of the log-layer mean velocity is dramatically modified. Furthermore, there is an upper limit on drag reduction referred as the maximum drag reduction asymptote (MDR) which depends on the Reynolds number [123]. The recent study of Choueiri et al. [14] has shown that polymers can reduce the

drag beyond the suggested asymptotic limit by re-laminarizing the flow. More detailed review on the topic can be found in Xi [126]. Introducing a second gaseous phase with surfactant contamination into this problem results in even more complex and exciting dynamics, as the two-fluid interface dynamics is tightly coupled with the elastic turbulence and the local surfactant concentration.

Direct numerical simulations (DNS) of bubbly flows in the absence of viscoelasticity and surfactant have been performed previously for both spherical bubbles [67] and deformable bubbles [66]. Simulations of turbulent bubbly channel flows [62, 65, 30, 18, 93, 9] have shown that the distribution of bubbles in the channel have significant effects on the overall flow dynamics. For instance, spherical bubbles tend to accumulate at the wall, forming bubble clusters that result in a significant reduction of the flow rate. The recent review by Elgobashi [28] encompasses the recent progress in the DNS of bubbly flows. Lu and Tryggvason [68, 69] have also performed DNS of turbulent bubbly flows undergoing topological changes. They examined the effects of various governing parameters on the evolution of flow statistics such as the average flow rate, wall shear, and interface area. The conventional Reynolds-averaged Navier-Stokes models for multiphase flows [8, 72, 35] are currently relying on high-quality DNS data.

Numerous industrial applications involve bubbly flows, for example, bubble column reactors and light-weight reactors. In such applications contamination/surfactant is naturally present or sometimes deliberately added to manipulate the dynamics of bubbly flows. Indeed, the presence of surfactants has a drastic effect on the behavior of bubbly flows [108]. Takagi et al. [110] observed bubble clustering phenomena in an upward bubbly channel flow, without surfactant and for small enough surfactant concentrations. Conversely, the presence of a large amount of surfactant, or a small amount of a strong surfactant type (Triton-X100), prevented the formation of bubble clusters near the wall. Lu et al. [64] examined the effects of insoluble surfactant on turbulent bubbly flows by DNS and showed that the contaminated bubbles remain distributed across the whole channel. Soligo et al. [99, 100] developed a modified phase field method (PFM) for simulations of turbulent flows with

large and deformable surfactant-laden droplets. They used this method to examine breakage/coalescence rates and size distribution of surfactant-laden droplets in turbulent flow.

The interaction of a dispersed phase with turbulent flows of viscoelastic fluids is object of active research due to its relevance to numerous environmental and engineering applications. Rosti et al. [89] studied the effect of finite-size rigid spherical particles on the viscoelastic turbulent channel flow. They found that the drag reducing effect of polymer additives is completely lost for semi-dense suspensions. They also observed that the drag increases more for suspensions in viscoelastic fluids than for suspensions in Newtonian fluids. Amir et al. [31] also performed the DNS of viscoelastic turbulent channel flow laden with neutrally rigid buoyant spherical particles. Similarly, they observed that the drag reducing effect of viscoelasticity is lost for suspensions, but only at low Weissenberg numbers.

In our previous work [1], we gave examples of the combined effect of surfactant and viscoelasticity on the behavior of pressure-driven, vertical turbulent bubbly flows at $Re_\tau = 127$. We found that the viscoelasticity promotes the formation of bubbly wall-layers and consequently the flow rate is reduced (i.e., drag increases). The formation of bubble wall-layers was related to the interplay of inertial and elastic, and Marangoni forces. In the present study, extensive simulations are performed to understand the effects of soluble surfactants on dynamics of turbulent bubbly flow at a higher Reynolds number, $Re_\tau = 180$, and a larger number of bubbles. The physical properties of Triton X-100 and 1-Pentanol are used to investigate the effects of sorption kinetics of surfactant on turbulent bubbly flows. We will then examine the effects of surfactants on polymer drag reduction in turbulent bubbly channel flows.

4.2 Computational setup and numerical method

Hereafter, unless otherwise stated, the superscript $*$ is used to denote dimensional quantities, and variables without the superscript are non-dimensional (e.g., p^* and p represent the dimensional and non-dimensional pressure, respectively). The com-

putational domain is illustrated in the Fig. A.1 and corresponds to a plane channel with streamwise, spanwise and wall-normal direction along y , x and z coordinates, respectively. The flow is periodic in the streamwise and spanwise directions, while no-slip/no-penetration boundary conditions are applied at each wall. The size of the domain ($L_y \times L_x \times L_z$) is $6h \times 3h \times 2h$ resolved by ($N_y \times N_x \times N_z$) $576 \times 288 \times 240$ points in streamwise, spanwise and wall-normal directions respectively, where $h = 1$ is the half channel width. The grid points are uniformly spaced in the spanwise and streamwise direction but stretched in the wall-normal direction by a hyperbolic tangent function

$$z(k) = 1 + \frac{\tanh\left(\gamma\left(\frac{2k}{N_z} - 1\right)\right)}{\tanh(\gamma)}, \quad (4.1)$$

where stretching parameter $\gamma = 1.43$ is used here which yields inner-scaled resolution of $\Delta x^+ = \Delta y^+ = 1.875$ and $0.498 \leq \Delta z^+ \leq 2.4$.

As an initial condition, spherical bubbles are randomly placed in a single-phase turbulent flow with a friction Reynolds number of $Re_\tau = v_\tau^* h^* / \nu_o^* = 180$. Here, the friction velocity is $v_\tau^* = \sqrt{\tau_{wall}^* / \rho_o^*}$, where ρ_o^* and ν_o^* are the density and kinematic viscosity of the suspending liquid, respectively. The inner-scale dimensions ($l_0^+ = \nu_o^* / v_\tau^* = 0.0055$) of the channel are $1090.9 \times 545.5 \times 363.6$ in the streamwise, spanwise and wall-normal directions, respectively. The flow is driven by a constant pressure gradient dp^*/dy^* . At a statistically steady state, the average wall shear stress τ_{wall}^* is related to the pressure gradient and the weight of the bubble/liquid mixture by a streamwise momentum balance:

$$\tau_{wall}^* = - \left(\frac{dp^*}{dy^*} + \rho_{av}^* g^* \right) h^* = -\mathcal{B}^* h^*, \quad (4.2)$$

where ρ_{av}^* is the average density of the mixture in the whole channel and h^* is the channel half-width. Note that the value of $\mathcal{B}^*$ dictates the bulk flow direction, i.e., upflow ($\mathcal{B}^* < 0$) and downflow ($\mathcal{B}^* > 0$).

A swarm of mono-dispersed bubbles ($N_b = 133$) is considered in this study, corresponding to a void fraction of 3%. The bubbles are initialized with a spherical shape with a diameter $d_b^* = 0.25$ (45.5 in viscous wall units) and Eötvös Number

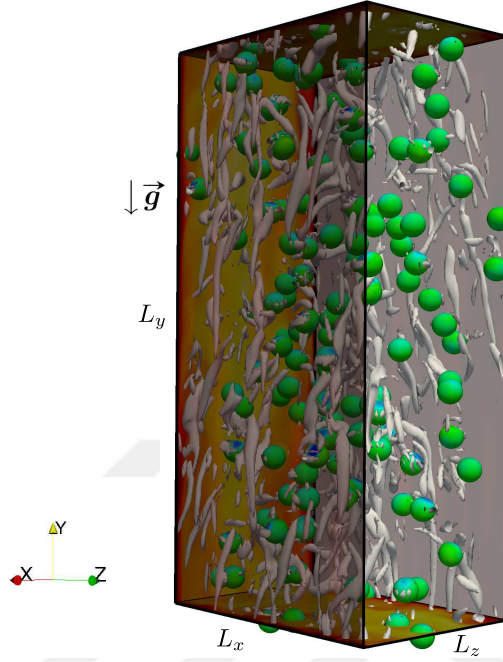


Figure 4.1: Schematic representation of the computational setup considered in the present work. The vortical structures are visualized using Q -criterion, i.e., the iso-contours of the normalized second invariant of the velocity-gradient tensor, $Q^*/(V_b^*/(h^*))^2 = 2.5$, are plotted. The contours on the plane represent streamwise velocity with the scale ranging from $V_b^* = 0$ (grey) to $V_b^* = 20$ (red). The contours on the bubble surface represent interfacial surfactant concentration with the scale ranging from 0 (blue) to 0.23 (red).

$Eo = \rho_o^* g^* d_b^{*2} / \sigma_s^* = 0.45$. The Morton number ($M = g^* \mu_o^{*4} / \rho_o^* \sigma_s^{*3}$) used here is $M = 6.17 \times 10^{-10}$, which is higher than the Morton number of $M = 2.52 \times 10^{-11}$ for an air bubble in water at 20°C, but could be matched by using an aqueous solution of sugar [101]. The physical parameters governing the flow are listed in Table 4.1 where subscripts “ i ” and “ o ” denote the properties of the inner (dispersed) and the outer (continuous) fluids, respectively, and λ^* is the polymer relaxation time.

Triton X-100 and 1-Pentanol surfactants are considered in the present work. The corresponding physical adsorption (k_a^*) and desorption (k_d^*) properties are taken from Takagi et al. [109]. For Triton X-100, $k_a^* = 50 \text{ m}^3 \text{mol}^{-1} \text{s}^{-1}$ and $k_d^* = 0.033 \text{ s}^{-1}$, whereas for 1-Pentanol, $k_a^* = 5.08 \text{ m}^3 \text{mol}^{-1} \text{s}^{-1}$ and $k_d^* = 110.24 \text{ s}^{-1}$. The corresponding non-dimensional numbers related to the surfactants physical properties are listed

Table 4.1: Physical and computational parameters governing the flow.

Density and viscosity ratio	$\rho_i^*/\rho_o^*, \mu_i^*/\mu_o^*$	0.02, 0.02
Total pressure gradient	$\mathcal{B}^* = \frac{dp^*}{dz^*} + \rho_{av}^* g^*$	-1
Surface tension	σ	3.334
Gravitational acceleration	g^*	-24
Weissenberg Number	$Wi = \lambda^* V_b^*/h^*$	0/4/8
Solvent viscosity ratio	$\beta = \mu_s^*/\mu_o^*$	0.9
Extensibility parameter	L	60

in Table 4.2. The C_∞ ($= \frac{C_\infty^*}{C_{ref}^*}$) and Γ ($= \frac{\Gamma^*}{\Gamma_{max}^*}$) represent the non-dimensional initial bulk surfactant concentration and the non-dimensional interfacial surfactant concentration, respectively. Here, C_{ref}^* denotes the reference bulk surfactant concentration, taken as the critical micelle concentration (CMC), and Γ_{max}^* represents the maximum packing concentration.

Table 4.2: Non-dimensional numbers for TritonX-100 & 1-Pentanol surfactant cases.

