

Computational Modeling of Viscoelastic Two-Phase Systems

by

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This is to certify that I have examined this copy of a doctoral dissertation by

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To my beloved wife, Madina.

ABSTRACT

A front-tracking method is developed for direct numerical simulations of viscoelastic two-phase systems in which one or both phases could be viscoelastic. One set of governing equations is written for the whole computational domain and different phases are treated as a single fluid with variable material and rheological properties. The method has been validated for various benchmark single-phase and two-phase viscoelastic flow problems. The method has been demonstrated to be grid convergent with a second-order spatial accuracy for all the cases considered in this paper.

Then, the method is applied to study two-phase viscoelastic systems in a pressure-driven flow in a capillary tube with a sudden contraction and expansion. The effects of viscoelasticity in drop and bulk fluids are investigated including high Weissenberg and Reynolds number cases up to $Wi = 100$ and $Re = 100$. The FENE-CR model is used to account for the fluid viscoelasticity. Extensive computations are performed to examine drop dynamics for a wide range of parameters. It is found that viscoelasticity strongly interacts with drop interface in a non-monotonic and complicated way.

Finally, the method is employed to investigate the effects of viscoelasticity on dynamics of a droplet impacting and spreading on flat solid surfaces. The contact angle is determined dynamically based on the empirical correlation proposed by Kistler (1993). The emphasis is placed on the influence of viscoelasticity and extensive simulations are performed for a wide range of parameters. It has been found that the viscoelasticity favors drop rebound in contrast with the well-known anti-rebound effects of polymer additives. Some recent experimental studies have suggested that the anti-rebound effects of polymeric additives are not due to the change in the bulk properties of the drop, but rather due to the modification of wetting properties of the substrate. A simple model is developed to test this hypothesis. The computational results are found to support this hypothesis and show that the anti-rebound behavior can be captured by the modification

of the surface wetting properties in the receding phase.

ÖZET

Bu doktora tezinde, iki fazlı viskoelastik akış sistemlerinin doğrudan sayısal simülasyonları için bir ara-yüz izleme yöntemi geliştirilmiştir. Bu yöntemde fazlardan herhangi biri veya her iki faz birlikte viskoelastik olabilmektedir. Ara-yüz izleme yönteminde bütün akış alanı için tek bir bünye denklemleri seti yazılmakta ama her bir faz bölgesinde o faza ait akışkan özellikleri kullanılmaktadır. Ayrıca ara-yüze etki eden yüzey gerilme kuvvetleri de hesaba katılmaktadır. Sayısal yöntem standart tek-fazlı ve çok-fazlı viskoelastik test problemlerine başarıyla uygulanarak doğrulanmıştır. Sayısal yöntemin çözüm ağı yakınsamasını sağladığı, fiziksel uzayda ve zamanda ikinci mertebeden doğru olduğu gösterilmiştir.

Daha sonra sayısal yöntem basınç-tahrikli ani daralan ve genişleyen kılcal bir kanal-daki çok fazlı akış sistemlerine uygulanmıştır. Damlacık ve ana akışkanın viskoelastik olma durumları ayrı ayrı incelenmiştir. Weissenberg ve Reynolds sayılarının 100 mertebesine kadar ulaştığı durumlar da başarıyla modellenmiştir. Bu simülasyonlarda viskoelastik etkiler FENE-CR modeli kullanılarak hesaba katılmıştır. Akış parametrelerinin etkilerini sistematik bir şekilde incelemek amacıyla çok sayıda simülasyon yapılmıştır. Simülasyonlar sonucunda viskoelastisitenin damlacık ara-yüzeyi ile kuvvetli bir şekilde etkileştiği ve bu etkileşimin son derece karmaşık ve tek düze olmayan formada (non-monotonic) olduğu bulunmuştur.

Son olarak sayısal yöntem kullanılarak viskoelastisitenin bir damlacığın katı bir yüzeye çarpması, yüzeyde yayılması ve yüzeyden geri sıçraması üzerindeki etkileri incelenmiştir. Kontak açısı dinamik bir şekilde Kistler (1993) tarafından önerilen korelasyon kullanılarak belirlenmiştir. Özellikle viskoelastik etkilerin üzerinde durulmasına karşın diğer akış parametrelerinin etkileri de incelenmiştir. Viskoelastisitenin damlacığın yüzeyden geri sıçramasını engelleyici bir etki yaptığı bilinmektedir. Fakat simülasyon sonuçları bunun tam aksine viskoelastisitenin damlacık geri sıçramasını artırdığını göstermiştir. Yakın

zamanda yapılan deneysel alıřmalar sonucunda, damlacıėın geri sıçramasını engelleyen esas etkinin damlacıėın sıvısının viskoelastisitesinden kaynaklanmadıėı ve bu etkinin esas itibarıyla polimerlerin yzeeye yapıřması sonucu yzey ıslatılabilirlik zelliklerinin deėiřmesi sonucu ortaya ıktıėı ynnde kuvvetli delillere ulařılmıřtır. Bu hipotezi test etmek iin bir model geliřtirilmiř ve modelin performansı incelenmiřtir. Yapılan simlasyonlar sonuları bu hipotezi destekler mahiyettedir. Ayrıca elde edilen sonular viskoelastik damlacıkların katı yzeyden geri sıçramama davranıřının yzeyin ıslatılabilirlik zelliklerinin deėiřtirilmesi suretiyle doėru bir řekilde modellenebileceėini gsterilmiřtir.

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Chapter 1

INTRODUCTION

Fluids are abundant in the nature and essential for the life. Many natural and engineering processes involve fluid flow. Fluids can be broadly characterized as Newtonian and non-Newtonian fluids based on their responses to an applied shear stress. Fluids that obey a linear relationship between shear stress and strain rate are called Newtonian fluids. Newtonian fluids usually have a simple molecular structure and many common fluids such as water and air can be considered as Newtonian fluids for practical purposes. However, non-Newtonian fluids are also common in natural and industrial processes. Non-Newtonian fluids are complex fluids involving complex microstructure such as toothpaste, saliva, mud and lava, polymer melts etc. In particular, the most of the biological fluids exhibit non-Newtonian behavior. These types of fluids can be found in various applications such as coating, tissue engineering, ink-jet printing, blood cells, polymer processing, oil recovery, to name a few. In these fluids, the stress has a non-linear relationship with the strain rate.

1.1 *Fluid Mechanical Preliminaries*

All fluid motion is governed by the conservation laws: the conservation of mass, linear and angular momentum and energy. When the flow is assumed to be incompressible, the mass and momentum conservation equations can be written as

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

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

where ρ , p , $\mathbf{u}$ and $\mathbf{T}$ denote the density of the fluid, the pressure, the velocity vector and the stress tensor, respectively. For a Newtonian fluid, the extra stress tensor is linearly

related to the rate of deformation tensor, i.e.,

$$\mathbf{T} = 2\mu\mathbf{D}, \quad (1.3)$$

where μ is the constant viscosity, and $\mathbf{D}$ is the rate of deformation tensor defined as

$$\mathbf{D} = \frac{1}{2}(\nabla\mathbf{u} + \nabla\mathbf{u}^T). \quad (1.4)$$

As mentioned above the non-Newtonian fluids have more complex relationship between the stress tensor and the rate of deformation.

1.2 Non-Newtonian Fluids

Non-Newtonian fluids have peculiar properties which are often surprising and different from those of Newtonian fluids. Here the behaviour of non-Newtonian fluids are described for a simple shear flow. In a shear flow, a non-Newtonian fluids have a nonlinear relationship between shear stress and the rate of strain [120]. The non-Newtonian fluids can be further subdivided into three classes: The shear thinning, shear thickening or dilatant, and yield-stress fluids. In the shear-thinning fluids, the apparent viscosity decreases with the rate strain. On the contrary, for the shear-thickening fluids, the viscosity increases with the shear-rate. The yield-stress fluids behave like an elastic solid until some critical (yield) stress and as a fluid above it. For some fluids, viscosity depends both on shear rate and duration of applied stress. For thixotropic fluids, material properties show time-dependent shear thinning property, i.e., viscosity decreases with time under constant shear stress. Whilst, some fluids exhibit anti-thixotropic (rheoplectic) behavior. In this kind of fluids, the viscosity increases or even can lead to solidification under a shear stress. 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.

1.2.1 Viscoelastic Fluids

The other type of non-Newtonian fluids is the viscoelastic fluid, which is main topic in this thesis. One important feature of viscoelastic fluids is the memory effect, i.e., it exhibits both viscous and elastic characteristics. Note that, the polymeric fluids are

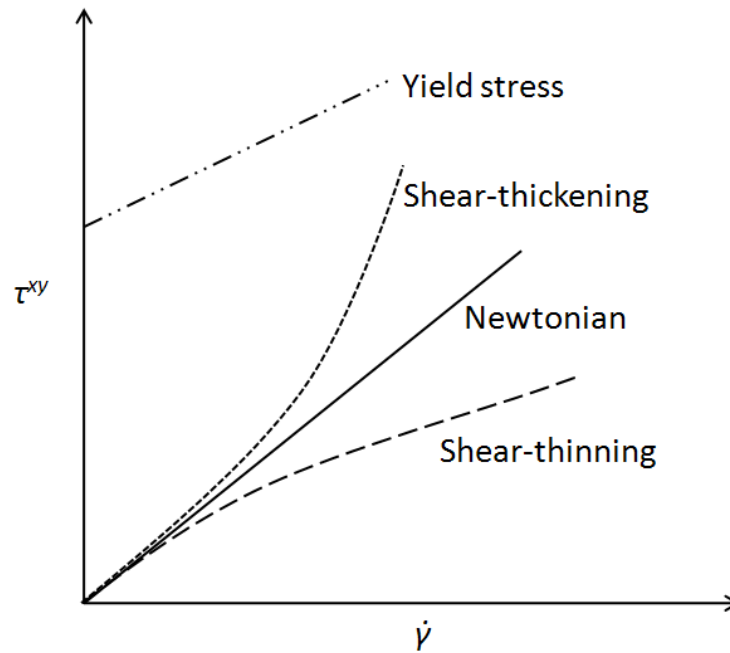


Figure 1.1: Classification of fluids.

also sometimes called as viscoelastic fluids since they are the most common industrial fluids exhibiting a viscoelastic behavior [14]. In addition to having non-Newtonian response to the rate of strain, the viscoelastic fluids also have non-zero normal stress differences. These non-zero normal stress differences are caused by the interaction of polymer molecules with 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 [60], the Weissenberg or rod climbing effect [45], die swell effect [120] and turbulence at low Reynolds number [48].

When a beaker with a fluid is spinned by a rotating disc on the surface, the direction of the secondary flow is found to be opposite for the Newtonian and the viscoelastic fluids [60]. For a Newtonian fluid, the flow is outwards due to inertia, whereas for a viscoelastic fluid, it is the opposite, as shown in Fig. 1.2. The normal stress differences

which oppose the inertia in the viscoelastic fluids are responsible for the reversal of the direction in the secondary flow.

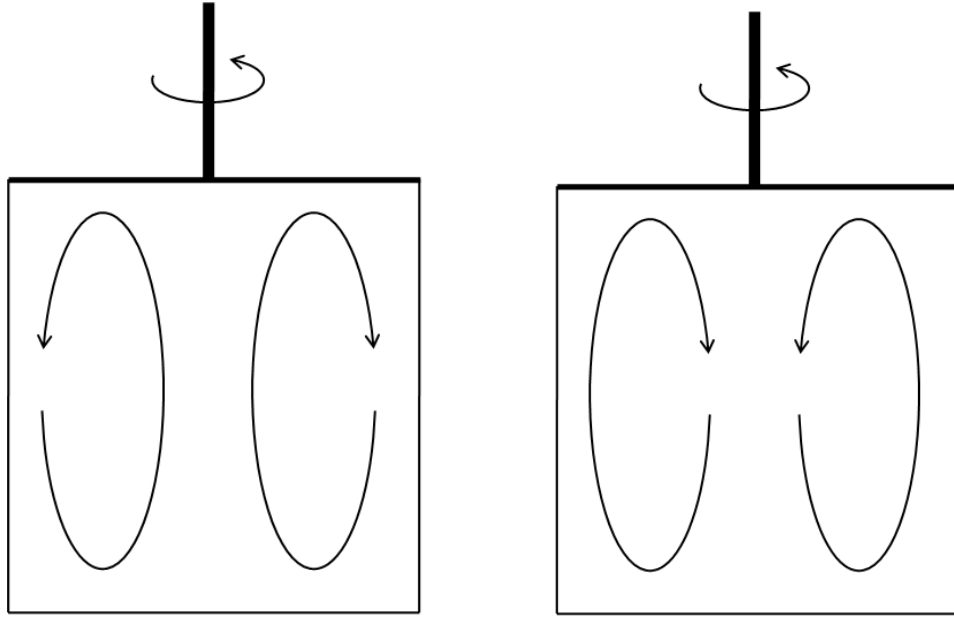


Figure 1.2: Secondary flow pattern in a Newtonian fluid (left) and a viscoelastic fluid (right).

Normal stress effects are also evident in the viscoelastic free surface flows. The Weissenberg effect [45] is well known phenomenon where the viscoelastic fluid climbs a rotating rod. When a rod is vertically placed and rotated in the beaker, Newtonian fluids rise on the walls of the beaker due to inertia while viscoelastic fluids climb the rotating rod due to normal stresses along the streamlines which prevails the centrifugal force as sketched in Fig. 1.3.

Another example of the normal stress effects is the die swell effect [120], it takes place when viscoelastic fluid is ejected from a tube (Fig. 1.4). At a low Reynolds number, the diameter of the viscoelastic extrudate increases twice or threefold of the capillary. This effect is more pronounced as the Reynolds number increases. A more detailed description and analysis of the phenomena mentioned above and other rheological phenomena can be found in Bird et al. [14] and Tanner [120].

Turbulent flows are ubiquitous in many engineering applications. Although turbu-

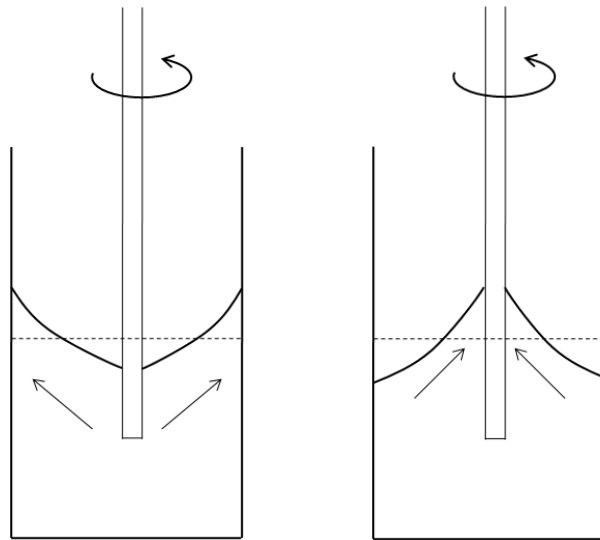


Figure 1.3: The Weissenberg effect in a viscoelastic fluid: Newtonian fluid (left) and a viscoelastic fluid (right) in the rotating rod experiment.

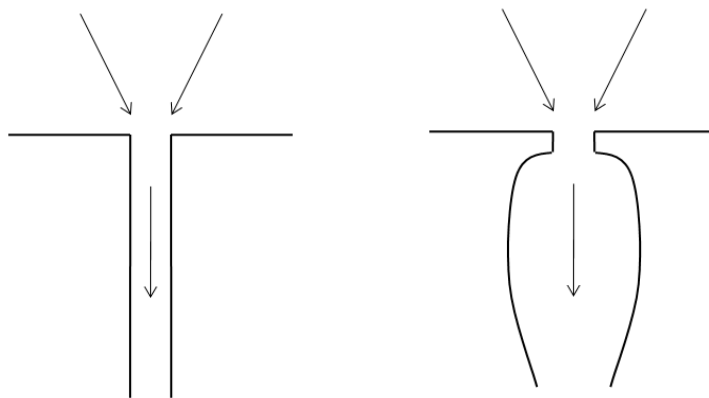


Figure 1.4: Schematic of the die swell effect: Newtonian (left) and viscoelastic fluid (right).

lence has been widely investigated since its discovery in 1880s, it has been not fully understood. Turbulence typically occurs at high Reynolds numbers as a result of instability of the laminar flows in Newtonian fluids. For instance, turbulence occurs at about $Re = 2000$ in a circular pipe flow. Groisman and Steinberg [48] have recently discovered that, in contrast to Newtonian fluids, viscoelastic fluids such as solutions of flexible long-chain polymers have nonlinear mechanical properties and the flow of a sufficiently elastic polymer solutions can become irregular even at an arbitrarily low Reynolds number, exhibiting a turbulent like chaotic behavior. The low Reynolds number or 'elastic' turbulence observed in polymer melts is accompanied by significant stretching of the polymer molecules, resulting in an increase in the elastic stresses of up to two orders of magnitude. This phenomena has a great promise in many applications particularly in mixing of liquids in microchannels.

Constitutive Relations

Development of rheological models have been a research topic for many decades. Different constitutive relationships between stress and strain have been developed since early works of Rivlin [108] and Oldroyd [96]. The generalized Newtonian fluid model has been designed so that it accounts for the shear thinning and shear thickening effects in a shear flow. This model has been mainly used to solve engineering problems for steady shear flows. However, the model is limited, as it does not predict the elastic effects and is not suited for extensional flows. The linear viscoelastic model involves the idea of memory and has been found to work well only up to medium strain rates and small displacement. As illustrated in Fig. 1.5, one dimensional Maxwell and Jeffrey models are examples of the linear viscoelastic models [37], consisting of combination of a spring and a dashpot. In this models, the spring and dashpot exhibit ideal elastic and purely viscous behavior, respectively. The retarded motion expansion method is derived by perturbation about the Newtonian solution, i.e., expanding in to a Taylor series about the Newtonian fluid [77]. It is suitable only for slightly elastic fluids and may not work for large velocity gradients cases.

The models described above are capable of describing only certain types of fluids due to their intrinsic limitations. To remedy these deficiencies, more sophisticated differential

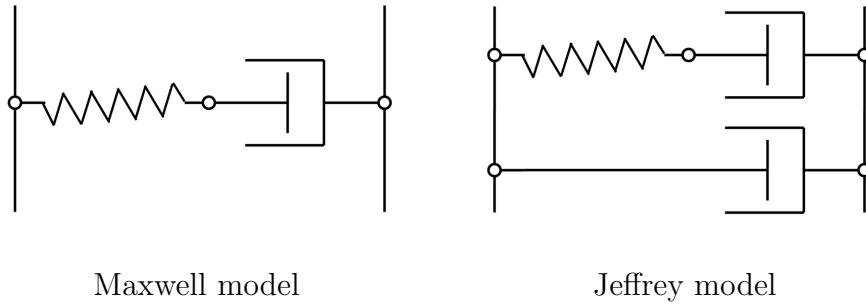


Figure 1.5: Representation of the Maxwell (left) and the Jeffrey (right) models with a spring (elastic behavior) and dashpot (viscous behavior).

models have been also designed for modelling of an arbitrary viscoelastic flow. Many of the differential constitutive models are derived from a kinetic theory of dilute polymer solutions. The polymer molecules are modelled as dumbbells having two beads connected by a massless spring as shown in Fig. 1.6. The interaction between the polymer molecules and the Newtonian fluid is modelled but the interaction among each other is ignored. The simplest models are the upper convected Maxwell model (UCM) and the Oldroyd-B model derived by Oldroyd [96]. Note that the UCM and Oldroyd-B models can be also derived by generalisation of the 1D Maxwell and Jeffrey models into a tensor formulations in 3D. Both models are appropriate for viscoelastic shear flows. However, in extensional viscoelastic flows, the dumbbells stretch infinitely thus having an unphysical singularity. To remove this deficiency, more sophisticated models have been developed by restricting the extensibility of the polymer chains. This kind of models is commonly known as the finitely extensible nonlinear elastic (FENE) type models. Such advanced models include the FENE-P model of Peterlin [102] and FENE-CR model of Chilcott and Rallison [25]. The FENE-P model captures the shear thinning effect. The Giesekus model [46] 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

$$\nabla \cdot \mathbf{u} = 0, \quad (1.5)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mu_s (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \nabla \cdot \boldsymbol{\tau}, \quad (1.6)$$

$$\boldsymbol{\tau} + \lambda \left(\frac{\partial \boldsymbol{\tau}}{\partial t} + \nabla \cdot (\mathbf{u} \boldsymbol{\tau}) - (\nabla \mathbf{u})^T \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \nabla \mathbf{u} \right) + \mathbf{f}(\boldsymbol{\tau}, \mathbf{D}) = 2\mu_p \mathbf{D}, \quad (1.7)$$

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

$$\mathbf{f}(\boldsymbol{\tau}, \mathbf{D}) = \begin{cases} 0 & \text{Oldroyd-B and UCM models} \\ \alpha \frac{\lambda}{\mu_p} \boldsymbol{\tau}^2 & \text{Giesekus model} \\ \epsilon \frac{\lambda}{\mu_p} \text{tr}(\boldsymbol{\tau}) \boldsymbol{\tau} + 2\xi \lambda (\mathbf{D} \boldsymbol{\tau} + \boldsymbol{\tau} \mathbf{D}) & \text{Phan-Thien Tanner (PTT) model,} \end{cases} \quad (1.8)$$

where α , ϵ and ξ are the model parameters. The FENE type models are considered in this thesis. The interested reader is referred to Owens and Phillips [99] for the details of these models and other constitutive equations.

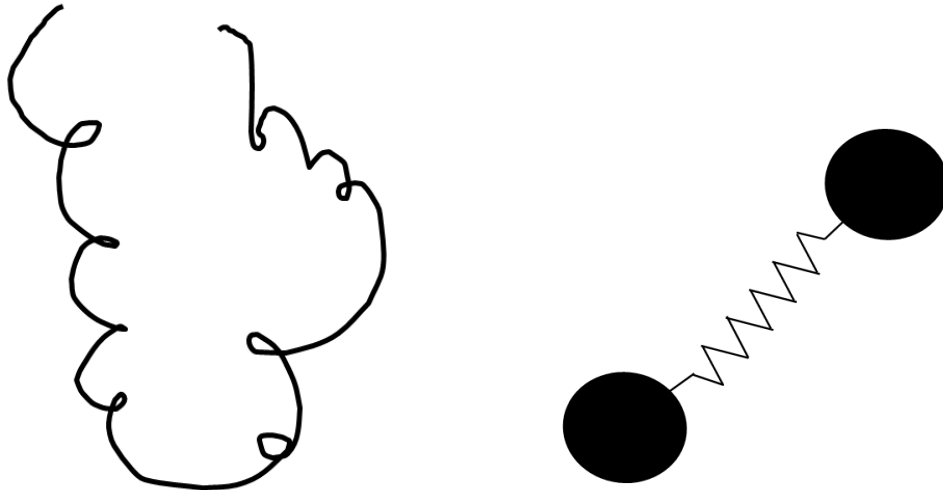


Figure 1.6: Modelling of polymer molecule (left) as a dumbbell (right).

Two-Phase Viscoelastic Systems

Many viscoelastic flows involve free surfaces with significant interfacial effects. Viscoelastic multiphase systems exhibit very rich dynamics mainly due to the strong interactions

between viscoelasticity and interfaces and thus pose a challenging problem for computational fluid dynamics. In particular, computational modeling of viscoelastic fluid flow is a difficult task due to the high Weissenberg number problem (The Weissenberg number is a non-dimensional measure of the fluid elasticity). This phenomenon causes computational methods to break down at low Weissenberg numbers. This stability problem is primarily caused by failure to properly approximate the exponential growth of viscoelastic stresses in regions of high shear rates. Various numerical approaches have been proposed to solve this phenomenon. The primary objective of the present work is to develop a stable finite-difference/front-tracking method for direct numerical simulation of viscoelastic two-phase flow systems. The method is designed to accommodate the generic family of viscoelastic model equations including the Oldroyd-B, FENE-CR and FENE-MCR. The convective terms in viscoelastic constitutive equations are approximated using a fifth-order upwinded WENO-Z schemes. The log-conformation method is employed to overcome high Weissenberg number problem.

1.3 Outline and Contribution of the Thesis

In Chapter 2, a front-tracking method is developed for direct numerical simulations of viscoelastic two-phase systems in which one or both phases could be viscoelastic. One set of governing equations is written for the whole computational domain and different phases are treated as a single fluid with variable material and rheological properties. The interface is tracked explicitly using a Lagrangian grid while the flow equations are solved on a fixed Eulerian grid. The surface tension is computed at the interface using the Lagrangian grid and included into the momentum equations as a body force. The Oldroyd-B, FENE-CR and FENE-MCR models are employed to model the viscoelasticity. The viscoelastic model equations are solved fully coupled with the flow equations within the front-tracking framework. A fifth-order WENO scheme is used to approximate the convective terms in the viscoelastic model equations and second-order central differences are used for all other spatial derivatives. A log-conformation method is employed to alleviate the high Weissenberg number problem (HWNP) and found to be stable and very robust for a wide range of Weissenberg numbers. The method has

been first validated for various benchmark single-phase and two-phase viscoelastic flow problems. The method has been demonstrated to be grid convergent with second-order spatial accuracy for all the cases considered in this paper.

In Chapter 3, two-phase viscoelastic systems are computationally studied in a pressure-driven flow with a sudden contraction and expansion using a finite-difference/front-tracking method. The effects of viscoelasticity in drop and bulk fluids are investigated including high Weissenberg and Reynolds number cases up to $Wi = 100$ and $Re = 100$. The FENE-CR model is used to account for the fluid viscoelasticity. Extensive computations are performed to examine drop dynamics for a wide range of parameters. It is found that viscoelasticity interacts with drop interface in a non-monotonic and complicated way, and the two-phase viscoelastic systems exhibit very rich dynamics especially in the expansion region. At high Re , the drop undergoes large deformation in the contraction region followed by strong shape oscillations in the downstream of the expansion. For a highly viscous drop, a re-entrant cavity develops in the contraction region at the trailing edge which, in certain cases, grows and eventually causes encapsulation of ambient fluid. The re-entrant cavity formation is initiated at the entrance of the contraction and is highly influenced by the viscoelasticity. Compared to the corresponding straight channel case, the effects of viscoelasticity are reversed in the constricted channel: Viscoelasticity in drop/continuous phase hinders/enhances formation of the re-entrant cavity and entrainment of ambient fluid into main drop. Encapsulation of ambient fluid into main droplet may be another route to produce a compound droplet in microfluidic applications.

In Chapter 4, the effects of viscoelasticity on drop impact and spreading on a flat solid surface are studied computationally using a finite-difference/front-tracking method. The FENE-CR model is used to account for the fluid viscoelasticity. It is found that viscoelasticity favors advancement of contact line during the spreading phase leading to a slight increase in the maximum spreading in agreement with the experimental observations of Huh et al. [64]. However, in contrast with the well-known anti-rebound effects of polymeric additives, the viscoelasticity is found to enhance the tendency of the drop rebound in the receding phase. These results suggest that the anti-rebound effects are mainly due to the polymer-induced modification of wetting properties of the substrate

rather than the change in the material properties of the drop fluid. A model is proposed to test this hypothesis. It is found that the model results in good qualitative agreement with the experimental observations and the anti-rebound behavior can be captured by the modification of surface wetting properties in the receding phase.

Finally, conclusions are drawn in Chapter 5.

Chapter 2

A FRONT-TRACKING METHOD FOR COMPUTATIONAL MODELING OF VISCOELASTIC TWO-PHASE FLOW SYSTEMS ¹

2.1 Introduction

Viscoelastic emulsions are ubiquitous in a wide range of engineering applications such as materials and food processing, pharmaceuticals, polymer blends and droplet-based microfluidics [121, 117]. In particular, almost all the particle-laden biological fluids in nature exhibit viscoelastic behavior. Therefore it is of crucial importance to understand the dynamics of an individual viscoelastic droplet in a viscoelastic or Newtonian medium [121].

Computational modeling of viscoelastic fluid flow is a difficult task mainly due to the large disparity in time scales especially at high Weissenberg numbers known as the high Weissenberg number problem (HWNP). The existence of a moving and deforming interface in two-phase systems makes the problem even more complicated and challenging. Viscoelasticity has been usually modeled based on the microstructure of dilute polymer solutions and expressed by various constitutive differential equations such as upper convected Maxwell (UCM)/Oldroyd-B [96], Giesekus [46] and finitely extensible nonlinear elastic (FENE-P [13], FENE-CR [25]) models for single and multiphase flow systems [121, 99]. Various numerical approaches have been proposed to solve these models coupled with the flow equations. However the conventional numerical algorithms usually failed to converge above a certain Weissenberg number limit [99]. This stability problem is primarily caused by the exponential growth of viscoelastic stresses in regions of high shear rates or near stagnation points [99]. The failure of the numerical meth-

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ods to properly approximate this exponential growth results in a numerical instability. Moreover this instability is pronounced if the positive definiteness of the conformation tensor is not preserved at the numerical solution level. The conformation tensor has a definite physical origin and interpretation stemming from the internal microstructure of polymer molecules in a continuum level [9] dictating the conformation tensor to be positive definite. Hulsen [65] proved that the conformation tensor must be initialized and remain positive definite for numerical stability. However, this condition can be violated in numerical approximations due to accumulation of numerical errors [99].