		TritonX-100	1-Pentanol
Peclet number	$Pe_c = Pe_s = h^* V_b^*/D_c^*$	777	777
Biot Number	$Bi = h^* k_d^*/V_b^*$	2×10^{-3}	7.0
Damkohler Number	$Da = \Gamma_{max}^*/h^* C_{ref}^*$	0.456	0.456
Langmuir number	$La = k_a^* C_{ref}^*/k_d^*$	2.2	7×10^{-4}
Elasticity Number	$\beta_s = R^* T^* \Gamma_\infty^*/\sigma_s^*$	0.5	0.5

Using Stokes drag, the bubble viscous response time can be estimated as $\tau_b^* = d_b^{*2}/36\nu_o^* = 0.3124$. To determine the Kolmogorov time scale of the turbulent flow $\tau_k^* = \sqrt{\nu_o^*/\epsilon^*}$, the turbulent energy dissipation rate (ϵ^*) can be calculated from the flow velocity field or can be estimated by $\epsilon^* = v_\tau^3/(\kappa z_b^*)$ where $\kappa = 0.42$ is the von Kármán constant and z_b^* is the bubble average distance to the wall [67]. Assuming $z_b^* = 0.5$, which yields $\tau_k^* = 0.03415$, and the Stokes number is therefore

$$St = \tau_b^*/\tau_k^* = 9.14.$$

The continuity and momentum equations for an incompressible viscoelastic fluid flow are discretized using a second-order finite-difference/front-tracking (FD/FT) method [119]. A single set of governing equations can be written for the entire computational domain provided the jumps in the material properties are taken into account and the effects of the interfacial surface tension are treated appropriately [119, 77, 49]. The governing equations are non-dimensionalized using a length scale $\mathcal{L}^*$, a velocity scale $\mathcal{U}^*$ and a time scale $\mathcal{T}^* = \frac{\mathcal{L}^*}{\mathcal{U}^*}$. The length and velocity scales are taken as $\mathcal{L}^* = h^*$ and $\mathcal{U}^* = V_b^*$ where V_b^* is the average liquid velocity of the Newtonian single-phase flow, i.e., $V_b^* = 15.56$. The density and viscosity are non-dimensionalized using the density ρ_o^* and total viscosity μ_o^* of the continuous phase while the surface tension is normalized by the surface tension of the surfactant-free gas-liquid interface σ_s^* . The non-dimensional momentum equation, accounting for interphase coupling, is then given by

$$\begin{aligned} \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \frac{(\rho - \rho_{av}) \mathbf{g}}{Fr^2} + \nabla \cdot \boldsymbol{\tau} + \frac{1}{Re} \nabla \cdot \mu_s (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \\ &+ \frac{1}{We} \int_A [\sigma(\Gamma) \kappa \mathbf{n} + \nabla_s \sigma(\Gamma)] \delta(\mathbf{x} - \mathbf{x}_f) dA, \end{aligned} \quad (4.3)$$

where ρ , $\mathbf{u}$, p , $\boldsymbol{\tau}$, μ_s and σ are the non-dimensional density, the velocity vector, the pressure, the polymer stress tensor, the solvent viscosity and the surface tension coefficient, respectively. The unit vector $\mathbf{g}$ points in the direction of the gravitational acceleration. In Eq. (4.3), the last term on the right hand side represents the surface tension where A is the surface area, κ is twice the mean curvature, $\mathbf{n}$ is the unit normal vector and ∇_s is the gradient operator along the interface. The non-dimensional numbers in Eq. (4.3) are Reynolds number ($Re = \rho_o^* \mathcal{U}^* \mathcal{L}^* / \mu_o^*$), Froude number ($Fr = \mathcal{U}^* / \sqrt{g^* \mathcal{L}^*}$) with g^* being the magnitude of the gravitational acceleration and the Weber number ($We = \rho_o^* \mathcal{U}^{*2} \mathcal{L}^* / \sigma_s^*$). We emphasize that the surface tension is a function of the interfacial surfactant concentration Γ and $\nabla_s \sigma(\Gamma)$ represents the surfactant-induced Marangoni stress. The present soluble surfactant methodology is the same as that developed by Muradoglu and Tryggvason [76, 77] and have been extensively used in various previous studies [80, 115, 2]. The rheo-

logical properties of the fluid are taken into account using the FENE-P model for the polymeric stress tensor $\boldsymbol{\tau}$. This constitutive equation and its numerical solution are described in details in our previous works [49, 50, 1].

The flow equations (Eq. (4.3)) are solved fully coupled with the FENE-P model and surfactant concentration equations using a front-tracking/finite-difference (FD/FT) method [119, 77, 49]. All the field equations are solved on a fixed Eulerian grid with a staggered arrangement where the velocity nodes are located at the cell faces while the material properties, the pressure, the bulk surfactant concentration and the extra stresses are all located at the cell centers. The interfacial surfactant concentration evolution equation is solved on a separate Lagrangian grid. The spatial derivatives are discretized with second-order central differences for the diffusive terms, while the convective terms are discretized using a QUICK scheme [60] in the momentum equation, and a fifth-order WENO-Z [10] scheme in the viscoelastic and the bulk surfactant concentration equations. The equations are integrated in time with a second-order predictor-corrector method in which the first-order solution (Euler method) serves as a predictor that is then corrected by the trapezoidal rule [119]. Poisson equation is solved by an efficient FFT-based direct solver for a constant-coefficients [16]. The details of the present numerical method are given in Ahmed et al. [1].

4.3 Results and Discussion

Simulations are first performed to examine the sole effects of surfactant for the Newtonian turbulent bubbly flow using the physical properties of Triton X-100 and 1-Pentanol. Then we examine the interplay and combined effects of surfactant and viscoelasticity. We particularly investigate the effects of surfactant and surfactant properties on polymer drag reduction in turbulent bubbly flows.

4.3.1 Newtonian flow: The sole effects of surfactants

Figure 4.2 shows the transient behavior of the skin friction coefficient c_f normalized by the value of the Newtonian single-phase flow, $c_{f,0} \approx 8.3 \times 10^{-3}$. The skin friction

coefficient is defined as $c_f = 2\tau_{wall}^*/\rho_o^*\bar{v}_o^{*2}$, where $\bar{v}_o^*$ is the average liquid velocity. The c_f for the clean case ($C_\infty = 0$) increases in time monotonically, until it reaches a steady state at $c_f/c_{f,0} \approx 3.25$. We first consider the initially clean cases, i.e., $\Gamma_{\text{initial}} = 0$. For Triton X-100, c_f first increases reaching a peak, followed by a decrease approaching the single-phase flow $c_f = c_{f,0}$ at the statistically steady state. The value at the peak and the time to reach the steady state decreases with C_∞ . For 1-Pentanol case however, the time-evolution of c_f is similar to the clean case. Moreover, high surfactant concentrations are needed to see any significant effect for the 1-Pentanol case. The curve for 1-Pentanol at $C_\infty = 1$ is almost identical to the clean case. When increasing the surfactant concentration further up to $C_\infty = 100$, the behaviour for 1-pentanol still remains the same, with only difference being that the upper limit of $c_f/c_{f,0}$ has decreased to ≈ 2.6 . Finally, we see a large effect of the initial conditions for Triton X-100. The $\Gamma_{\text{initial}} = \Gamma_{eq}$ cases for Triton X-100 follow a nearly straight line. The vast variation between different initial conditions could be attributed to the very low desorption rate of Triton X-100. Surfactant molecules at the leading part of bubble surface are transported to the trailing part of the bubble surface. Thus, large surface concentration gradient generates strong Marangoni stresses which prevent the lateral migration of the bubbles toward the wall.

Table 4.3: Case specifications for contaminated cases.

Name	Surfactant	Γ_i	C_∞
Case 1	Triton X-100	0	0.05 – 1.0
Case 2	1-Pentanol	0	1.0 and 100
Case 3	Triton X-100	Γ_{eq}	0.1, 0.25 and 0.5

The increase in drag for a turbulent bubbly flow, compared to the corresponding turbulent single-phase flow, could be attributed to the formation of bubble-wall layers which can be seen for the clean case ($C_\infty = 0$) in Fig. 4.3. The lateral migration of the bubbles to the wall is due to the inertial lift force. The lift force

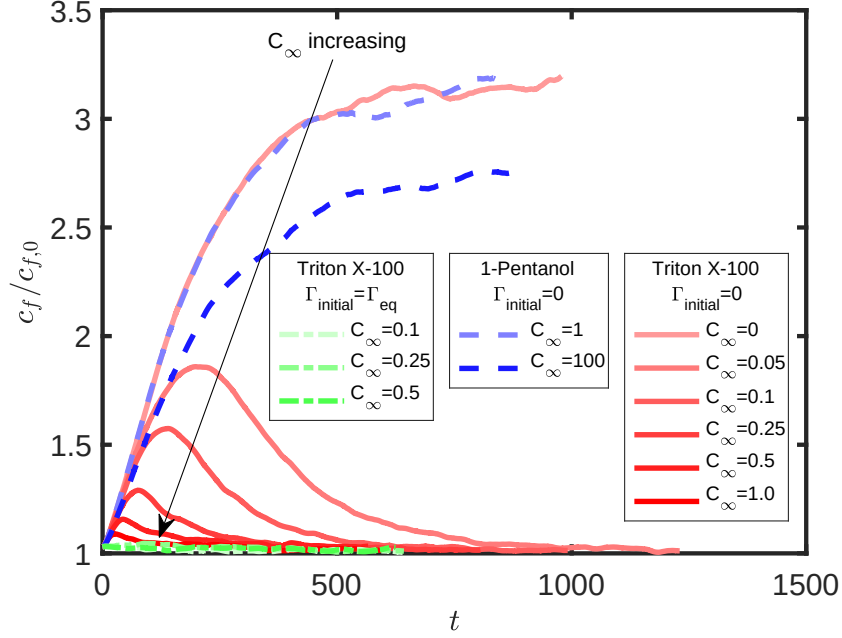


Figure 4.2: Skin friction coefficient (c_f) of the bubbly flow normalized by the statistically steady state value of the corresponding single-phase flow ($c_{f,0}$).

acts perpendicular to both the direction of motion and the rotation of the spherical bubble, which is also known as the Magnus effect [2]. The presence of a bubble wall-layer affects the liquid velocity profile, as shown in Fig. 4.3. The velocity profile for the clean case $C_{\infty} = 0$ is more flat near the wall due to the presence of the bubble clusters. The terminal velocity of the bubbles moving within the cluster is higher than that of the bubbles moving individually [67]. Surfactant prevents the formation of these bubble wall-layers and thus, alleviates the increase in drag. Clearly, flow dynamics strongly depends on the specific kinetics of surfactant absorption, as a minute amount of Triton X-100 is sufficient to prevent the bubble wall-layers, but 100 times more concentration of 1-Pentanol is not very effective. This is due to the amount of surfactant adsorbed on the bubble surface, which is much larger for the Triton X-100 than the 1-Pentanol, as can be seen in the Fig. 4.4. The adsorption rate of the Triton X-100 is hence about 10 times larger than that of the 1-Pentanol, and the desorption rate is about 3300 times smaller. In the case of Triton X-100,

a larger amount of surfactant and its non-uniform distribution on the surface of bubble generates a strong Marangoni induced force which prevents the motion of bubbles toward the channel wall. For $C_\infty = 1$, Triton X-100, the void fraction near the wall slightly increases, as the surfactant distribution becomes more uniform. Figure 4.4 also shows the iso-contours of vortices. The vortices are identified by the Q-criterion [53] ($Q^*/(V_b^*/(h^*))^2 = 0.8$). It is clear that for $C_\infty = 0$ and for $C_\infty = 1.0$ (1-Pentanol), the flow relaminarizes, whereas for Triton X-100, the flow is in a turbulent state.

Figure 4.5 shows the liquid velocity fluctuations for the clean and contaminated bubbly flow (Triton X-100). For all C_∞ values, the contaminated bubbles increase the liquid velocity fluctuations in all directions with respect to the corresponding single-phase flow. This can be attributed to the fact that in the presence of enough surfactant, a spherical bubble behaves as a rigid sphere [110]. For the clean case ($C_\infty = 0$), the fluctuations in all directions are much lower than the single-phase flow due to the significant reduction in the flow rate. However, a small peak can be seen near the wall in the spanwise direction (u'_{rms}). This is due to the presence of horizontal bubble clusters in the spanwise direction.

Averaging Eq. 4.3 over planes parallel to the walls and integrating in z -direction (wall-normal), over the both fluids [87], gives

$$\begin{aligned} \int_0^z \frac{\partial \rho V}{\partial t} dz &= - \int_0^z \left(\left(\frac{\rho - \rho_{av}}{Fr^2} \right) \mathbf{g} \right) dz + \frac{\mu}{Re} \frac{dv}{dz} - \overline{\rho v' w'} + \bar{\tau}_p \\ &+ \int_0^z \frac{1}{We} F_\sigma dz, \end{aligned} \quad (4.4)$$

$$F_\sigma = \int_A [\sigma(\Gamma) \kappa \mathbf{n} + \nabla_s \sigma(\Gamma)] \delta(\mathbf{x} - \mathbf{x}_f) dA, \quad (4.5)$$

for $V(z)$, average velocity in the vertical direction. The terms on the right-hand side of Eq. 4.5 (starting from the second term) are buoyancy stress ($\bar{\tau}_B$), viscous stress ($\bar{\tau}_N$), Reynolds stress ($\bar{\tau}_R$), polymeric stress (τ_p) and surface stress ($\bar{\tau}_S$) respectively. For the Newtonian flow, τ_p is zero. At statistically steady state, the left-hand side of Eq. 4.5 is zero and the total pressure gradient $\mathcal{B} = \tau_{23}$, where τ_{23} is the total shear

stress. Figure 4.6 shows the stress balance for the clean and contaminated bubbly flows at the statistically steady state. For $C_\infty = 0$, the formation of bubble clusters near the wall completely alters the stress balance comparing to the single-phase flow. The major contributions to the total shear stress come from the buoyancy and surface stresses. Due to the high void fraction near the wall, the applied pressure gradient is balanced by the weight of the mixture in the middle of the channel. The Reynolds stress remains lower than the corresponding single-phase. For $C_\infty = 0.1$, the stress balance of contaminated bubbly flow becomes similar to the single-phase flow, major contributors to the total shear stress are the viscous and the Reynolds stress. Reynolds stress is even slightly higher than that of the single-phase flow but, for $C_\infty = 1.0$, it slightly decreases due to the increase in the void fraction near the wall. Surface stress for both $C_\infty = 0.1$ and $C_\infty = 1.0$ cases becomes nearly zero and the bouncy term becomes slightly negative near the wall due to very low void fraction and elimination of the bubble clusters.

4.3.2 viscoelastic flow: The combined effects of Viscoelasticity and Surfactant

Next, simulations are performed to examine the combined effects of viscoelasticity and surfactant (Triton X-100) on dynamics of bubbly flows. For this purpose, single-phase viscoelastic turbulent flow is first simulated for $Wi = 4$ and $Wi = 8$. The drag reduction (DR) for $Wi = 4$ and $Wi = 8$ is found to be approximately 23% and 37%, respectively, which falls in the low drag reduction regime (LDR) of the polymeric drag reduction [26]. The drag reduction for the single-phase flow is determined as $DR = (c_{f,0} - c_{f,0,Wi})/c_{f,0}$ where $c_{f,0}$ is the skin friction coefficient for the Newtonian single-phase case while $c_{f,0,Wi}$ is for the corresponding viscoelastic case characterized by the Weissenberg number (Wi). The effects of bubbly flow on the polymer drag reduction are determined by introducing the spherical bubbles to the viscoelastic turbulent flow for $Wi = 4$ and $Wi = 8$ in the absence of the surfactant (clean bubbles). For the contaminated bubbles cases, i.e., in the presence of surfactant, simulations are performed by varying the surfactant concentrations of $C_\infty = 0.1, 0.25$ and 0.5 , at a fixed Weissenberg number ($Wi = 4$). Next, the Weissenberg number

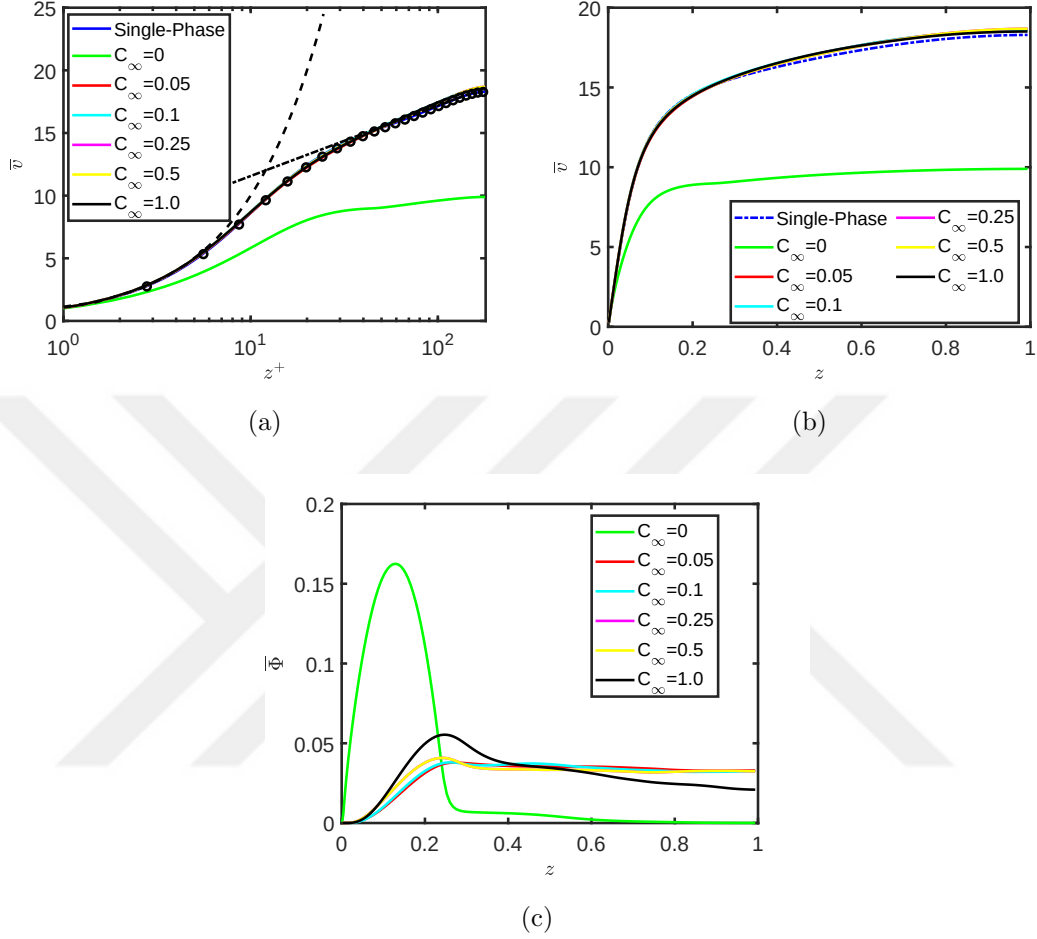


Figure 4.3: Surfactant Triton X-100: (a) Average liquid velocity scaled by v_τ^* vs wall-normal distance (b) mean velocity profiles (c) average void fraction at a statistically steady state. The computed inner-scaled mean velocity profile (solid line) compared with the law of the wall (dashed and dash-dotted lines). The law of the wall plots in the laminar sub-layer ($v^+ = z^+$) and in the logarithmic region ($v^+ = 2.5 \ln z^+ + 5.5$). The solid lines represent the current results and the symbols are the DNS data of Kim et al. [57]

is changed from $Wi = 4$ to $Wi = 8$, while keeping $C_\infty = 0.5$. Figure 4.7 shows the transient behavior of the skin friction coefficient (c_f) for the clean and contaminated bubbly flows. The addition of clean bubbles to the viscoelastic turbulent flow has drastic effects on the polymeric drag reduction. As can be seen, c_f scaled by corresponding single-phase skin friction coefficient, increases with increasing Weissenberg number ($Wi = 4$ and $Wi = 8$). Hence, viscoelasticity results in a significant drag

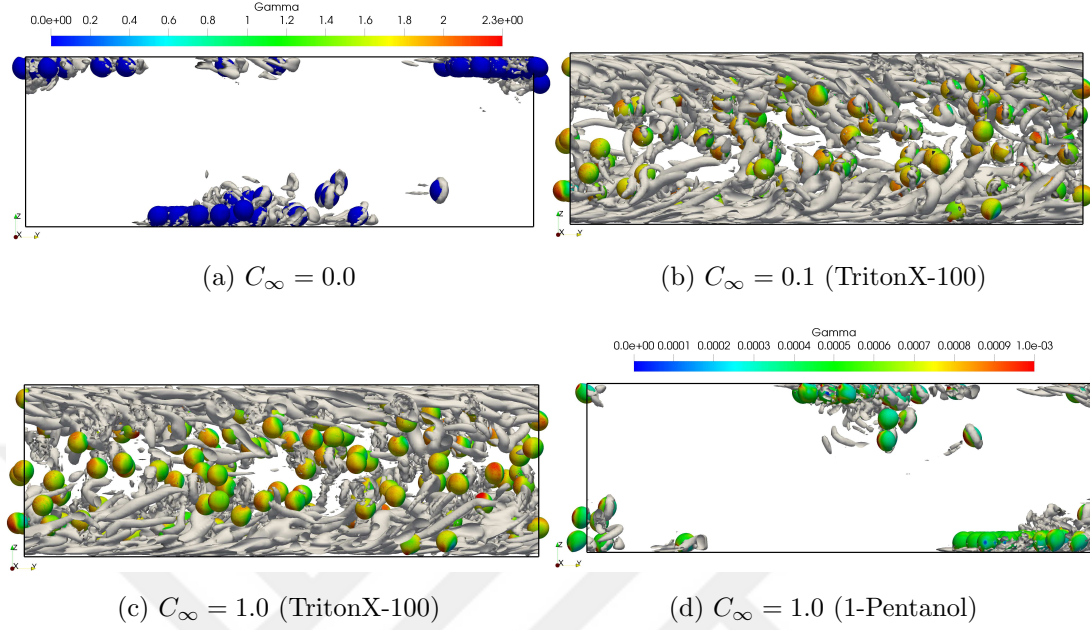


Figure 4.4: Newtonian Flow: Vortical structures at a statistically steady state. The vortical structures are visualized using Q -criterion, i.e., the iso-contours of the normalized second invariant of the velocity-gradient tensor, $Q^*/(V_b^*/(h^*))^2 = 0.8$, are plotted. The contours on the bubble surface represent interfacial surfactant concentration (Γ).