In a pioneering study, Keunings [72] observed failure of existing numerical methods at high Weissenberg numbers and attributed this failure to the inappropriate numerical methodologies. Since then, a number of stabilization approaches have been proposed to overcome the HWNP in viscoelastic flow simulations as recently discussed in details by Chen et al. [24]. Marchal and Crochet [80] developed one of the first successful numerical methods for simulations of viscoelastic flows at high Weissenberg numbers using upwind discretization of the convective terms in a mixed finite-element framework. Mompean and Deville [84] developed a finite-volume method and successfully performed simulations of Oldroyd-B fluid flow in a 3D planar contraction at high Weissenberg numbers. More recently, Fattal and Kupferman [41] developed the log-conformation method (LCM) based on reformulation of the constitutive equations using a logarithmic transformation of conformation tensor. The LCM has been shown to be stable and accurate at high Weissenberg numbers, i.e., as high as $Wi = 100$ [66]. This representation makes the problem more stable at numerical solution level since it preserves the positive definiteness of the conformation tensor and successfully captures sharp elastic stress layers. Sarkar and Schowalter [110] proposed a semi-analytical method (SAM) in which the exponential time variation is retained explicitly. In contrast with the LCM, the SAM does not require any eigen-decomposition so it has an advantage of having lower computation cost and implementation simplicity. However the positive definiteness of the conformation tensor is not preserved automatically in the SAM. Thus it may diverge at high Weissenberg numbers unless special treatments are done to guarantee the positive definiteness at numerical solution level. The SAM has been successfully used for two-phase viscoelastic flow simulations including shear [1, 85] and buoyancy-driven [86] flows. However we

found that, although the SAM is efficient at low or moderate Weissenberg numbers, it diverges when Weissenberg number exceeds a certain limit, i.e., $Wi > 2$, in simulating a viscoelastic droplet in a pressure-driven constricted channel. Therefore the SAM is used for low or moderate Weissenberg numbers while the LCM is employed at high Weissenberg numbers in the present study.

In spite of significant progress made for viscoelastic single-phase flow simulations, numerical methods have not yet reached maturity for simulating multiphase viscoelastic flows especially at high Weissenberg numbers. Tanner [119] performed a pioneering numerical study of die-swell problem using a Maxwell fluid model. Later Crochet and Keunings [33] simulated a circular and slit die-swell problem using the Oldroyd-B fluid model. Keunings and co-worker have also performed numerical simulations of various free-surface viscoelastic flows [19, 20, 72]. Kolte et al. [76] used a Lagrangian method to simulate the transient filament stretching rheometer. More recently various one-field formulations have been employed to perform direct numerical simulations of interfacial viscoelastic flows. Examples include the level-set [6, 103], the volume of fluid (VOF) [27, 53, 59], marker and cell [100, 125, 126], phase-field [18, 140, 149], the conservative semi-Lagrangian advection scheme of constrained interpolation profile method with rational function (CIP-CSLR) [44] and the front-tracking methods [30, 31, 110]. In addition, versions of the arbitrary Lagrangian-Eulerian (ALE) [28, 72, 132, 141, 142] and the Lagrangian [105, 137] methods have been also employed. Lind and Phillips [79] recently studied the effect of viscoelasticity on a rising gas bubble using a boundary element method. These methods have been used to investigate a wide range of interfacial viscoelastic flow problems including the jet buckling [16, 92, 126], extrudate swell [28, 125, 126], viscoelastic drop dynamics [30, 31, 85, 100] and the cross-slot flow [100], among others.

The front-tracking method developed by Unverdi and Tryggvason [130] has been widely used to examine many aspects of Newtonian interfacial flows [127, 88, 122, 89, 97, 91]. The method was extended to treat viscoelastic interfacial flows first by Sarkar and Schowalter [110] and has been successfully used to study viscoelastic drop dynamics in shear and buoyancy-driven flows [1, 85, 86, 87]. Sarkar and Schowalter [110] used the semi-analytical method that is limited to low or moderate Weissenberg numbers as

mentioned earlier. Chung et al. [30, 31] developed a finite-element/front-tracking method for simulation of viscoelastic interfacial flows in two-dimensional planar geometries using the log-conformation approach but the method is restricted to low Reynolds number (creeping) flows. This method has been successfully applied to study viscoelastic two-phase systems in a planar channel with a sudden constriction.

In the present study, a finite-difference/front-tracking method is developed for direct numerical simulation of viscoelastic two-phase flow systems including a Newtonian droplet in a viscoelastic medium (NV), a viscoelastic droplet in a Newtonian medium (VN) and a viscoelastic droplet in another viscoelastic medium (VV). Although the method is general and applicable to virtually any interfacial flow involving viscoelastic fluids, our main goal is to simulate the drop dynamics encountered or inspired by micro/bio-fluidic applications [122, 131, 146, 147]. The method is designed to accommodate the generic family of viscoelastic model equations including the Oldroyd-B, FENE-CR of Chilcott Rallison [25] and FENE-MCR of Coates et al. [23]. The convective terms in viscoelastic constitutive equations are approximated using a second-order ENO [55] and fifth-order upwinded WENO-Z [17] schemes. It is found that the WENO-Z scheme outperforms the ENO scheme in resolving thin high viscoelastic stress layers near the interface. All the other spatial derivatives are approximated using central differences on a staggered grid. Both the semi-analytical and log-conformation methods are employed to overcome high Weissenberg number problem. It is found that the SAM is computationally more efficient than the LCM but fails to achieve convergence at high Weissenberg numbers especially for the pressure-driven viscoelastic two-phase flows in constricted capillary tubes. On the other hand, the LCM successfully achieves convergence for much higher Weissenberg numbers, e.g., as high as $Wi = 100$ without any difficulty but with a higher computational cost and increased implementation complexity. The method has been first validated for two benchmark single-phase problems. The first problem deals with the start-up Poiseuille flow of an Oldroyd-B fluid in a circular capillary tube. For this case, the numerical results are found to be in excellent agreement with the analytical solution obtained by Waters and King [134] both for the transient and steady state cases. The second benchmark problem concerns with a pressure-driven single-phase FENE-MCR fluid flow through an abrupt 4:1 constricted pipe. The re-

sults are compared and found to be in good agreement with the computational results of Coates et al. [23]. Then the method is applied to simulate the motion and deformation of a buoyancy-driven droplet in viscoelastic two-phase systems moving through a capillary tube studied computationally by You et al. [142]. The results are found to be in good agreement with You et al. [142] especially when the WENO-Z scheme is used to discretize the convective terms in the viscoelastic model equations. Finally the method has been successfully applied to a more challenging case involving motion and deformation of a droplet in pressure-driven viscoelastic two-phase systems flowing through a capillary tube with a sudden contraction and expansion. This test case holds a great promise to be a benchmark problem for testing performance of numerical methods developed to simulate viscoelastic two-phase systems of practical interest. The present numerical algorithm has been found to be very robust and grid convergent with second-order spatial accuracy for all the cases considered in this paper.

The main contributions of the present work can be summarised as follows:

1. The front-tracking method is extended for simulations of viscoelastic interfacial flows with significant inertial effects at high Weissenberg numbers using the log-conformation approach.
2. A fifth-order WENO-Z scheme is used for convective terms of the viscoelastic model equation, and found to be instrumental for resolving thin viscoelastic stress boundary layers especially near the interface. Note that the usual second-order central differences are unstable while second-order ENO schemes are excessively dissipative.
3. The method is general and applicable to two-phase systems in which phases can be all Newtonian, Newtonian-viscoelastic and viscoelastic-viscoelastic. It can accommodate virtually any viscoelastic model for each phase. Moreover, the method is readily extendible for simulation of multiphase systems in which more than two-phases may exist.
4. To the best of our knowledge, it is the first time that the front-tracking method is applied to pressure-driven viscoelastic interfacial flows in axisymmetric geome-

tries with sudden contraction and expansion at finite Reynolds and Weissenberg numbers. The previous applications were restricted to 2D planar channels [30, 31, 59]. Moreover, simulations are performed for Newtonian-Newtonian, viscoelastic-Newtonian, Newtonian-viscoelastic and viscoelastic-viscoelastic cases.

The rest of this paper is organized as follows: In the next section, we briefly describe the governing equations including the constitutive models for viscoelasticity. The numerical method is presented in Section 3. The emphasis is placed on the numerical solution of viscoelastic model equations within the framework of the front-tracking method. The results are presented and discussed in Section 4. The method is first validated for single-phase and two-phase viscoelastic test problems, and then applied to viscoelastic two-phase systems in a pressure-driven flow through a circular pipe with a sudden contraction and expansion. Finally conclusions are drawn in Section 5.

2.2 Mathematical Formulation

The governing equations are described in the context of the finite difference/front tracking method. The flow is assumed to be incompressible. Following Unverdi and Tryggvason [130], a single set of governing equations can be written for the entire computational domain provided that the jumps in the material properties such as density, viscosity and relaxation time are taken into account and the effects of the interfacial surface tension are treated appropriately.

The continuity and momentum equations can be written as follows:

$$\nabla \cdot \mathbf{u} = 0, \quad (2.1)$$

$$\begin{aligned} \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot \mu_s (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \nabla \cdot \boldsymbol{\tau} + \Delta \rho g + \\ &\int_A \sigma \kappa \mathbf{n} \delta(\mathbf{x} - \mathbf{x}_f) dA, \end{aligned} \quad (2.2)$$

where μ_s , ρ , g , p , $\mathbf{u}$ and $\boldsymbol{\tau}$ denote the solvent viscosity and the density of the fluid, the gravitational acceleration, the pressure, the velocity vector and the extra stress tensor, respectively. The last term in Eq. (2.2) represents the body force due to surface tension where σ is the surface tension coefficient, κ is twice the mean curvature, and $\mathbf{n}$ is the unit vector normal to the interface, respectively. 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 points at which the equation is evaluated and a point at the interface, respectively.

The Oldroyd-B, FENE-CR and FENE-MCR models are adopted as the constitutive equations for the viscoelastic extra stresses. These models can be written in a generic transport equation form as

$$\frac{\lambda}{F} \left(\frac{\partial \mathbf{E}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{E}) - (\nabla \mathbf{u})^T \cdot \mathbf{E} - \mathbf{E} \cdot \nabla \mathbf{u} \right) + \mathbf{E} = \mathbf{S}, \quad (2.3)$$

where $\mathbf{E}$ can be extra stress or conformation tensor and $\mathbf{S}$ is a source term. In Eq. (2.3), F , $\mathbf{S}$ and $\boldsymbol{\tau}$ are specified in Table 2.1 for the three viscoelastic models considered in the present study. In this table, μ_p , λ , L , F , $\mathbf{I}$ and $\boldsymbol{\tau}$ are the polymeric viscosity, the

Table 2.1: Specification of the parameters F , $\mathbf{S}$ and $\boldsymbol{\tau}$ in Eq. (2.3).

Model	F	$\mathbf{S}$	$\boldsymbol{\tau}$
Oldroyd-B	1	$\mathbf{I}$	$\mu_p F (\mathbf{E} - \mathbf{I}) / \lambda$
FENE-CR	$L^2 / (L^2 - \text{trace}(\mathbf{E}))$	$\mathbf{I}$	$\mu_p F (\mathbf{E} - \mathbf{I}) / \lambda$
FENE-MCR	$(L^2 + \lambda \text{trace}(\mathbf{E}) / \mu_p) / (L^2 - 3)$	$\mu_p (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$	$\mathbf{E}$

relaxation time, the ratio of the length of a fully extended polymer dumbbell to its equilibrium length, the stretch function, the identity and extra stress tensors, respectively. The conformation tensor is then defined as

$$\mathbf{A} = \frac{\lambda}{\mu_p F} \boldsymbol{\tau} + \mathbf{I}. \quad (2.4)$$

It is also assumed that the material properties remain constant following a fluid particle, i.e.,

$$\frac{D\rho}{Dt} = 0; \frac{D\mu_s}{Dt} = 0; \frac{D\mu_p}{Dt} = 0; \frac{D\lambda}{Dt} = 0, \quad (2.5)$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$ is the material derivative. The density, polymeric and solvent viscosities, and the relaxation time vary discontinuously across the fluid interface and

are given by

$$\begin{aligned}\mu_p &= \mu_{p,i}I + \mu_{p,o}(1 - I); \mu_s = \mu_{s,i}I + \mu_{s,o}(1 - I); \\ \rho &= \rho_iI + \rho_o(1 - I); \lambda = \lambda_iI + \lambda_o(1 - I),\end{aligned}\tag{2.6}$$

where the subscripts i and o denote the properties of the drop and bulk fluids, respectively, and I is the indicator function defined such that it is unity inside the droplet and zero outside.

2.3 Numerical Method

The viscoelastic flow equations are solved using the front-tracking method developed by Unverdi and Tryggvason [130]. This method is based on a single-field formulation of the flow equations for the entire computational domain and treats different phases as a single fluid with variable material properties. The emphasis is placed on describing the new ingredients and essential features of the method as it is applied to two-phase viscoelastic systems and specifically to the numerical solution of the viscoelastic model equations within the front-tracking framework.

2.3.1 Front-Tracking Method

The interface between different phases is represented by separate, non-stationary computational marker points connected to form a Lagrangian grid that lies within a stationary Eulerian grid as sketched in Fig. 2.1. The marker points move with the local flow velocity interpolated from the neighboring Eulerian grid points. Each piece of the interface between two neighboring marker points is called an interface (or front) element. The surface tension force is first computed at the centroids of the front elements using a third-order Legendre polynomial fit through the end points of each element and the end points of the adjacent elements. These forces are then distributed on the neighboring staggered Eulerian grid points in a conservative manner and added to the discrete momentum equations as source terms in a similar way as discussed by Tryggvason et al. [127].

The front is also used to advect the discontinuous material property fields at each time step. First, the indicator function is computed. Based on the locations of the

interface marker points, unit magnitude jumps are distributed in a conservative manner on the Eulerian grid points near the interface and are then integrated to obtain the indicator function everywhere. This procedure involves solution of a separable Poisson equation on the Eulerian grid and yields a smooth transition of the indicator function across the interface. Once the indicator function distribution is determined, the material properties are set as a function of the indicator function according to Eq. (2.6).

As the interface evolves, it greatly deforms and stretches. Thus some front elements become too large resulting in a lack of resolution while some become too small resulting in formation of wiggles much smaller than the grid size. To maintain accuracy, the Lagrangian grid is restructured at every time step by deleting the front elements that are smaller than a prespecified lower limit and by splitting the front elements that are larger than a prespecified upper limit to keep the front element size nearly uniform and comparable to the Eulerian grid size. The curvature of the interface is accounted for using a third-order Legendre polynomial fit in deleting and adding a front element as described by Tryggvason et al. [127].

Information must be passed between the Lagrangian and Eulerian grids at each time step since the locations of the marker points do not necessarily coincide with the stationary Eulerian grid points. This is achieved by approximating the infinitely thin interface by a smooth distribution function that is used to distribute the interfacial surface tension forces computed on the interface over the Eulerian grid points near the interface and also to interpolate the velocity onto the locations of the marker points from the Eulerian grid. Thus the front is given a finite thickness comparable to the mesh size in order to maintain stability and smoothness. This also prevents numerical diffusion since this thickness remains constant for all time. The Peskin's cosine distribution function [101] is employed for this purpose and found to perform well.

The details of the front-tracking method can be found in the original paper by Unverdi and Tryggvason [130], the review paper by Tryggvason et al. [127] and the recent book by Tryggvason et al. [128].