increase in a clean bubbly flow. This is in sharp contrast with the expectations from the single-phase flow, where we observe drag reduction by the viscoelasticity. Conversely, for the bubbly flow in the presence of surfactant, the drag reduction of viscoelastic turbulent flow is restored, in line with the corresponding single-phase flows. This revival of the drag reduction for the contaminated bubbly flow depends on the net effect of Marangoni and elastic forces. The loss of drag reduction for the clean bubbly flow is due to the formation of the bubble wall-layers. The clean bubbles are pushed toward the channel wall not only due to the aerodynamic force but also due to the elastic induced lift forces [2]. Thus, the addition of polymers into the clean turbulent bubbly flow results in a drag increase due to the elastic induced lift forces, which increase with Wi . In the presence of surfactant, Marangoni forces prevent the formation of bubble clusters by opposing the aerodynamic and elastic induced forces. Thus, for the $Wi = 4$ & $C_\infty = 0.1$ case, the skin friction coefficient c_f approaches the corresponding single-phase value. For $Wi = 8$ & $C_\infty = 0.5$ on the

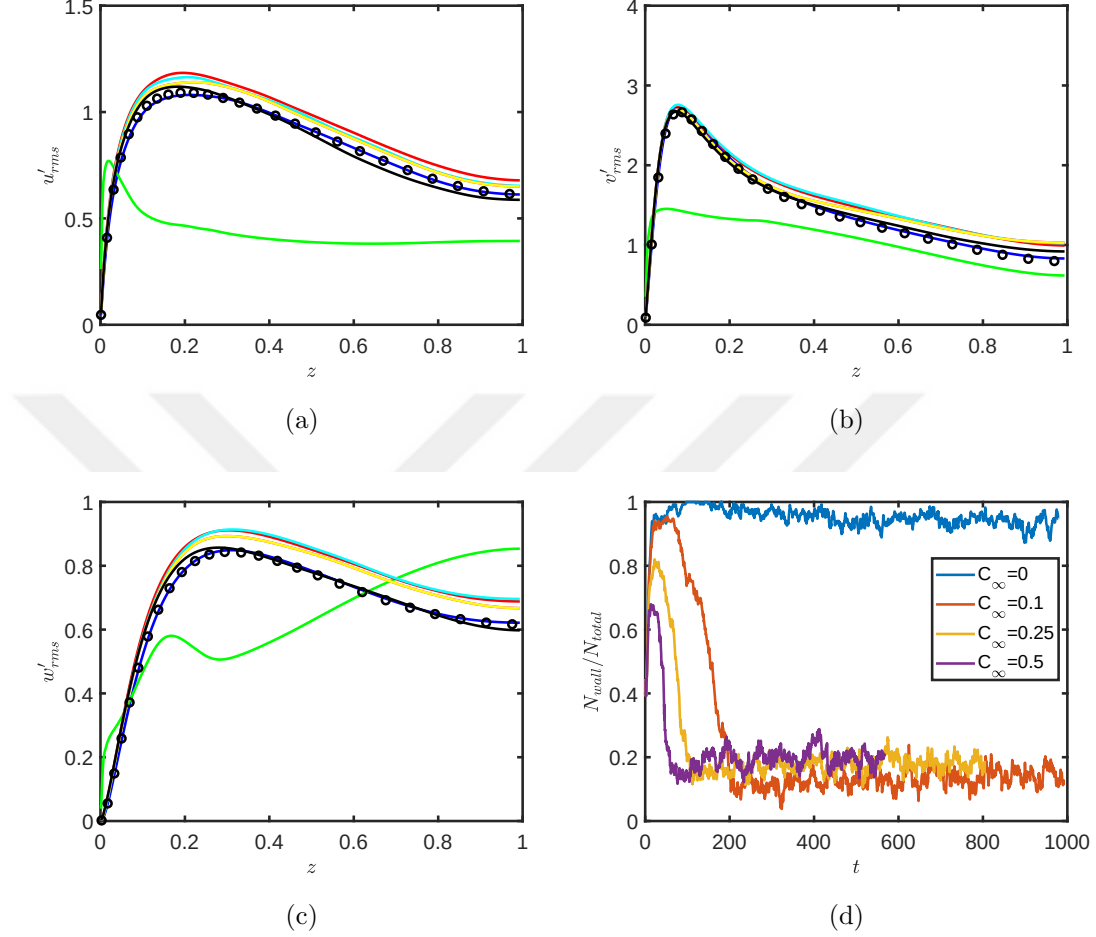


Figure 4.5: Newtonian Flow: (a)-(c) Effect of surfactant (Triton X-100) on liquid velocity fluctuations scaled by v_τ versus wall-normal distance at statistically steady state. u'_{rms} , v'_{rms} , and w'_{rms} are the fluctuations in the spanwise, streamwise and wall-normal direction, respectively. (d) transient result: N_{wall}/N_{total} is the number of bubbles in the bubble wall-layer. The wall layer is defined as one diameter distance from the wall. The solid lines represent the current results and the symbols represent the DNS data of Kim et al. [57].

other hand, c_f increases again showing that the Marangoni forces are not strong enough to counter the elastically induced lift force. In the presence of surfactant, the polymer drag reduction hence depends on the interplay of the Marangoni and elastic forces.

The drag-reducing property of polymers is attributed to the polymer stretching. Figure 4.8 shows that the polymeric stretching in viscoelastic turbulent bubbly flows

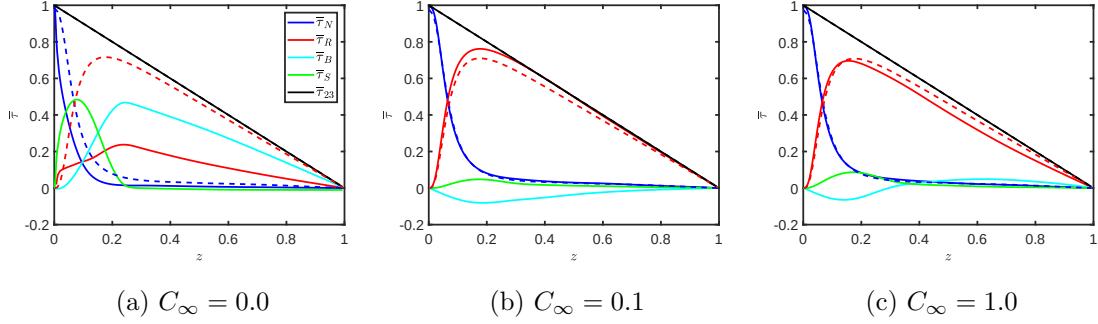


Figure 4.6: Newtonian Flow (Triton X-100): Stress balance at a statistically steady state. Dotted lines show the corresponding single-phase stress balance. $\bar{\tau}_N$ is viscous stress, $\bar{\tau}_R$ is Reynolds stress, $\bar{\tau}_B$ is buoyancy stress, $\bar{\tau}_S$ is surface stress, $\bar{\tau}_{23}$ is total shear stress.

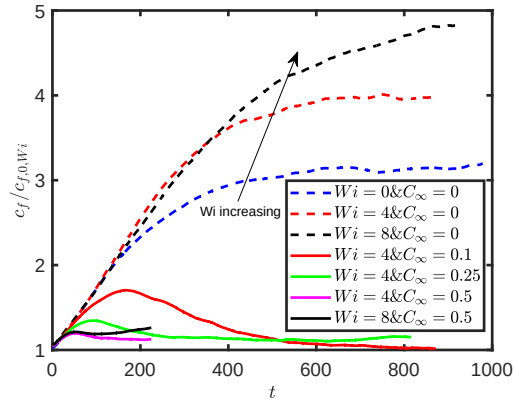


Figure 4.7: Skin friction coefficient (c_f) of the viscoelastic bubbly flow normalized by the value of the corresponding single-phase flow at a statistically steady state.

is highly affected by the formation of bubble clusters. As can be seen, the polymeric stretching becomes minimal for the clean case, for which there is a clear peak of average void fraction near the wall. For contaminated cases, the average void fraction peak vanishes and the polymer stretching is similar to the single-phase flow resulting in the restoration of drag reduction. The formation of bubble wall-layers not only affects the drag reducing property of polymers, but also causes a significant drag increase for clean bubbly flows.

It is known for the LDR regime of polymer drag reduction (single-phase) that

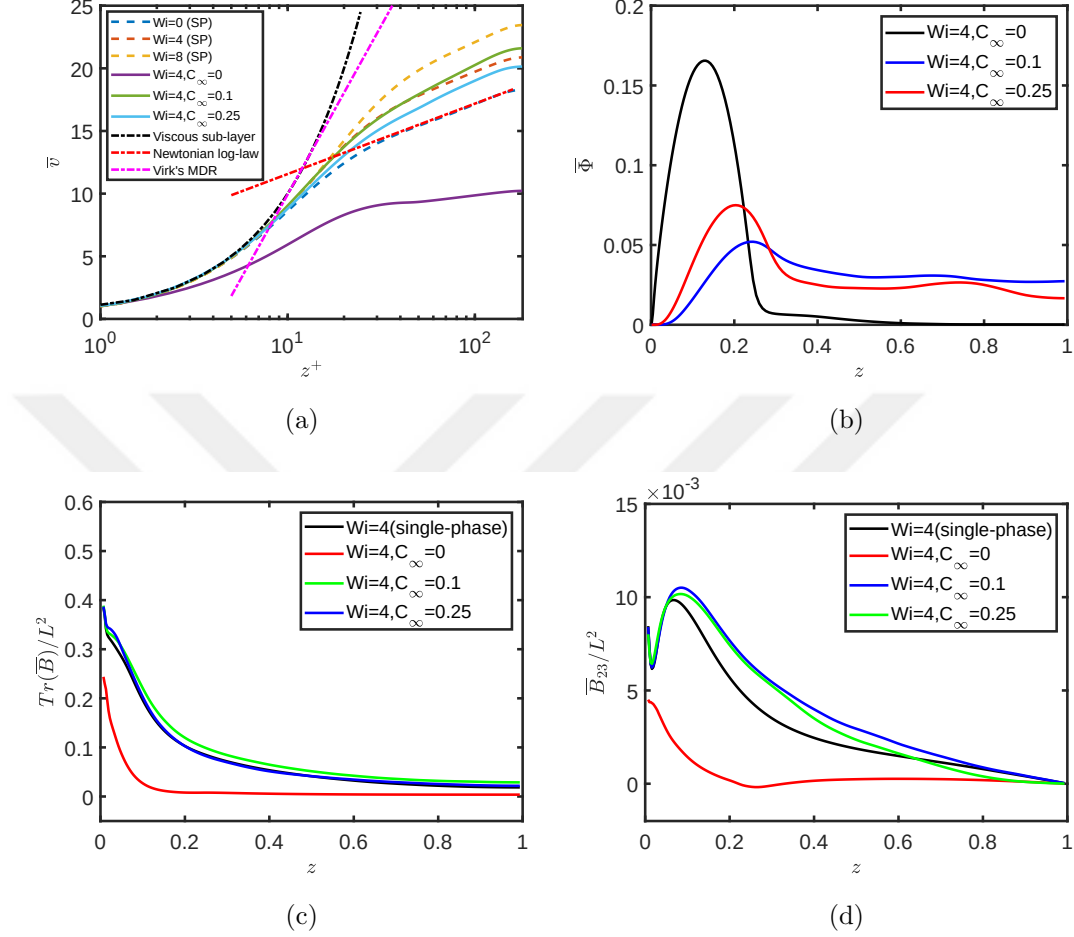


Figure 4.8: Various statistics at statistically steady state versus wall-normal direction (a) Mean velocity profiles (b) average void fraction (c) polymeric stress (d) B_{23} stress.

the velocity fluctuations (v'_{rms}) increase in the streamwise and decrease in the other directions [26, 25]. Figure 4.9 shows the liquid velocity fluctuations for a viscoelastic turbulent bubbly flow at a statistically steady state. The fluctuations for the clean case are the same as that observed for the Newtonian bubbly flow. It is interesting to observe that v'_{rms} decreases for the contaminated bubbly flow ($Wi = 4, C_\infty = 0.1$) near the wall, even though the polymer stretching and the skin friction coefficient are almost the same as for $Wi = 4$ single-phase flow. For $Wi = 4, C_\infty = 0.25$, v'_{rms} further decreases near the wall as the void fraction increases there. The reduction of v'_{rms} near the wall can be attributed to the increase in the frequency of bubbles leav-

ing/entering in the bubble wall-layer. Thus, the presence of contaminated bubbles modifies the streamwise velocity fluctuations near the wall. Reynolds stress is also shown in Fig. 4.9. As expected, the Reynolds stress decreases for the single-phase flow while the near-wall peak further decreases for the contaminated bubbly flows at $Wi = 4$. It is also known for the single-phase flows that the polymeric shear stress increases while Reynolds stress decreases for the viscoelastic turbulent flows. To quantify and further explore this observation, the shear stress balance across the channel is shown in Fig. 4.10. For the clean case ($Wi = 4, C_\infty = 0$, Fig. 4.10 a), the stress balance is completely different from the corresponding single-phase flow (shown by dotted lines). For the clean bubbly flow, the major components contributing to the total shear stress ($\bar{\tau}_{23}$) are the surface stress ($\bar{\tau}_S$) and buoyancy stress ($\bar{\tau}_B$). Due to the significant reduction in the flow rate, the viscous stress ($\bar{\tau}_N$) near the wall also reduces. The polymeric stress ($\bar{\tau}_P$) almost vanishes for the clean bubbly flow. Conversely, for the $Wi = 4, C_\infty = 0.1$ case, the stress balance becomes similar to the corresponding single-phase flow, as the major components to the total shear stress ($\bar{\tau}_{23}$) are Reynolds stress ($\bar{\tau}_R$) and viscous stress ($\bar{\tau}_N$). However, Reynolds stress is slightly lower for contaminated bubbly flow than in the corresponding single-phase flow, and further decreases for higher surfactant concentrations ($Wi = 4, C_\infty = 0.25$). Furthermore, Fig. 4.11 shows the iso-surfaces of vortices for the clean and contaminated viscoelastic turbulent flows, compared with the corresponding Newtonian case. The vortices are identified by the Q-criterion method [53]. As can be seen, the clean ($C_\infty = 0$) Newtonian (4.11 a) and viscoelastic ($(Wi = 4)$, 4.11 b) bubbly flows have re-laminarized. The vortical structures are only concentrated around the bubbles. For the contaminated bubbly flows ($C_\infty = 0.1$), turbulent structures reappear, but are stronger in the Newtonian case (4.11 c) than in the viscoelastic case ($Wi = 4$, 4.11 d).

Figure 4.12 shows the one-dimensional energy spectrum of the streamwise velocity fluctuations (E_{vv}) defined as

$$E_{vv} = \int_{kx} \hat{v}_i'^* \hat{v}_i' dx, \quad (4.6)$$

where “ $'$ ” indicates the fluctuating component of the velocity field, $\hat{\cdot}$ indicates the Fourier transform, and “ $\star$ ” indicates the complex conjugate. Energy spectra is plotted against the streamwise wave number (k_y) at different distances from the wall. As can be seen that the single-phase Newtonian and viscoelastic turbulent flow follow the $-5/3$ scaling, reconfirming the flow is turbulent and well resolved. The presence of bubbles certainly modify the energy spectrum. For bubbly flow cases, spectra follows $-5/3$ scaling before the wave number based on bubble diameter. After this wave number the scaling changes for the bubbly flows.

4.4 Conclusions

An efficient fully parallelized finite-difference/front-tracking method has been used to examine the effects of clean and contaminated spherical bubbles on the Newtonian and viscoelastic turbulent channel flows. For the clean case, the earlier findings are verified: The clean bubbles move towards the wall due to hydrodynamic lift force and form a bubble-rich wall layer. Prevention of bubble clusters near the wall in the presence of surfactant were examined by using physical sorption properties of Triton X-100 and 1-Pentanol. It is found that, the sorption kinetics highly affect the dynamics of turbulent bubbly flow. $C_\infty = 1.0$ (Triton X-100), is enough to prevent the formation of bubble clusters but $C_\infty = 100$ (1-Pentanol) is not sufficient. For viscoelastic turbulent flows, it is found that, in the presence of clean bubbles, the polymer drag reducing property of viscoelastic fluid is completely lost. It is also shown that the addition of small amount of surfactant (contaminated bubbles) can revive the polymer drag reduction effect for turbulent bubbly flows. The drag reduction for contaminated bubbly flows depends on the interplay of the elastic and Marangoni-induced forces. For $Wi = 4$ and $C_\infty = 0.5$, almost same drag reduction is achieved as observed in the respective single-phase flow but for $Wi = 8$, the drag reduction does approaches respective single-phase as elastic forces increase which promotes the formation of bubble-wall layers and Marangoni-induced force is not sufficient to counter it.

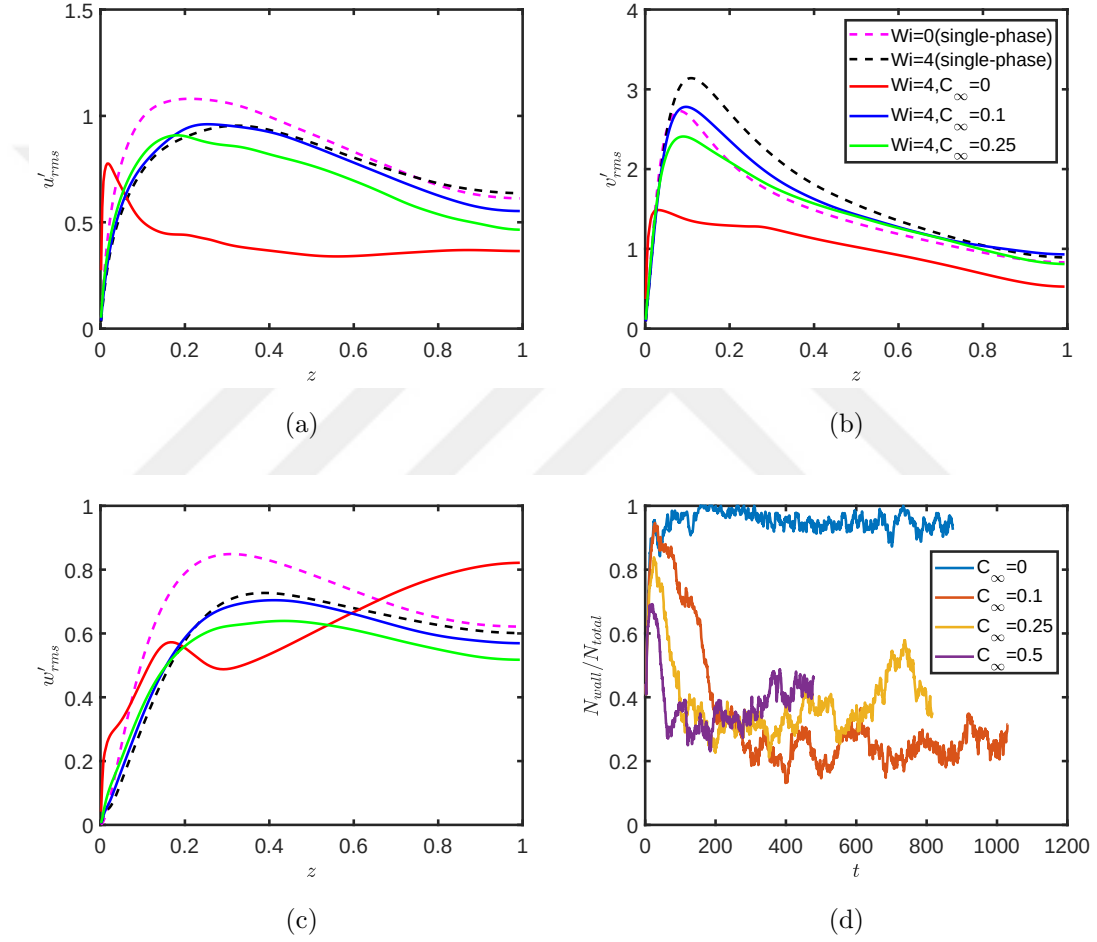


Figure 4.9: (a)-(c) Liquid velocity fluctuations scaled by v_τ versus wall-normal distance at statistically steady state. u'_{rms} , v'_{rms} , and w'_{rms} are the fluctuations in the spanwise, streamwise and wall-normal direction, respectively. (d) transient result for $Wi = 4$: N_{wall}/N_{total} is the number of bubbles in the bubble wall-layer. The wall layer is defined as one diameter distance from the wall.