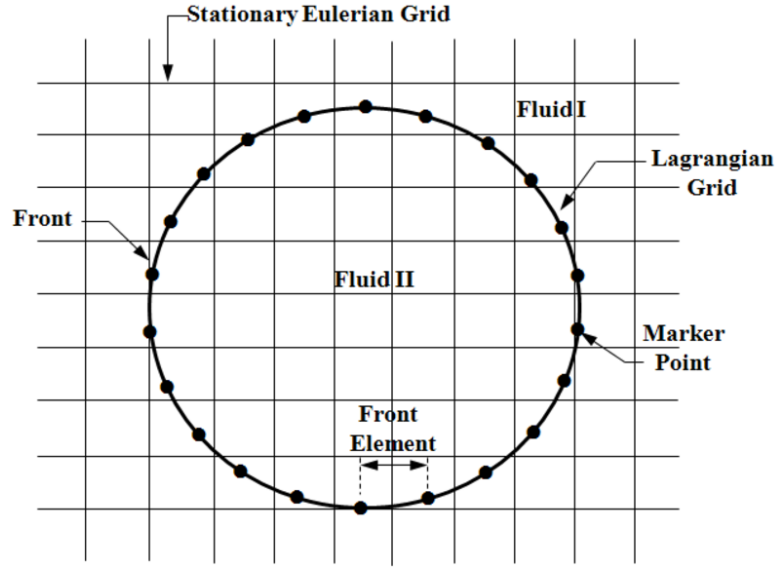


Figure 2.1: The Lagrangian and Eulerian grids used in computations. The flow equations are solved on the fixed Eulerian grid. The interface between different phases is represented by a Lagrangian grid consisting of connected marker points.

2.3.2 Flow Solver

The flow equations are solved using a projection method on a staggered fixed Eulerian non-uniform Cartesian grid in which the velocity nodes are located at the cell faces while the material properties, the pressure and the extra stresses are all located at the cell centers. The spatial derivatives are approximated using central differences and time integration is performed using the projection method developed by Chorin [29]. Although a second-order accuracy in time can be easily achieved using a predictor-corrector scheme [127], a very conventional first order scheme is employed and briefly described here for completeness. In advancing solutions from time level n to level $n + 1$, first the interface is advanced for a time step using an explicit Euler method and the density field is updated based on the new locations of the marker points to obtain ρ^{n+1} . Then the momentum equation is integrated in two steps. In the first step, the pressure

gradient is ignored and the unprojected velocity field is computed as

$$\frac{\rho^{n+1}\mathbf{u}^* - \rho^n\mathbf{u}^n}{\Delta t} = \left[-\nabla_h \cdot (\rho\mathbf{u}\mathbf{u}) + \nabla_h \cdot (\mu_s(\nabla_h\mathbf{u} + \nabla_h^T\mathbf{u})) + \Delta\rho g + \nabla \cdot \boldsymbol{\tau} + \int_A \sigma\kappa\mathbf{n}\delta(\mathbf{x} - \mathbf{x}_f)dA \right]^n, \quad (2.7)$$

where Δt is the time step, ∇_h is the discrete version of the nabla operator and $\mathbf{u}^*$ is the unprojected velocity vector. In the second step, the velocity field is corrected as

$$\frac{\rho^{n+1}\mathbf{u}^{n+1} - \rho^{n+1}\mathbf{u}^*}{\Delta t} = -\nabla_h p^{n+1}. \quad (2.8)$$

Taking divergence of Eq. (2.8) and using the incompressibility condition $\nabla_h \cdot \mathbf{u}^{n+1} = 0$, a non-separable Poisson equation is obtained for the pressure field in the form

$$\nabla_h \cdot \frac{1}{\rho^{n+1}} \nabla_h p^{n+1} = -\frac{1}{\Delta t} \nabla_h \cdot \mathbf{u}^*, \quad (2.9)$$

which is solved on the fixed Eulerian grid using a multigrid method as described by Tryggvason et al. [127].

2.3.3 Solution of the Viscoelastic Model Equations

Numerical solution of the viscoelastic constitutive equations is notoriously difficult especially in two-phase systems mainly due to the large disparity in time scales and discontinuous variation of viscoelastic properties across the interfaces. To overcome these difficulties, two approaches are adopted in the present study. In the first approach, a semi-analytical method (SAM) developed by Sarkar and Schowalter [110] is used and found to be effective for Weissenberg numbers up to order of unity. For larger Weissenberg numbers, the log-conformation method (LCM) developed by Fattal and Kupferman [41] is employed.

In the SAM, the viscoelastic constitutive equations (e.g., Eq. (2.3)) are first written as

$$\frac{\lambda}{F} \frac{\partial \mathbf{E}}{\partial t} + \mathbf{E} = \mathbf{K}(t), \quad (2.10)$$

where

$$\mathbf{K}(t) = \mathbf{S} - \frac{\lambda}{F} \left[\nabla \cdot (\mathbf{u}\mathbf{E}) - (\nabla\mathbf{u})^T \cdot \mathbf{E} - \mathbf{E} \cdot \nabla\mathbf{u} \right]. \quad (2.11)$$

Equation (2.10) is integrated from time level n to level $n + 1$ for a time step Δt to get

$$\mathbf{E}^{n+1} = \mathbf{E}^n e^{-\Delta t F/\lambda} + \mathbf{K}^n (1 - e^{-\Delta t F/\lambda}), \quad (2.12)$$

where $\mathbf{K}$ and F are assumed to remain constant during the integration. This scheme is equivalent to an explicit Euler method as $\Delta t \rightarrow 0$ and consistent everywhere (including the regions where $\lambda = 0$). The convective terms are approximated using a second-order ENO [55] or a fifth-order upwinded WENO-Z [17] scheme while central differences are used for all other spatial derivatives. In contrast with the LCM, the SAM does not automatically preserve positive definiteness of the conformation tensor. Thus the SAM becomes unstable at high Weissenberg numbers due to accumulation of numerical errors unless special treatments are done to ensure positive definiteness.

The LCM is used to overcome the well known high Weissenberg number problem (HWNP). In this approach, Eq. (2.3) is rewritten in terms of the logarithm of the conformation tensor through eigen-decomposition, i.e., $\Psi = \log \mathbf{A}$. This representation ensures the positive definiteness of the conformation tensor. The core feature of the formulation is the decomposition of the gradient of divergence free velocity field $\nabla \mathbf{u}^T$ into two anti-symmetric tensors denoted by Ω (pure rotation) and $\mathbf{N}$, and a symmetric tensor denoted by $\mathbf{C}$ which commutes with the conformation tensor [41], i.e.,

$$\nabla \mathbf{u}^T = \Omega + \mathbf{C} + \mathbf{N} \mathbf{A}^{-1}. \quad (2.13)$$

Inserting Eq. (2.13) into Eq. (2.3) and replacing the conformation tensor with the new variable Ψ , the transformed constitutive equations can be written as

$$\frac{\partial \Psi}{\partial t} + \nabla \cdot (\mathbf{u} \Psi) - (\Omega \Psi - \Psi \Omega) - 2\mathbf{C} = \frac{F}{\lambda} (e^{-\Psi} - \mathbf{I}). \quad (2.14)$$

This equation is integrated using an explicit Euler scheme, i.e.,

$$\Psi^{n+1} = \Psi^n + \Delta t \left(-\nabla \cdot (\mathbf{u} \Psi) + (\Omega \Psi - \Psi \Omega) + 2\mathbf{C} + \frac{F}{\lambda} (e^{-\Psi} - \mathbf{I}) \right)^n, \quad (2.15)$$

where the spatial derivatives are again approximated using central differences except for the convective terms for which a second-order ENO [55] or a fifth-order upwinded WENO-Z [17] scheme is employed. The conformation tensor is then obtained using the inverse transformation as $\mathbf{A} = e^{\Psi}$.

When the log-conformation method is used in the straightforward one-field formulation framework as described above, numerical difficulties arise at the viscoelastic/Newtonian interface since Eq. (2.15) becomes singular as $\lambda \rightarrow 0$ on the Newtonian side. To circumvent this problem, a simple procedure is employed here and found to be very robust. In this approach, the viscoelastic model equations are solved only in the viscoelastic region identified by the indicator function that is slightly truncated to avoid the singularity. For instance, the viscoelastic model equations are solved in the region where $I \geq \epsilon_I$ and $I \leq 1 - \epsilon_I$ for the VN and NV cases, respectively, and the viscoelastic stresses are set to zero otherwise. Since the viscoelastic stresses are zero in the Newtonian region, the conformation tensor equals to the identity tensor, (i.e., $\mathbf{A} = \mathbf{I}$) and $\Psi = 0$ there. The cut off parameter ϵ_I is used to avoid the singularity on the Newtonian side and set to $\epsilon_I = 0.005$ in the present study. Note that the results are found to be insensitive to the value of the cut off parameter as long as $\epsilon_I < 0.01$.

2.4 Results and Discussion

2.4.1 Single-Phase Flow

The method is first validated for viscoelastic single-phase flows. For this purpose, two test cases are considered. The first test case concerns with the start-up Poiseuille flow of an Oldroyd-B fluid in a circular pipe of radius R . The flow is assumed to be axisymmetric so a cylindrical coordinate system is adopted with z representing the axial direction aligned with the pipe axis and r the radial direction. Waters and King [134] studied this problem and provided analytical solutions both for the transient and steady-state cases. Thus it serves an ideal test case for validation of the present numerical method. In this problem, the fluid is initially at rest and set into motion by a constant applied pressure gradient $G = -\frac{dp}{dz} = \text{const.}$ in the axial direction. No-slip and periodic boundary conditions are applied at the pipe wall and in the axial direction, respectively. Following dimensionless variables are introduced:

$$R^* = \frac{r}{R}; T = \frac{t}{\lambda}; V = \frac{v_z}{v_0}; \beta = \frac{\mu_s}{\mu_0}; Re = \frac{\rho v_0 R}{\mu_0}; Wi = \frac{\lambda v_0}{R}, \quad (2.16)$$

where v_z is the axial velocity and $\mu_0 = \mu_s + \mu_p$ is the total viscosity. In Eq. (2.16), the velocity scale v_0 is defined as $v_0 = -\frac{R^2}{8\mu_0} \frac{dp}{dz}$. Computations are performed on a uniform

grid with grid size $\Delta r = R/128$ for three different Weissenberg numbers, i.e., $Wi = 1, 10$ and 100 . The other dimensionless parameters are kept constant at $Re = 1$ and $\beta = 0.1$. Figure 2.2a shows the velocity profiles at various dimensionless times for $Wi = 10$. The evolution of the centerline velocity is plotted in Fig. 2.2b for $Wi = 1, 10$ and 100 . As can be seen in these figures, there is excellent agreement between the computational and analytical results indicating the accurate solution of the viscoelastic model equations. Note that, although not shown here due to space consideration, the steady state results of the viscoelastic stresses and velocity are also found to be in good agreement with the analytical solutions.

The second test case deals with a single-phase viscoelastic fluid flow through an abrupt axisymmetric 4:1 contraction. This flow has been widely used as a benchmark problem for validation of computational methods, see e.g., Owens and Phillips [99]. The FENE-MCR model is employed here to facilitate comparison of the present results with Coates et al. [23]. The semi-analytical method is used for this test problem. The channel consists of two circular tubes. The fluid passes from the larger channel of radius R_1 into the narrower channel of radius R_2 . The relevant dimensionless parameters are the viscosity ratio $\beta = \mu_s/\mu_0$, the Reynolds number $Re = \rho U R_2/\mu_0$ and the Weissenberg number $Wi = \lambda U/R_2$, where $\mu_0 = \mu_s + \mu_p$ is the total viscosity and U is the average velocity in the narrow channel. The present results are compared with the computational simulations of Coates et al. [23]. For this purpose, the streamline patterns are shown in Fig. 2.3 in the vicinity of the constriction for two different Weissenberg numbers. As can be seen in the figure, the present results are overall in good agreement with those of Coates et al. [23], i.e., the vortex stretches towards the reentrant corner and grows in upstream direction with increasing Weissenberg number and the vortex lengths compare well in both simulations. Although not included in the paper, there is also good quantitative agreement between the present simulations and the results of Coates et al. [23] for all flow quantities including the mean velocity and the extra stress components.

2.4.2 Multiphase Flow

After validating the numerical algorithm for the benchmark single-phase viscoelastic flows, the method is now applied to study two-phase viscoelastic flow systems. For

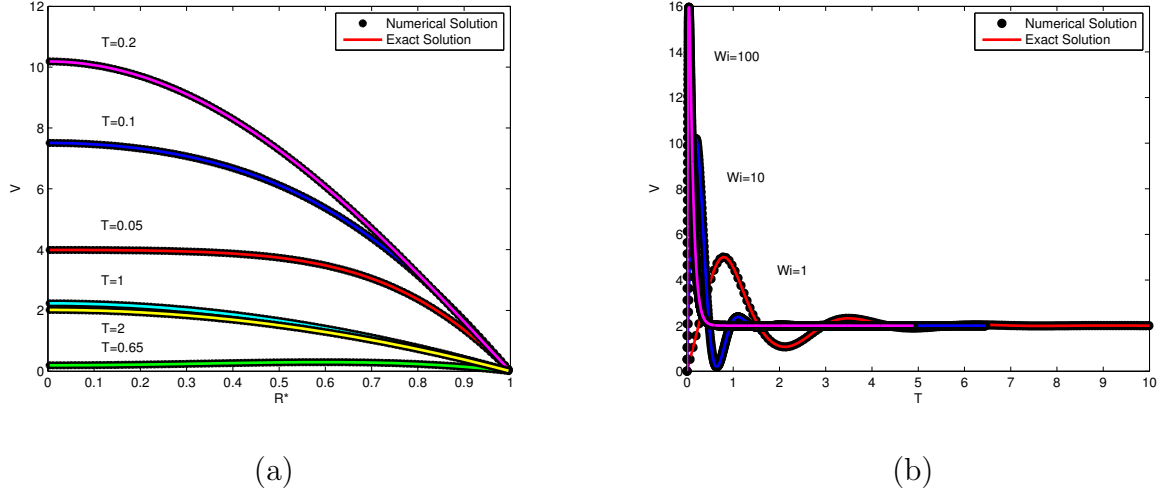


Figure 2.2: The start-up Poiseuille flow: (a) The velocity profiles at different non-dimensional times for $Wi = 10$. (b) The evolution of centerline velocity for $Wi = 1, 10$ and 100 . The symbols represent the computational results and the solid lines are the analytical solution of Waters and King [134].

this purpose, the method is first validated for the buoyancy-driven viscoelastic droplet systems studied computationally by You et al. [142]. Then the performance of the numerical method is demonstrated for a more challenging two-phase viscoelastic flow system involving the motion and deformation of a droplet in a pressure-driven constricted channel.