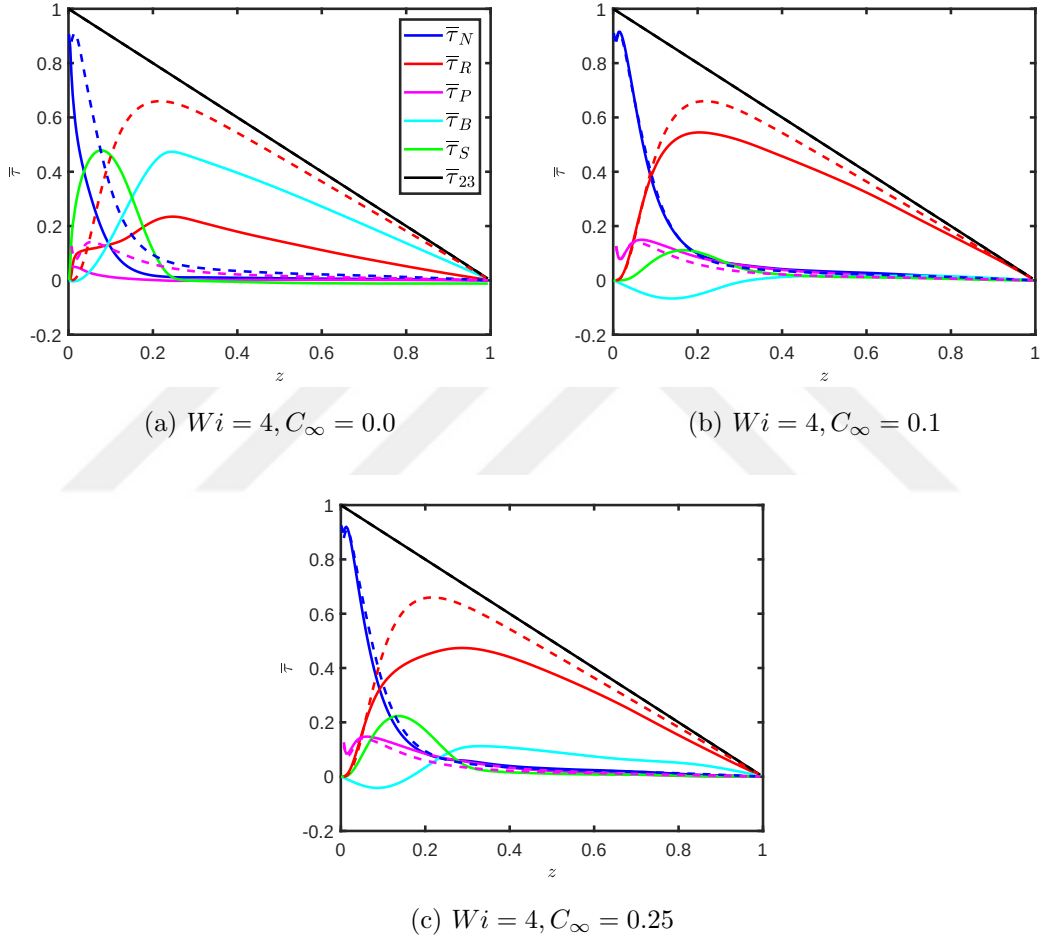


Figure 4.10: Stress balance at statistically steady state. Dotted lines show the corresponding single-phase stress balance. $\bar{\tau}_N$ is viscous stress, $\bar{\tau}_R$ is Reynolds stress, $\bar{\tau}_P$ is polymeric stress, $\bar{\tau}_B$ is buoyancy stress, $\bar{\tau}_S$ is surface stress, $\bar{\tau}_{23}$ is total shear stress.

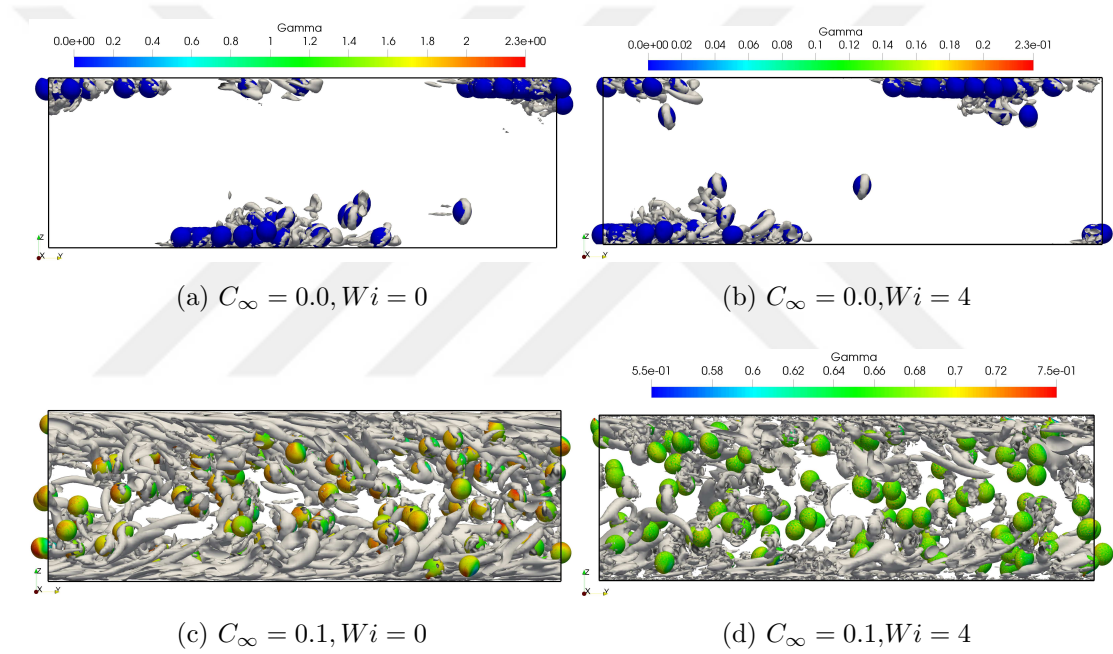


Figure 4.11: The vortical structures at statistically steady state. The vortical structures are visualized using Q -criterion, i.e., the iso-contours of the normalized second invariant of the velocity-gradient tensor, $Q^*/(V_b^*/(h^*))^2 = 0.8$, are plotted. The contours on the bubble surface represent interfacial surfactant concentration (Γ)

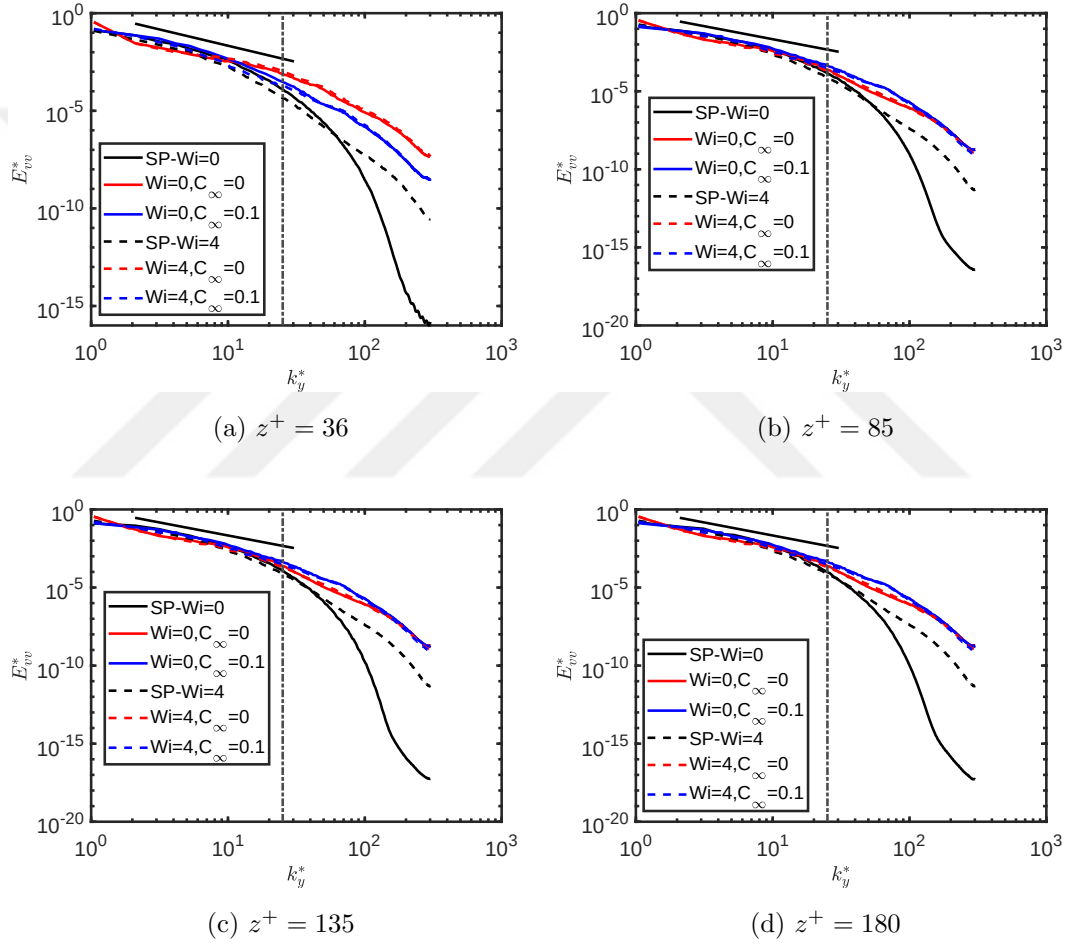


Figure 4.12: Energy spectra is plotted against the streamwise wave number (k_y) at different distances from the wall. The vertical line shows the wave number based on the diameter of bubble.

Chapter 5

CONCLUSIONS

An efficient fully parallelized finite-difference/front-tracking method has been used to examine the effects of soluble surfactant and viscoelasticity on turbulent bubbly channel flows.

Effects of surfactant on the lateral migration of a bubble in a pressure driven show that a small amount of surfactant can alter direction of lateral migration of a bubble. The clean bubble moves toward the wall and maintains a steady separation distance depending on the deformability (Ca) of the bubble. On the contrary, the contaminated bubble migrates toward the center of the channel and its steady separation distance is nearly independent of the deformability (Ca) of the bubble. By comparing soluble and insoluble surfactant cases for different capillary numbers, it is observed that the lateral migration of the bubble is faster in case of insoluble surfactant than the soluble surfactant during the transient period and this difference in both cases increases with the capillary number. The effects of the bulk surfactant concentration (C_∞) and the elasticity number (β_s) on the lateral migration of the bubble are examined by extensive simulations. It is found that in both cases, the bubble migrates toward the center of channel after a critical value of $C_\infty = 0.25$ and $\beta_s = 0.25$. Finally the effect of *Eötvös* number on the lateral migration is examined. For the clean case, the bubble moves away from the wall only at high $Eo = 3$, whereas it migrates towards it at smaller values. In the presence of surfactant, the bubble reverses the direction of lateral migration for $Eo = 0$ and $Eo \geq 1.5$, while it moves towards the wall in the values in between. Path instability is observed for rising bubbles in both clean and contaminated cases. It is observed that the surfactant reduces the critical values at which a path instability is triggered.