Buoyancy-Driven Viscoelastic Two-Phase Systems in a Capillary Tube

You et al. [142] considered buoyancy-driven droplet systems in which either the droplet or the bulk fluid could be viscoelastic. In addition to these two flow systems, we also consider the case in which both the phases are viscoelastic with different rheological properties. The FENE-CR model is employed in the present simulations to facilitate direct comparison with the results of You et al. [142]. The physical problem is shown schematically in Fig. 3.1. The tube has a diameter of $1.4d_d$ and a length of $6.5d_d$, and are closed at both ends. A spherical droplet of diameter d_d is initially located at the centerline of the tube with a $1.5d_d$ distance from the bottom wall. Flow is assumed to be axisymmetric and no-slip boundary conditions are applied at the walls. For the

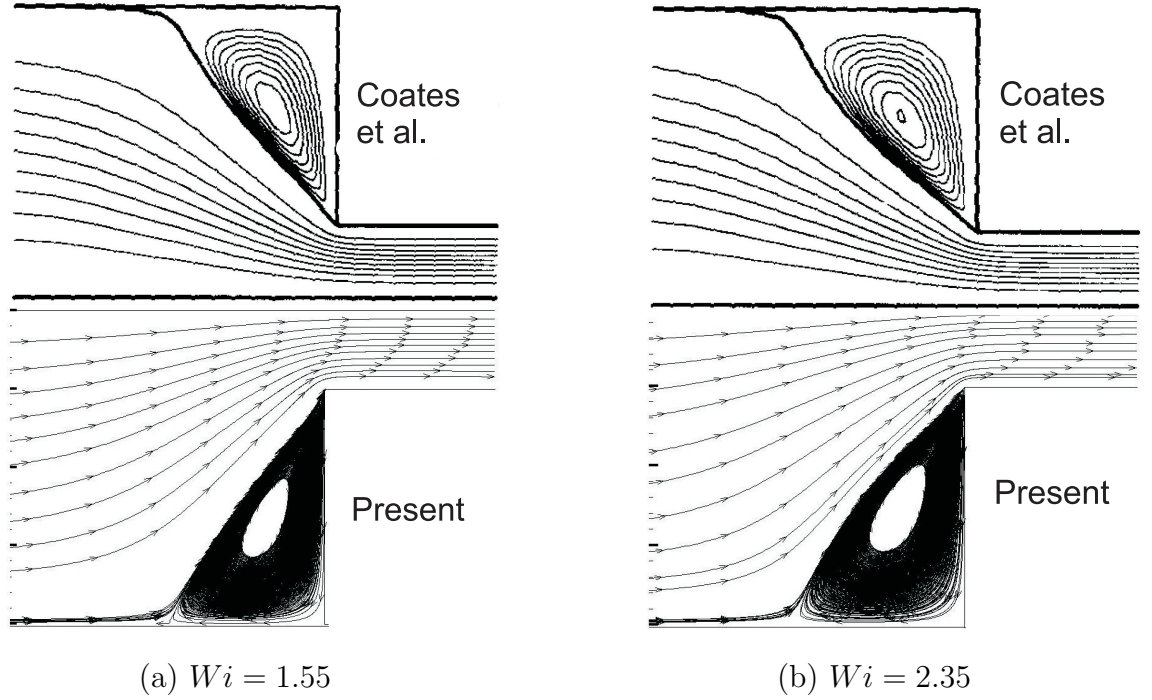


Figure 2.3: The vortices computed in the corner of the 4:1 contraction using the FENE-MCR model. (a) $Wi = 1.55$ and (b) $Wi = 2.35$. The present results (bottom portion) are compared with the results of Coates et al. [23] (top portion). ($Re = 0.1$, $\beta = 0.01$, and Grid: 128×320)

conformation tensor, the Neumann and axisymmetric boundary conditions are applied on the walls and at the centerline, respectively. The droplet starts moving due to buoyancy from rest in an otherwise quiescent ambient fluid. Following You et al. [142], the non-dimensional parameters are defined as follows:

$$\begin{aligned}
 Re &= \frac{\rho V^* d_d}{\mu_s}; Ca = \frac{\mu_s V^*}{\sigma}; Wi = \frac{\lambda V^*}{d_d}; \\
 \theta &= \frac{\mu_{s,i}}{\mu_{s,o}}; \alpha = \frac{\rho_i}{\rho_o}; k = \frac{\lambda_i}{\lambda_o},
 \end{aligned} \tag{2.17}$$

where Re , Ca , and Wi represent the Reynolds, capillary and Weissenberg numbers, respectively. In Eq. (2.17), the velocity scale is defined as $V^* = (\rho_o - \rho_i)gd_d^2/\mu_s$ where g is the gravitational acceleration. The other parameters θ , α and k denote the solvent viscosity, the density and the relaxation time ratios, respectively. Unless specified otherwise, the viscosity and density ratios are fixed at $\theta = 0.5$, $\beta = 0.77$, and $\alpha = 0.5$ for the results presented in this section. The computations are performed using dimensional

quantities but the results are made dimensionless with the length scale d_d and time scale $t^* = d_d/V^*$. Note that You et al. [142] defined a slightly different conformation tensor that is related to $\mathbf{A}$ as $\mathbf{B} = \mathbf{A} - \mathbf{I}$.

Extensive computations are performed to examine the effects of the viscoelasticity on drop mobility and deformation. The viscoelastic constitutive equations are solved using the semi-analytical method. The computational domain is resolved by a 128×1184 grid. The constant contours of the components of the conformation tensor are plotted in Figs. 2.5 and 2.6 in the vicinity of the droplet in a steady motion for a viscoelastic droplet in a Newtonian medium (VN) and a Newtonian droplet in a viscoelastic medium (NV), respectively, together with the computational results of You et al. [142]. These figures show that a Newtonian drop immersed in a viscoelastic fluid experiences an extending trailing edge while a viscoelastic drop in a Newtonian fluid develops an indentation around the rear stagnation point. Moreover, in both cases, there is a thin layer at the interface in the leading and trailing edges of the droplet where the viscoelastic stress concentration occurs with a sharp gradient due to large polymer extensions. These results are overall in good qualitative and quantitative agreement with the computational simulations of You et al. [142]. The slight difference in the maximum magnitudes of some components of the conformation tensor between the present results and the results of You et al. [142] is mainly attributed to the lack of resolution of the thin viscoelastic layer at the interface in the present simulations. Note that You et al. [142] used a separate body-fitted curvilinear grid for each phase. Therefore they were able to greatly stretch the grids near the interface resulting in a good resolution of the thin viscoelastic layers there for these particular flow systems. The terminal velocities of the VN and NV systems are shown in Fig. 2.7 where the steady drop shapes are also plotted. The terminal velocity is slightly under predicted for the VN system while it is over predicted for the NV system. However, the steady drop shapes are in good agreement with those of You et al. [142]. Further simulations are also performed to examine dynamics of a buoyancy-driven viscoelastic droplet immersed in another viscoelastic medium for a wide range of elasticity ratio $k = \lambda_i/\lambda_o$. Two sample results are shown in Fig. 2.8 for $k = 0.2$ and $k = 5$ to demonstrate the ability of the present method for simulation of viscoelastic-viscoelastic two-phase systems. As can be seen in this figure, $k = 0.2$ case

resembles the NV system while $k = 5$ resembles the VN system.

The properties of the numerical algorithm are also examined for this test case. For this purpose, first the second-order ENO and the fifth-order upwinded WENO-Z schemes are compared for the VN and NV systems in Fig. 2.9. Considering the results of You et al. [142] shown in Figs. 2.5 and 2.6, Fig. 2.9 clearly demonstrates that the WENO-Z scheme outperforms the ENO scheme in resolving the thin viscoelastic layer at the interface. The WENO-Z scheme is particularly successful for the VN case providing a comparable resolution with the results of You et al. [142] whereas the ENO scheme results in about 40% under prediction in terms of the maximum magnitude of $B_{\theta\theta}$ and B_{rr} on the same grid. It is also emphasized here that the extra stress boundary conditions are more easily implemented for the VN case since the viscoelasticity is essentially confined in the flow domain far from the tube walls. Then the consistency of the semi-analytical and log-conformation methods is examined. The semi-analytical and log conformation methods are mathematically identical so they must be consistent at the numerical solution level within the spatial and temporal discretization errors. This is verified in Fig. 2.10 where the constant contours of $B_{\theta\theta}$ and B_{zz} obtained by the two methods are compared. As can be seen from this figure, both methods yield essentially the same results indicating good consistency of two approaches. We also note that, although not shown here, both methods have been comprehensively compared for a wide range of flow conditions and found to be in excellent agreement for all the cases. It is worth stressing that no HWNP related instability has been observed for this buoyancy-driven flow case when the SAM is employed even for very high Weissenberg numbers, i.e., as high as $Wi = 1000$.

It is well known that the vanishing solvent viscosity poses a significant challenge for most numerical methods and often leads to numerical instabilities [4] mainly due to the loss of the elliptic nature of the governing equations as $\mu_s \rightarrow 0$. The performance of the present numerical method is examined through extensive simulations for a range of solvent viscosity ratios (β) while keeping the other parameters fixed. For this purpose, the solvent viscosity ratio is varied in the range $\beta = 0.1$ and $\beta = 10^{-4}$ by successively increasing the polymeric viscosity and reducing solvent viscosity such that the total viscosity remains the same. The steady drop shapes and corresponding constant contours of $\text{trace}(\mathbf{B})$ are shown in Figs. 2.11 and 2.12 for the VN and NV systems, respectively.

Note that the results for $\beta = 10^{-4}$ case are not shown in Figs. 2.11 and 2.12 since the effects of β become negligible after $\beta < 0.01$ and thus the results of $\beta = 10^{-3}$ and $\beta = 10^{-4}$ cases are indistinguishable for both NV and VN cases. It is found that the present method remains very robust even for $\beta = 10^{-4}$ case without any sign of instability. As β decreases, the viscoelastic stresses grow and can dominate over the surface tension. In the VN case, when β is reduced below a threshold value, the surface tension cannot balance the viscoelastic stresses anymore and the dimple created at the trailing edge penetrates through the droplet and eventually forms a toroidal shape as seen in Fig. 2.11. Similar drop deformation was also observed by Mukherjee and Sarkar [86] for a viscoelastic drop falling through a viscous medium. It is also interesting to observe that the droplet mobility increases and the terminal velocity becomes more oscillatory for smaller β values as shown in Fig. 2.13. These results are consistent with the results of Pillapakam et al. [104] and Lind and Phillips [79]. We finally note that, in the NV case, the increased viscoelastic stresses sharpen the trailing edge of the droplet as β decreases as seen in Fig. 2.12.

Finally the spatial and temporal accuracy of the numerical method is examined for the VN case. In the present method, the numerical error can be generally decomposed into spatial and time-stepping errors. First, computations are performed using various grid resolutions ranging between 32×296 and 128×1184 to show the overall dependence of the numerical results on grid refinement. The terminal velocity is plotted against the non-dimensional time in Fig. 2.14a while $\text{trace}(\mathbf{B})$ is computed at the drop centerline and plotted against the local vertical position of drop measured from the trailing edge in Fig. 2.15a. As can be seen in these figures, differences between successive grid resolutions decrease as grid is refined indicating grid convergence. Furthermore, the terminal velocity and $\text{trace}(\mathbf{B})$ are plotted in Fig. 2.14b and 2.15b, respectively, as a function of square of non-dimensional grid size. The approximate linear relation indicates expected second-order spatial accuracy of the method. Figure 2.14b also shows that a 64×592 grid is sufficient to reduce the maximum spatial error in terminal velocity below 1%. However, much finer grid is required to resolve the thin viscoelastic stress boundary layer near the interface. For instance, even the finest grid can reduce the spatial error only below 4% for $\text{trace}(\mathbf{B})$ at the leading edge stagnation point.

Since the present numerical method is explicit, the time step is strictly restricted by the stability conditions so the time stepping error is expected to be small compared to the spatial error. To check this, simulations are performed for various time steps using a 64×592 grid. The results are shown in Fig. 2.16 where the non-dimensional axial coordinate of droplet centroid is plotted against the non-dimensional time (Fig. 2.16a) and $\text{trace}(\mathbf{B})$ is plotted along the droplet centerline in steady motion (Fig. 2.16b) for various time steps. As can be seen in this figure, the temporal error is negligible even for the maximum time step allowed by the stability constraints.

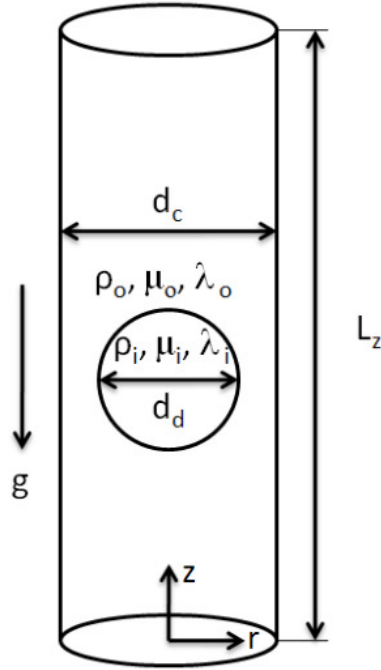


Figure 2.4: Schematic illustration of a buoyancy-driven viscoelastic two-phase system.

Pressure-Driven Viscoelastic Two-Phase Systems in a Capillary Tube with Sudden Contraction and Expansion

The method is finally applied to study the viscoelastic two-phase systems in a capillary tube with a sudden contraction and expansion. A viscoelastic droplet in a Newtonian medium (VN), a Newtonian droplet in a viscoelastic medium (NV) and a viscoelastic droplet in another viscoelastic medium (VV) cases are considered. In addition to the

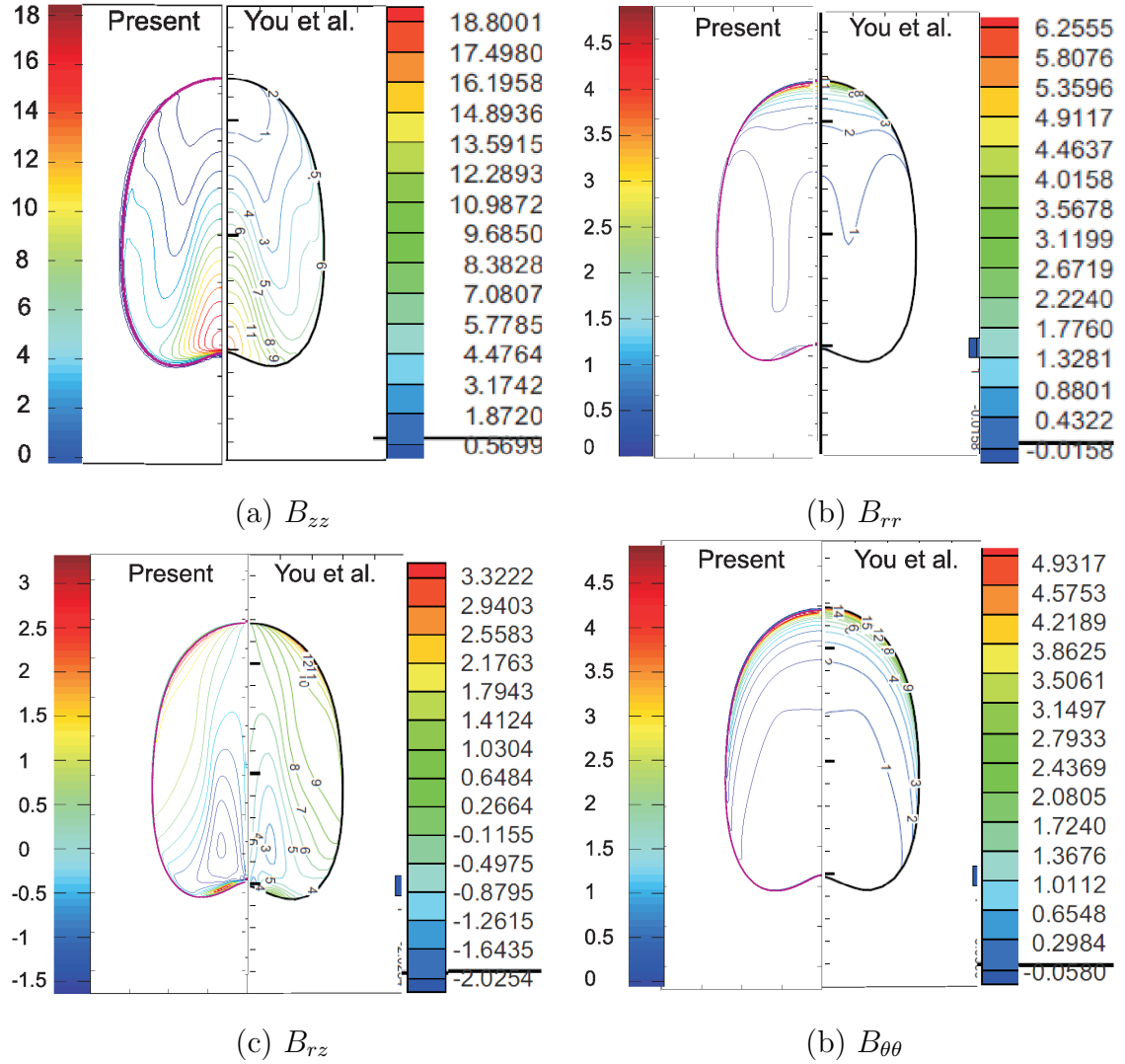


Figure 2.5: The steady droplet shapes and the constant contours of the conformation tensor $\mathbf{B}$ for a buoyancy-driven FENE-CR droplet rising in a Newtonian fluid. The present results (left portion) are compared with the results of You et al. [142] (right portion). ($Re = 10, Ca = 50, Wi = 50, Grid : 128 \times 1184$).

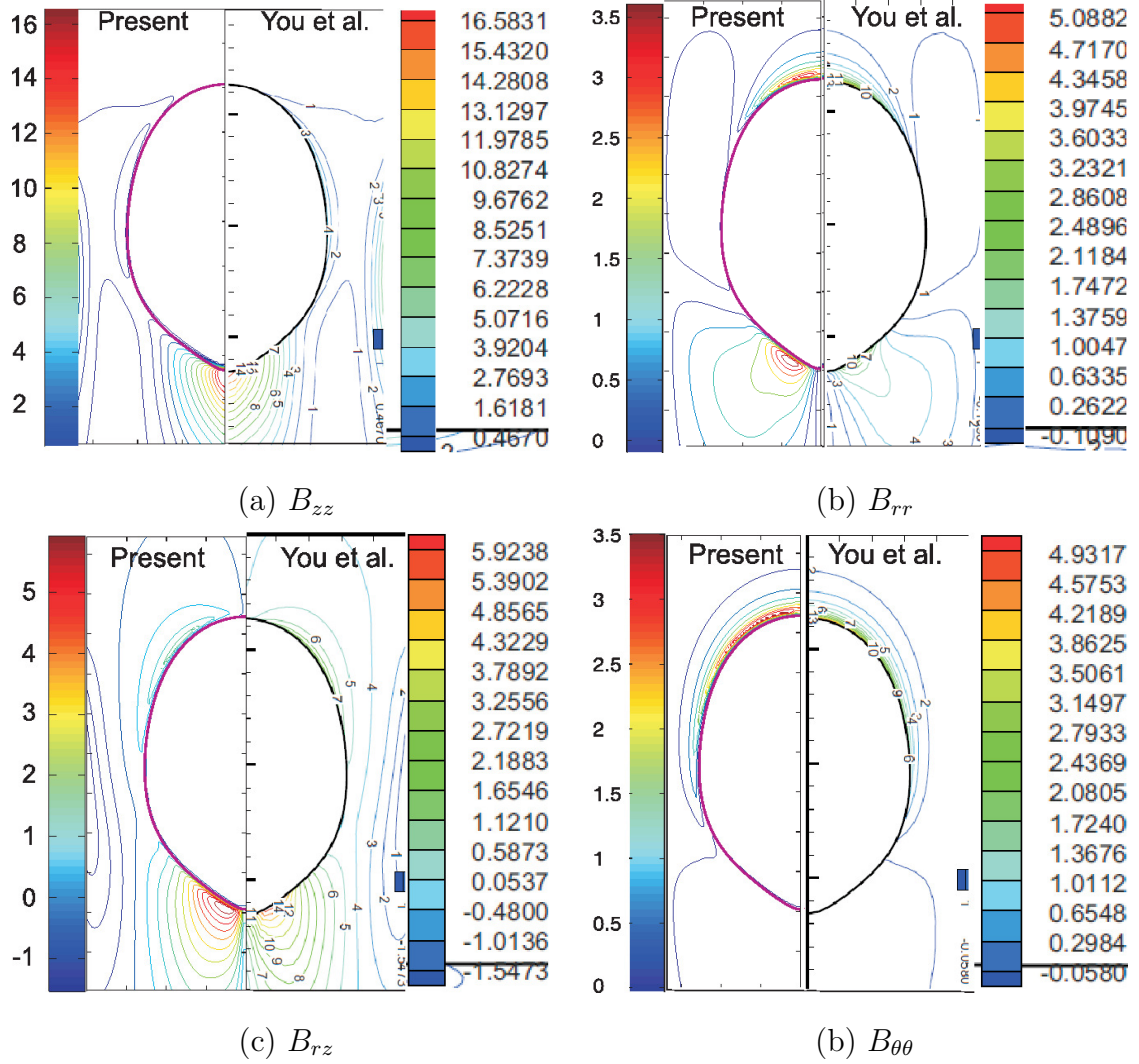


Figure 2.6: The steady droplet shapes and the constant contours of the conformation tensor $\mathbf{B}$ for a buoyancy-driven Newtonian droplet rising in a FENE-CR fluid. The present results (left portion) are compared with the results of You et al. [142] (right portion). ($Re = 10, Ca = 20, Wi = 50, Grid : 128 \times 1184$).

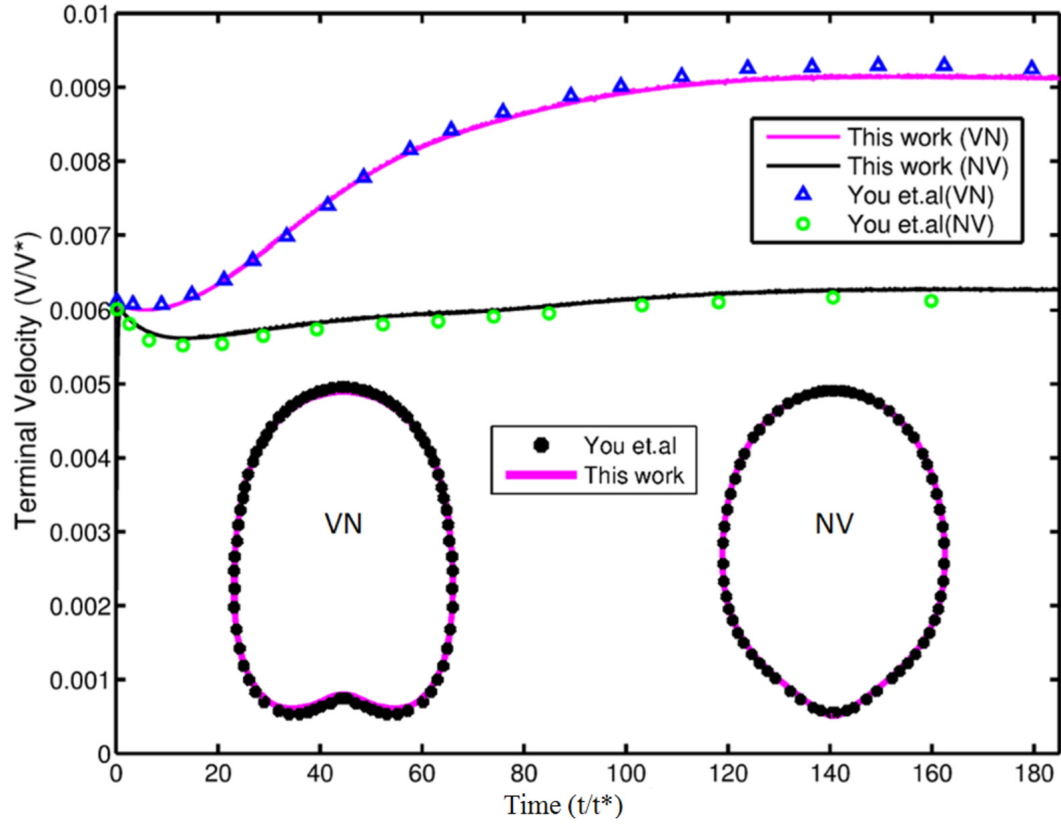


Figure 2.7: The terminal velocity versus the non-dimensional time for a droplet in the VN and NV systems, and their respective steady shapes. Solid lines are the present results and the symbols are the results of You et al. [142]. The results are obtained using a 128×1184 grid. (VN case: $Re = 10, Ca = 50, Wi = 50$; NV case: $Re = 10, Ca = 10, Wi = 100$).

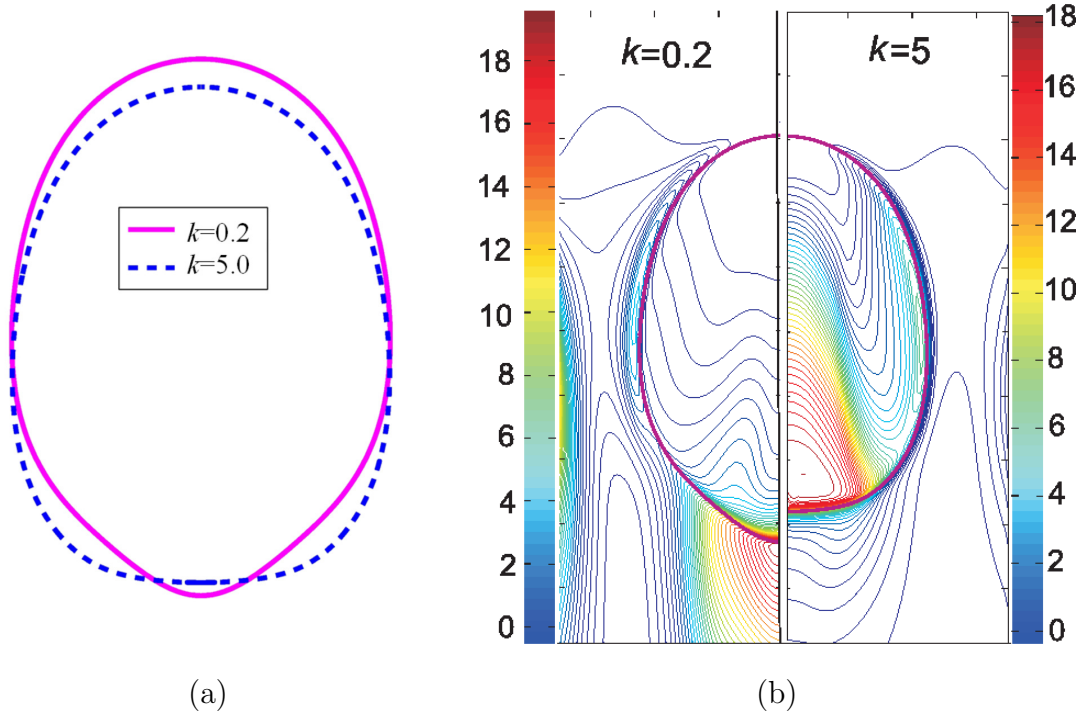


Figure 2.8: A buoyancy-driven FENE-CR droplet rising in another FENE-CR fluid for $k = 0.2$, $Wi_i = 20$ and $Wi_o = 100$ and for $k = 5$, $Wi_i = 100$ and $Wi_o = 20$. (a) The steady shapes, and (b) the constant contours of the conformation tensor component B_{zz} . ($Re = 10$, $Ca = 20$, $Grid : 64 \times 592$).

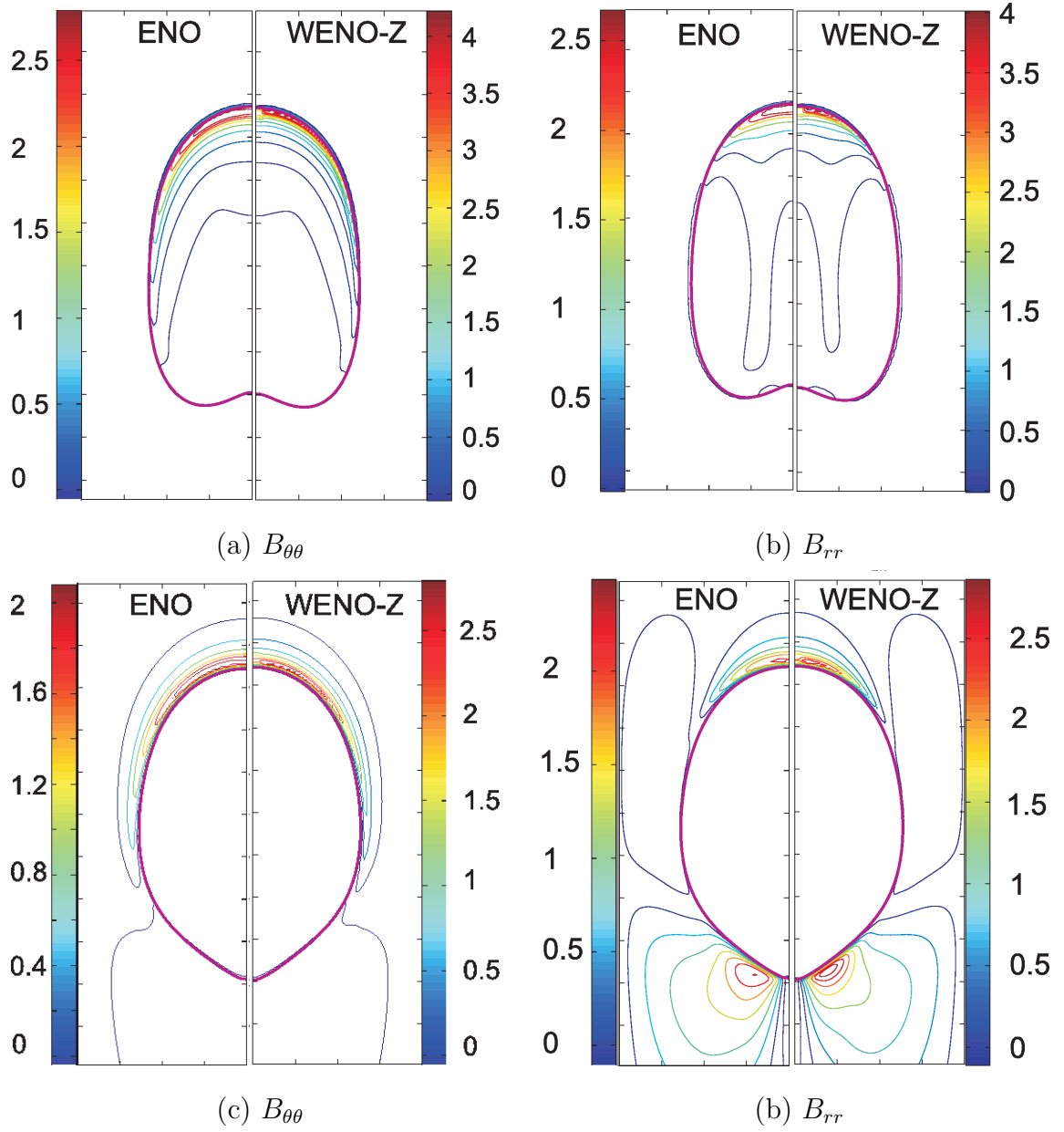


Figure 2.9: The second-order ENO versus the fifth-order upwind WENO-Z schemes. The constant contours of the conformation tensor components $B_{\theta\theta}$ and B_{rr} for VN and NV cases. (VN case: $Re = 10$, $Ca = 50$, $Wi = 50$; NV case: $Re = 10$, $Ca = 20$ and $Wi = 50$; Grid: 64×592).