The sole and combined effects of soluble surfactant and viscoelasticity on tur-

bulent bubbly channel flows show that for the clean case, the earlier findings are verified: The clean bubbles move towards the wall due to hydrodynamic lift force and form a bubble-rich wall layer. It is found that addition of surfactant has significant influence on the overall flow structure of turbulent bubbly channel flow. Surfactant-induced Marangoni stresses counteract the hydrodynamic lift force and push the bubbles away from the wall region. At a high enough surfactant concentration $C_\infty = 0.5$, the formation of bubble wall layer is completely prevented resulting in a uniform void fraction distribution across the channel cross-section. The present results are in agreement with the earlier experimental Takagi et al. [110] and the numerical Lu et al. [64] studies, i.e., the addition of surfactant prevents the formation of the wall-layers. For $C_\infty = 1$, the trend reversal is also observed i.e., reforming of bubble clusters due to a more uniform interfacial surfactant concentration. For the clean viscoelastic case, bubbles move toward the channel wall, similarly to the Newtonian case. The elastic force promotes the formation of the bubble wall-layer resulting in the reduction of the flow rate, which is consistent with the computational results of Mukherjee et al. [74]. Thus, the drag reduction effect of viscoelasticity observed for the single-phase flows diminishes due to the formation of bubble wall-layers. Finally, in the presence of combined effects of surfactant and viscoelasticity, similar wall-layer formation is observed, but the bubbles in the horizontal clusters show a more sparse distribution compared to the clean case.

Prevention of bubble clusters near the wall in the presence of surfactant were examined by using physical sorption properties of Triton X-100 and 1-Pentanol. It is found that, the sorption kinetics highly affect the dynamics of turbulent bubbly flow. $C_\infty = 1.0$ (Triton X-100), is enough to prevent the formation of bubble clusters but $C_\infty = 100$ (1-Pentanol) is not sufficient. For viscoelastic turbulent flows, it is found that, in the presence of clean bubbles, the polymer drag reducing property of viscoelastic fluid is completely lost. The flow rate for the both $Wi = 4$ and $Wi = 8$, becomes similar to the Newtonian bubbly flow. It is also shown that the addition of small amount of surfactant (contaminated bubbles) can revive the polymer drag reduction effect for turbulent bubbly flows. The drag reduction for

contaminated bubbly flows depends on the interplay of the elastic and Marangoni-induced forces. For $Wi = 4$ and $C_\infty = 0.5$, almost same drag reduction is achieved as observed in the respective single-phase flow but for $Wi = 8$, the drag reduction does approaches respective single-phase as elastic forces increase which promotes the formation of bubble-wall layers and Marangoni-induced force is not sufficient to counter it.



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Appendix A

EFFECTS OF SURFACTANT ON POLYMER DRAG REDUCTION FOR VISCOELASTIC POLY-DISPERSED TURBULENT BUBBLY CHANNEL FLOWS

A.1 Introduction

Direct numerical simulations (DNS) have been used to examine several bubbly multiphase flows revealing considerable new insights. First, a brief overview of studies conducted without considering the effects of surfactant and viscoelasticity is presented here. Lu et al. [63] studied the effects of few large bubbles on the wall drag in a turbulent channel flow for friction Reynolds number of $Re_\tau = 135$ using front-tracking method. They found that the deformable bubbles lead to a significant reduction in the wall drag whereas the spherical bubbles increase the wall drag. Lu and Tryggvason [66, 67] performed simulations to study the effects of nearly spherical and deformable bubbles on the dynamics of turbulent bubbly flows. They performed the simulations considering “minimum turbulent channel” (i.e., $Re_\tau = 127.2$) and void fraction of 3 percent. They observed that the spherical bubbles move towards the wall and form horizontal clusters and thus, result in the reduction of liquid flow rate whereas the deformable bubbles tend to move toward the center of the channel and remain there. Later, they also performed simulations for bubbly flow at a much higher Reynolds number ($Re_\tau = 250$) with the same void fraction. They found that the overall structure of the bubbly flow remains similar to the smaller system. They also observed the formation of bubble clusters similar to the experimental observations of Takagi et al. [108] for the turbulent flows laden with nearly spherical bubbles. Santarelli and Frohlich [92, 93] also examined the collective motion of mono-dispersed and bi-dispersed bubbles in a turbulent channel

flow ($Re_\tau = 172$ and $Re_\tau = 194$, respectively) and void fraction of 2.14 percent. Their results did not show the strong lateral migration as seen for the clean bubbles but rather their results were similar to that of fully contaminated bubbles in the experiments. Tryggvason et al. [121] performed the DNS of poly-dispersed bubbly flow for much larger system at a higher Reynolds number ($Re_\tau = 500$). They used 3 percent void fraction containing bubbles of different sizes (spherical and deformable). Due to large computational time requirement to attain a statistically steady state, they have shown the results for only transient period. Their results show that the small bubbles quickly migrate to the wall but the bulk flow takes much longer to adjust the new bubble distribution. Bois [8] has recently performed the simulations using realistic fluid properties to represent saturated steam and water in pressurized water reactor (PWR) conditions at $Re_\tau = 180$ and void fraction of 10 percent.

Bubbly flows are, however, only one of several possible flow regimes like slug flow, churn flow, and annular flow. The structure of such flows is sensitive to governing parameters, specially, to the average void fraction and gas flow velocity. Samaras et al. [91] have presented a brief overview of the different maps that have been proposed to show the boundary between different flow regimes as functions of the governing parameters. Although DNS has been used extensively to study the bubbly flows, the DNS simulations of more complex multiphase flows involving multiphysics effects are not common, [68] have performed DNS of multiphase turbulent channel flow ($Re_\tau = 127.2$) undergoing extensive topology changes. They examined the effects of various governing parameters on the evolution of flow statistics such as the average flow rate, wall shear, and interface area. More recently, Soligo et al. [99, 98] have presented a modified phase field method (PFM) and performed simulations of turbulent bubbly channel flow ($Re_\tau = 590$) to examine the effects of surfactant on bubble coalescence. They performed simulations for a very short time interval without providing any statistics of turbulent bubbly flows.

For the present study, extensive simulations are performed to investigate the effects of surfactant and viscoelasticity on the structure of poly-dispersed turbulent two-phase flow.

A.2 Computational setup

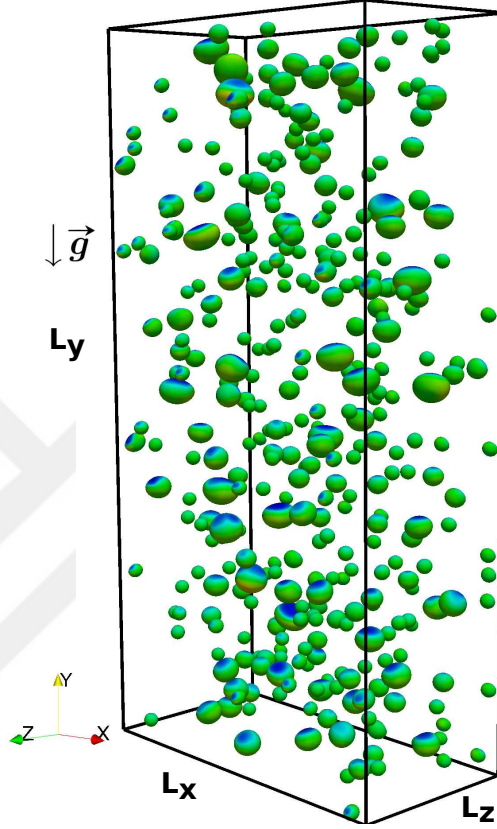


Figure A.1: Schematic representation of the computational setup considered in the present work. The contours on the bubble surface represent interfacial surfactant concentration with the scale ranging from 0 (blue) to 0.23 (red).

Computational domain shown in the Fig. A.1 is a rectangular channel with streamwise, spanwise and wall-normal direction along y , x and z coordinates, respectively. The flow is periodic in the spanwise (x) and streamwise (y) directions, while no-slip/no-penetration boundary conditions are applied at the walls (z direction). The size of the domain ($L_y \times L_x \times L_z$) is $8h \times 4h \times 2h$ resolved by a $1280 \times 640 \times 384$ in streamwise, spanwise and wall-normal directions respectively, where $h = 1$ is the half width of the channel. The flow is driven by an imposed constant pressure gradient $\frac{dp^*}{dy^*}$. Note that dimensional quantities are denoted by the superscript $*$ in the present study, e.g., p^* and p represent the dimensional and

non-dimensional pressure, respectively. The single-phase turbulent channel flow is generated by initializing the flow field with a streamwise-aligned vortex pair [46], which effectively triggers transition to turbulence.

To depict the scenario, where some bubbles have coalesced during the rising process or formation of different size of bubbles in a controlled experiment, the simulations are performed for poly-dispersed flows. The physical parameters are selected such that the total void fraction is 3 percent. Further, the void fraction is divided into four equal portions of 0.75 percent for four different sizes of bubbles, yielding the Eotvos numbers (Eu) ranging from 0.5 to 2.5. The literature review suggests that, for the bubbly flow without surfactant and viscoelasticity, $Eu = Eu_{cr} = 2.5$ is the critical value: The bubbles tend to move towards the center of the channel when $Eu \geq 2.5$ while they are more likely to move towards the channel wall otherwise. Hence, we have three sets of bubbles which are likely to accumulate at the channel wall while the bubbles in the other set move away from the wall for the clean case. The details of this configuration are given in Table A.1.

Table A.1: Configuration of poly-dispersed flow. Eu , R_b^* , Vol_b^* and N_b denote the Eotvos number, the initial bubble radius, the bubble volume and number of bubbles, respectively

Eu	R_b	Vol_b	N_b
0.5	0.08	2.14×10^{-3}	224
1.0	0.11	5.58×10^{-3}	86
2.0	0.14	0.011	42
2.5	0.18	0.024	20

A.3 Results and Discussion

Simulations are performed to examine the effects of surfactant and viscoelasticity on poly-dispersed turbulent flow. Figure A.2 shows the transient behavior of skin friction coefficient normalized with the skin friction coefficient of Newtonian single-

phas flow ($C_{f,0}$ and average void fraction profile. The results are shown for on-going simulations, therefore the cases have not reached a statistically steady state yet. For the clean case ($C_\infty = 0, Wi = 0$), the drag increases as observed for the bubbly flow simulatons of the mono-dispersed bubbles. This increase in the drag is because of the small bubbles have formed a wall clusters near the wall. It can also be seen that the most deformable bubbles are away from the wall. In the presence of polymers, for $Wi = 20$, a similar trend is observed but it is different to what has been observed for the mono-dispersed clean bubbles. Though the drag increase for viscoelastic bubbly flow but it is slightly lower than the clean Newtonian bubbly flow. In presence of surfactant ($C_\infty = 0.1$) (Triton X-100), both the Newtonian and viscoelastic bubbly flow dynamics is completely altered. The Newtonian bubbly flow, for $C_\infty = 0.1$, maintains the same average flow rate as observed for the single-phase flow whereas, for the viscoelastic bubbly flow, the polymer drag reduction is effective and the drag is further reduced compares to the corresponding single-phase flow.