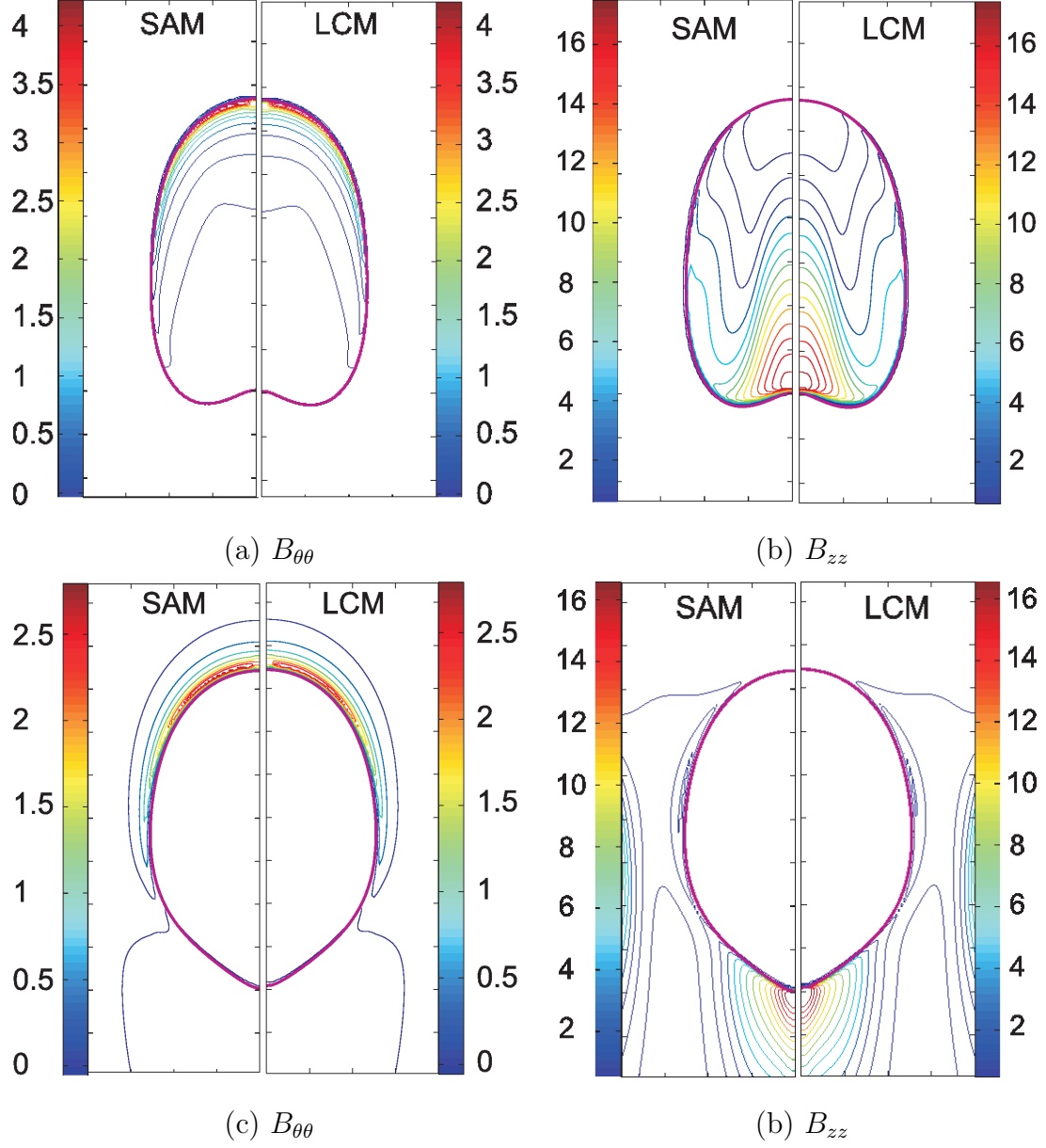


Figure 2.10: The semi-analytical method (SAM) versus the log-conformation method (LCM). The constant contours of the conformation tensor components $B_{\theta\theta}$ and B_{zz} for VN and NV cases. (VN case: $Re = 10$, $Ca = 50$, $Wi = 50$; NV case: $Re = 10$, $Ca = 20$ and $Wi = 50$; Grid: 64×592).

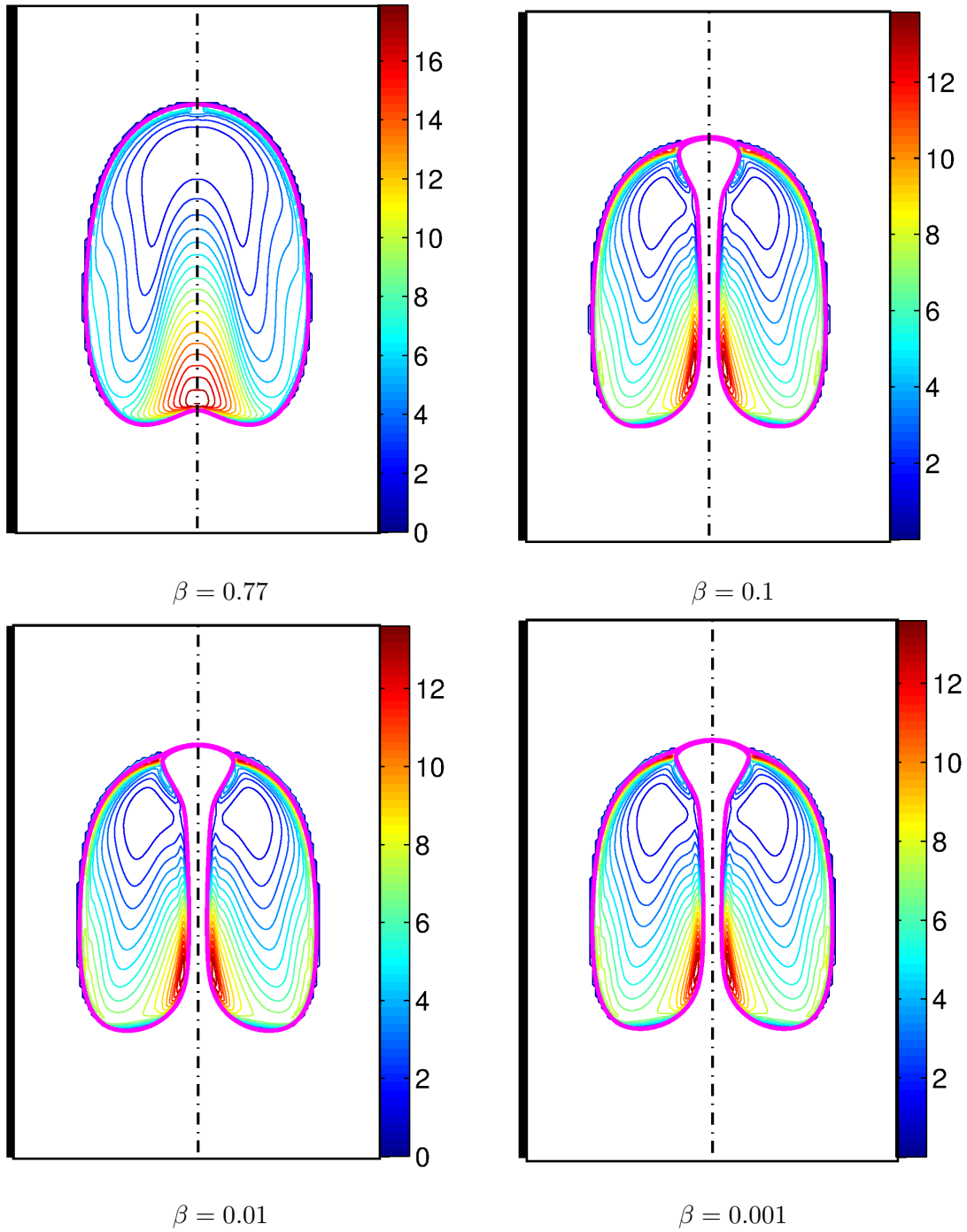


Figure 2.11: The effects of solvent viscosity ratio (β) for the VN case. The steady droplet shapes are shown together with the constant contours of $\text{trace}(\mathbf{B})$ for a buoyancy-driven FENE-CR droplet rising in a Newtonian fluid. ($Re = 10, Ca = 50, Wi = 50, Grid : 64 \times 592$).

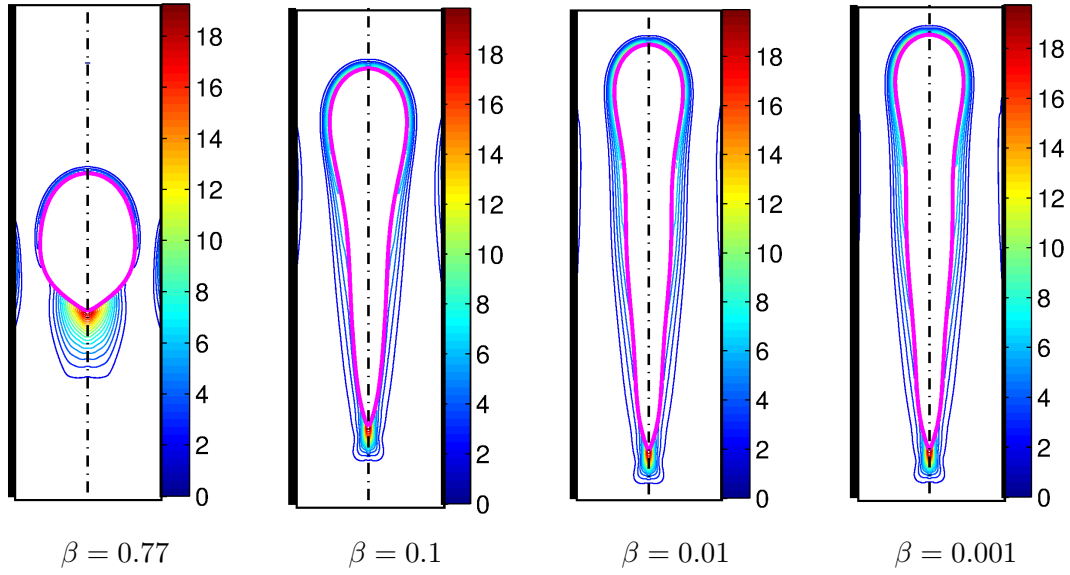


Figure 2.12: The effects of solvent viscosity ratio (β) for the NV case. The steady droplet shapes are shown together with the constant contours of $\text{trace}(\mathbf{B})$ for a buoyancy-driven Newtonian droplet rising in a FENE-CR fluid. ($Re = 10, Ca = 20, Wi = 50, Grid : 64 \times 592$).

well known stress singularities at the corners of the constriction, the strong droplet-constriction interactions and the subsequent large droplet deformations pose a challenge for the numerical solution algorithms. In particular, when a large droplet is forced to squeeze through the constriction at low capillary and high Weissenberg numbers, it undergoes large deformations leading to significant viscoelastic stress build ups especially near the corners of the constriction. It is worth mentioning here that the Oldroyd-B model is used for this test case in order to demonstrate the robustness of the present numerical method since the numerical solution of Oldroyd-B model equations is generally deemed to be more difficult than that of the FENE type models.

The physical problem is schematically shown in Fig. 2.17a. The flow is assumed be axisymmetric so only one half is used as the computational domain. This geometry is motivated by the recent computational studies of Chung et al. [30, 31] who simulated motion of a two-dimensional viscoelastic droplet in a creeping flow through a planar constricted channel using a finite-element/front-tracking method. A similar problem has been also studied by Harvie et al. [59] who performed volume-of-fluid simulations for a viscoelastic droplet in a Newtonian fluid moving through a pressure-driven 2D

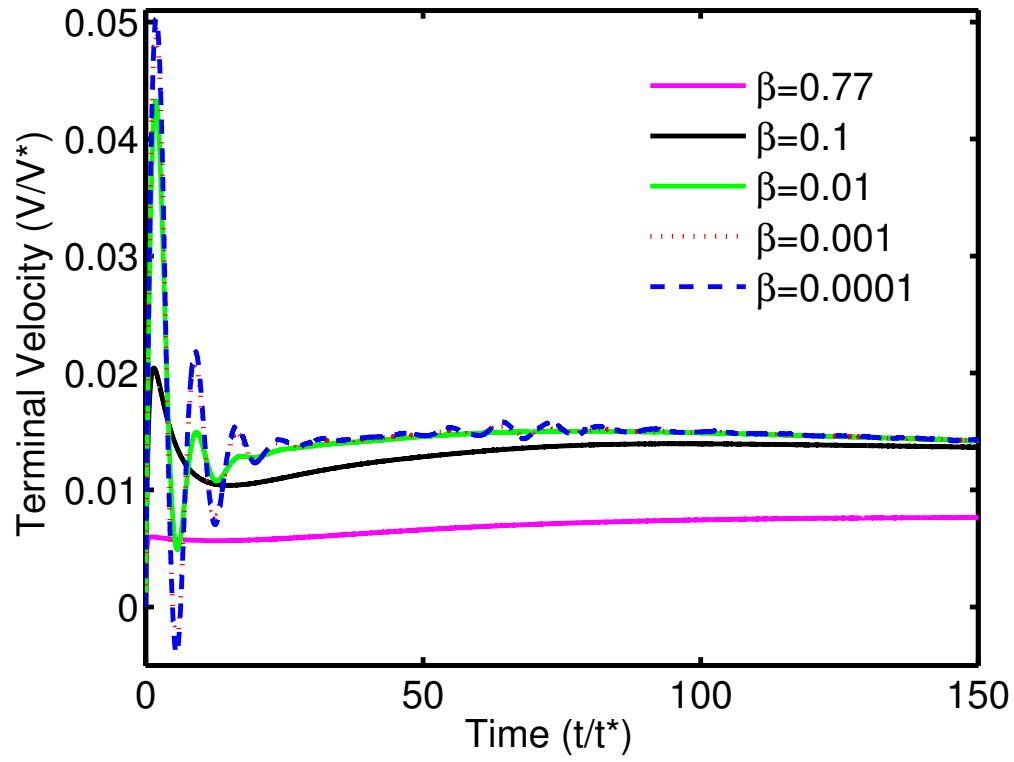


Figure 2.13: The effects of solvent viscosity ratio (β) for the NV case. The terminal velocity is plotted against the non-dimensional time for various β ranging between $\beta = 0.77$ and $\beta = 0.0001$. ($Re = 10, Ca = 10, Wi = 100$, Grid: 64×592 .)