Next, the effect of Wi number is examined on the poly-dispersed bubbly flow in the presence of surfactant. The $C_\infty = 0.1$ is fixed and the Wi is varied from 5 to 40. Also, two mono-dispersed bubble cases are for $Wi = 20$ and $C_\infty = 0.1$. The smallest $Eo = 0.5$ and the largest bubbles $Eo = 2.5$ are chosen for these cases. As can be seen, the results are still at early times but the difference in the cases is already visible. Increasing Wi number, reduces the drag but for $Wi = 40$, the drag reduction is same as for $Wi = 20$. This might be due to the MDR limit of polymer drag reduction, but it is early to claim this. Comparing to the mono-dispersed bubble cases, as expected the smallest bubbles $Eo = 0.5$ have formed the bubble clusters and thus the drag increases whereas the largest mono-dispersed $Eo = 2.5$ stays at the center have the maximum drag reduction among all the cases. The bubble distribution and interfacial surfactant concentration Γ is shown in the Fig. A.3 and Fig. A.4 for the various cases.

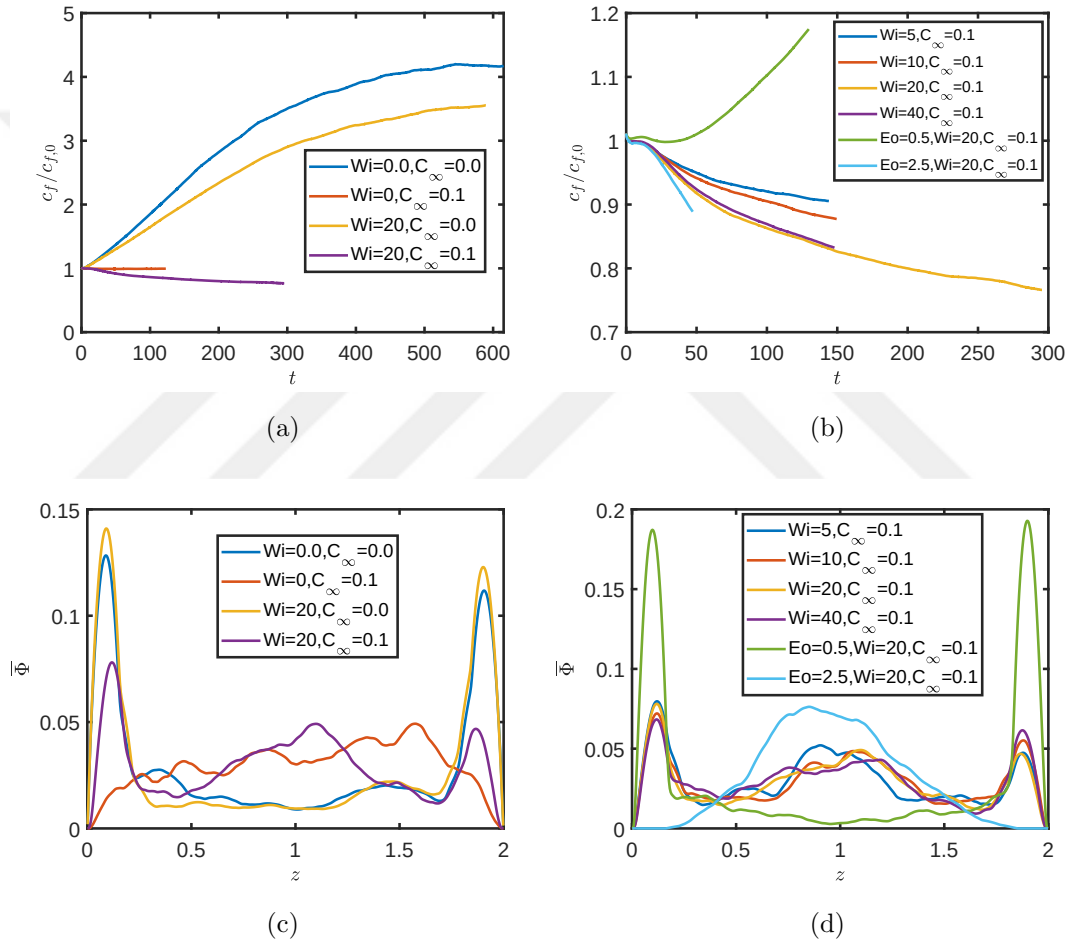


Figure A.2: (a)-(b) Skin friction coefficient (c_f) of the bubbly flow normalized by the statistically steady state value of the Newtonian single-phase flow ($c_{f,0}$). (c)-(d) Average void fraction against wall-normal direction at latest time.

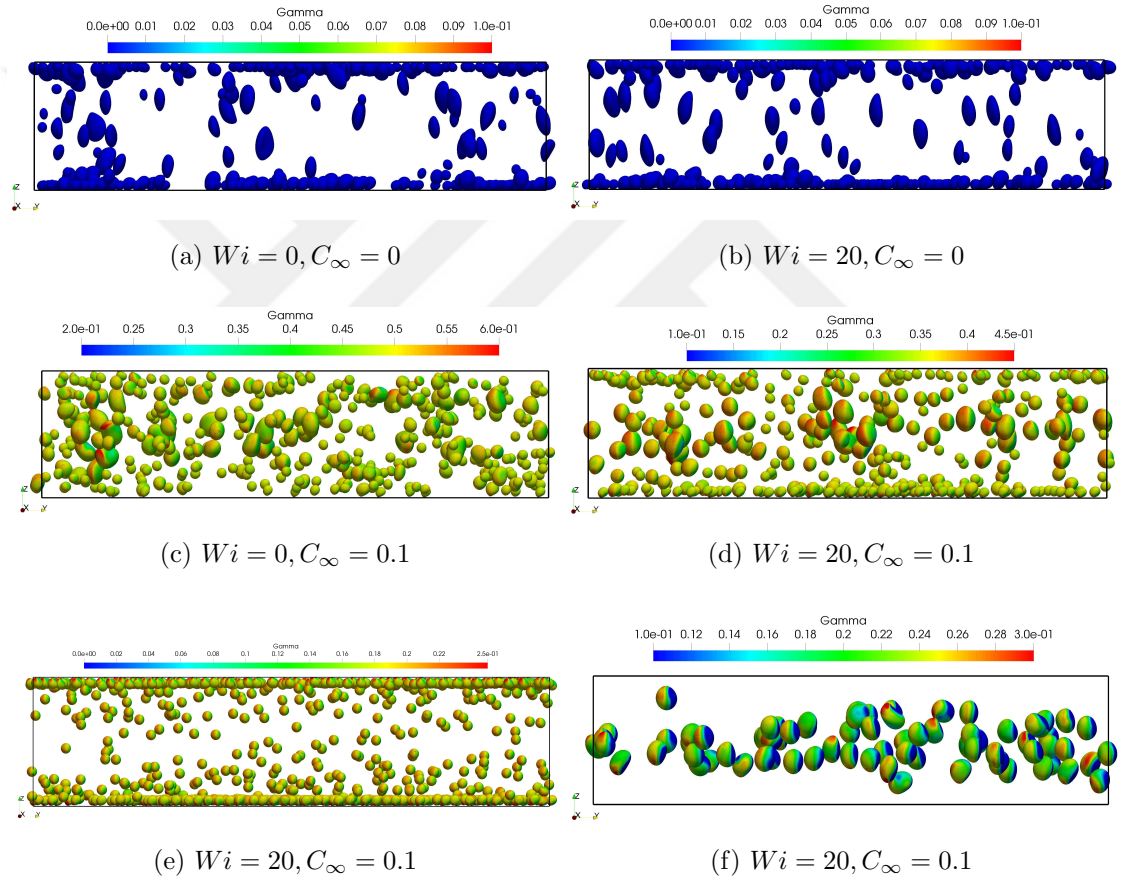
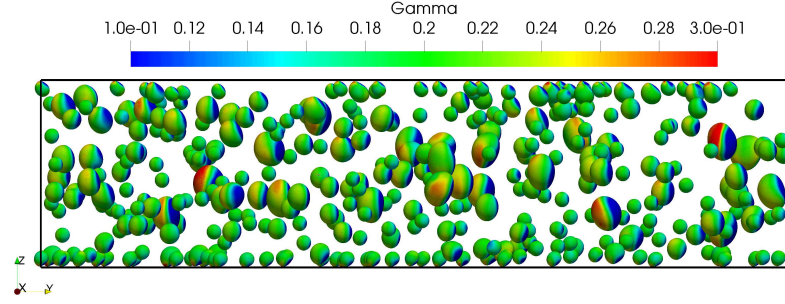
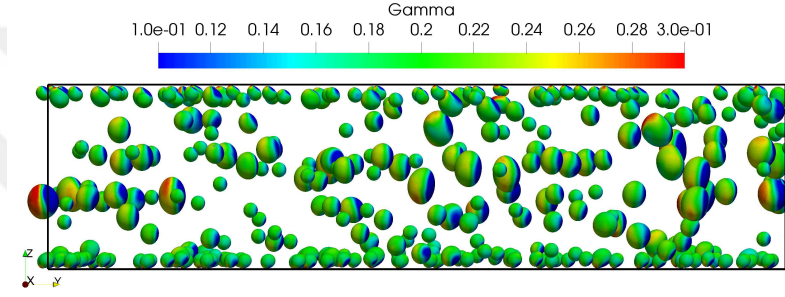


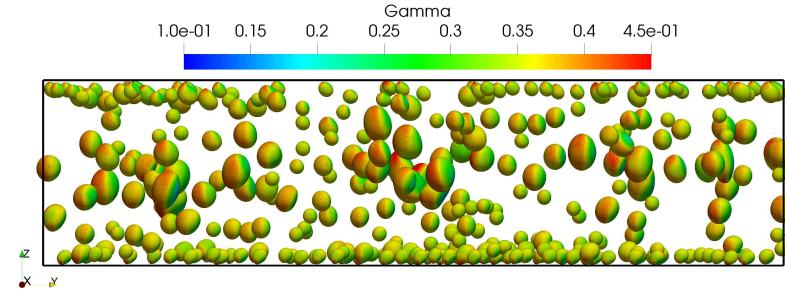
Figure A.3: Bubble distribution for various cases at latest time available. The contours on the bubble surface represent interfacial surfactant concentration (Γ).



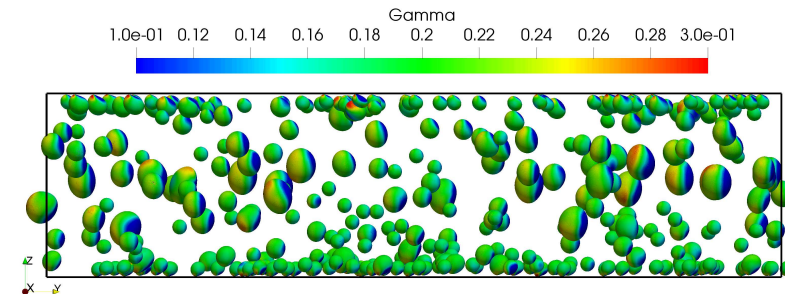
(a) $Wi = 5$



(b) $Wi = 10$



(c) $Wi = 20$



(d) $Wi = 40$

Figure A.4: Effect of Wi on the contaminated ($C_\infty = 0.1$) bubble distribution for various cases at latest time available. The contours on the bubble surface represent interfacial surfactant concentration (Γ).