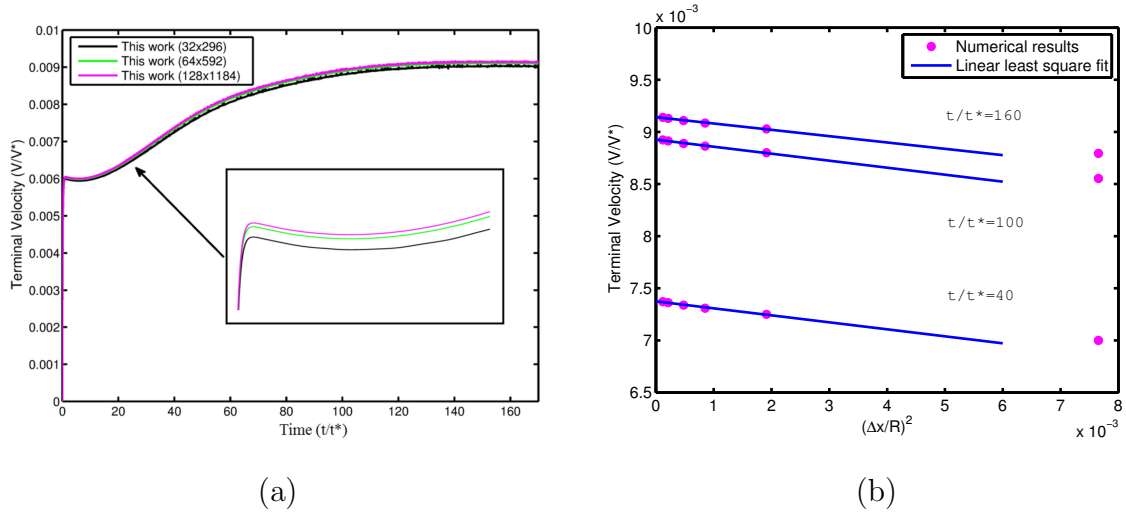


Figure 2.14: Grid convergence for the VN case. (a) The terminal velocity of the droplet against the non-dimensional time. The results are obtained using 32×296 , 64×592 and 128×1184 grids. (b) Variation of normalized terminal velocity with the square of the non-dimensional grid size $(\Delta x/R)^2$ at $t/t^* = 40, 100$ and 160 . The solid lines are the linear least squares fits to the computational results indicating the expected second-order accuracy of the method. ($Re = 10, Ca = 50, Wi = 50$).

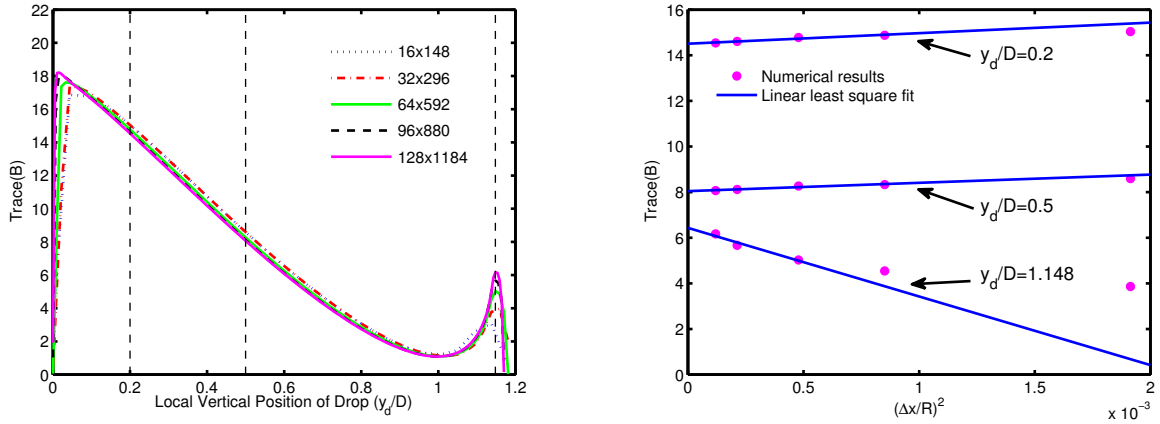


Figure 2.15: Grid convergence for the VN case. (a) Steady solution of $\text{trace}(\mathbf{B})$ is plotted along the drop centerline. The results are obtained using various grid resolutions ranging between 16×148 and 128×1184 . (b) Variation of $\text{trace}(\mathbf{B})$ with the square of the non-dimensional grid size $(\Delta x/R)^2$ at $y_d/2R_2 = 0.2, 0.5, 1.148$. The solid lines are the linear least squares fits to the computational results indicating the expected second-order accuracy of the method. ($Ca = 50, Re = 10, Wi = 50$).

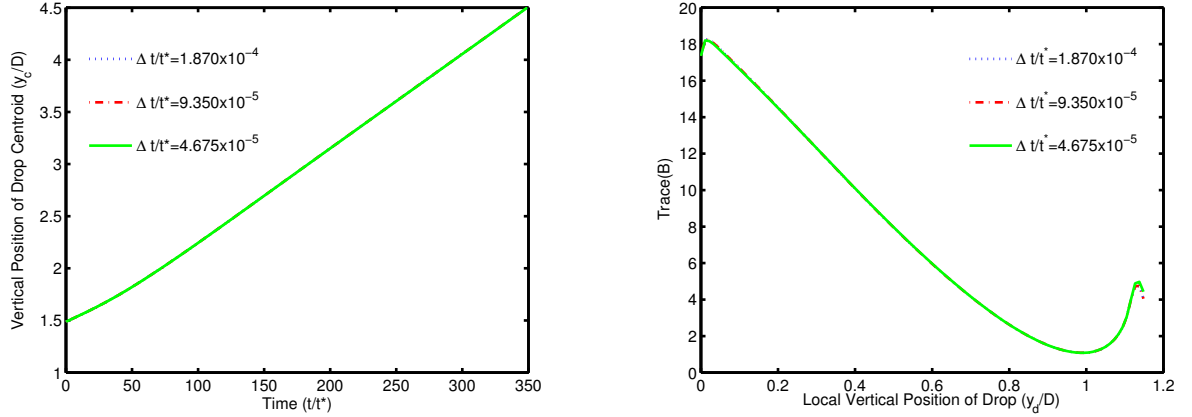


Figure 2.16: Time-stepping error convergence for the VN case. Simulations are performed using the non-dimensional time steps $\Delta t/t^* = 1.870 \times 10^{-4}$, 9.350×10^{-5} and 4.675×10^{-5} . (a) The non-dimensional axial location of droplet centroid is plotted against the non-dimensional time. (b) The steady solution of trace($\mathbf{B}$) is plotted along the drop centerline. ($Ca = 50$, $Re = 10$, $Wi = 50$; Grid: 64×592).

planar channel with a constriction. To the best of our knowledge, the only axisymmetric simulations of a viscoelastic droplet through a constricted channel have been performed by Zhou et al. [147] as a model for neutrophil deformation and transport in capillaries. Following Chung et al. [30], the constriction ratio is selected in the present study as 5:1:5, i.e., the ratio of the tube radius to that of the constriction is $R_1/R_2 = 5$. Note that this constriction ratio is more severe in the present axisymmetric case than that in the planar flow. The tube has a total length of $60R_2$. A sudden constriction of length $20R_2$ is located at the middle of the tube as shown in Fig. 2.17a. A spherical droplet of diameter $d_d = 2.5R_2$ is placed instantly at the axis of the channel with a distance of $10R_2$ upwards from the inlet. A parabolic fully developed velocity profile is specified at the channel entrance and the pressure is fixed at the exit. The viscoelastic stresses are specified at the inlet based on the analytical solution assuming a fully developed pipe flow, i.e.,

$$\tau_{rr} = 0; \tau_{\theta\theta} = 0; \tau_{rz} = \mu_p \frac{\partial v_z}{\partial r}; \tau_{zz} = 2\lambda \tau_{rz} \frac{\partial v_z}{\partial r}. \quad (2.18)$$

The Neumann boundary conditions are applied at the other boundaries.

In addition to the property ratios defined in Eq. (2.17), the relevant dimensionless

parameters are the capillary (Ca), the Weissenberg (Wi) and the Reynolds (Re) numbers defined as

$$Ca = \frac{\mu_o U}{\sigma}; Wi = \frac{\lambda U}{R_2}; Re = \frac{\rho_o U R_2}{\mu_o}, \quad (2.19)$$

where U is the mean velocity in the narrow part of the tube. Drop deformation is defined as

$$\text{deformation} = \frac{W_b - H_b}{W_b + H_b}, \quad (2.20)$$

where W_b and H_b are the maximum droplet dimensions in the axial and radial directions, respectively. The capillary number, the Reynolds number and the property ratios are fixed at $Ca = 0.1$, $Re = 1$, $\beta = 0.5$, $\theta = 0.5$ and $\alpha = 1.17$ in all the results presented in this section. The computations are again performed using dimensional quantities but the results are made dimensionless using the length scale R_2 and time scale $t^* = 125R_2/U$.

The simulations are first performed for the dimensionless numbers that are of the same order of those in Chung et al. [30, 31]. The computational grid is stretched near the walls and in the vicinity of the constriction similar to the single-phase flow case (Fig. 2.17b). The semi-analytical method is found to be convergent only up to $Wi = 2$ for the Oldroyd-B fluid model for this flow. Thus computations are performed using the log-conformation in all the results presented in this section. Figures 2.18 and 2.21 show the evolution of an Oldroyd-B droplet moving in a Newtonian fluid (VN system) through the constriction for $Wi = 0.4$ and $Wi = 2$, respectively.

Before presenting further results, a comprehensive study is conducted to demonstrate the grid convergence and determine the appropriate grid resolution for this pressure-driven case. Sample results are presented here for the VN system only. For this purpose, simulations are performed for the VN system shown in Fig. 2.18 using various grid resolutions ranging between 32×384 and 128×1536 . The evolution of drop deformation and the steady solution of $A_{zz} - A_{rr}$ along the drop centerline are plotted in Figs. 2.19a and 2.20a, respectively. As can be seen in these figures, differences between successive grid resolutions decrease as grid is refined indicating grid convergence. To quantify the spatial error, values of drop deformation and $A_{zz} - A_{rr}$ are plotted at selected locations against the square of non-dimensional grid size in Figs. 2.19b and 2.20b, respectively. The

approximate linear relationship confirms the expected second order spatial accuracy of the method. These figures show that a 96×1152 grid is required to reduce the maximum spatial error below 4% for $A_{zz} - A_{rr}$ while only a 64×768 grid is sufficient to reduce the spatial error below 1% in the drop deformation. Note that the results presented in this paper are obtained using a 96×1152 grid for which the maximum spatial error is reduced below 4% in all the flow quantities.

In order to demonstrate the robustness of the numerical method, simulations are also performed for much higher Weissenberg numbers and sample results are plotted in Figs. 2.22 and 2.23 for $Wi = 50$ and $Wi = 100$, respectively. The constant contours of $\sqrt{\text{trace}(\mathbf{A})}$ are used to quantify the evolution of the viscoelastic stresses. It is seen that, as the leading tip of the drop enters the contraction, the region in the vicinity of the front stagnation point contains significantly extended polymers due to extensional flow leading to accumulation of viscoelastic stresses there. As the droplet further progresses into the constriction, significant stress concentration also occurs on the side of the droplet due to high shear stresses exerted by the ambient fluid near the wall. These viscoelastic stresses are then convected toward the trailing edge mainly by the internal circulation and accumulated near the centerline when the droplet reaches a nearly steady motion in the constriction. As droplet leaves the constriction, the fluid decelerates resulting in negative extensional strain that reduces droplet length forming a part-moon shape. The droplet eventually relaxes to a nearly spherical shape due to surface tension. The stress patterns are similar for all Weissenberg number cases but the viscoelastic effects are more pronounced as Wi increases. Similar simulations are also performed for a Newtonian droplet in a viscoelastic medium (NV) and a viscoelastic droplet in another viscoelastic medium (VV). Figures 2.24 and 2.25 show the evolution of the NV and VV systems, respectively. Similar to the VN case, in the NV system, the viscoelastic stresses concentrate near the leading edge as drop enters the constriction and then move toward the side of the droplet near the tube wall mainly due to the shear stresses exerted by the ambient fluid. In the case of VV, the stress patterns are a combination of the VN and NV cases. The constant contours of $A_{zz} - A_{rr}$ are plotted in Fig. 2.26 both for the VN and NV cases in the middle of constriction when the droplet reaches a nearly steady motion. For the VN case, the normal stress differences develop inside the drop on the

sides close to the wall as well as near the rear stagnation point. For the NV case, the normal stress differences are significantly higher in the film region as seen in Fig. 2.26a. In the both cases, the high stress difference on the sides helps the drop swell at the exit of the constriction since the normal stress difference exerts force in the radial direction.

Typical deformation patterns are illustrated in Fig. 2.27a for the all Newtonian case (NN), i.e., $Wi = 0$. The deformation is plotted against the moving distance y_d defined as the distance that the droplet travels in the axial direction relative to its initial position. For the same case, the deformations in the axial and radial directions are plotted separately in Fig. 2.27b. The drop deforms as it moves into the constriction and becomes more elongated due to increased confinement. Once the centroid of the drop is within the capillary its rear is held by the contraction while its front continues to elongate. After some time the rear of the drop clears the contraction and drop attains a nearly steady shape in the narrow channel. As drop leaves the constriction, it swells as indicated by the negative deformation in Fig. 2.27a. Finally, the droplet restores its spherical shape due to surface tension in the expansion region. Drop deformation is compared in Fig. 2.28 for NV, VN and VV cases both for the Oldroyd-B and FENE-CR models. As can be seen in this figure, the drop deformation is almost identical for NV, VN and VV systems irrespective of the elastic properties of the fluids. Note that the present results are qualitatively similar to the 2D planar simulations of Chung et al. [31].

Finally simulations are performed for a high Weissenberg number case, i.e., $Wi = 25$, to demonstrate the difference between the Oldroyd-B and FENE-CR models. The results are shown in Fig. 2.29 where the constant contours of $A_{zz} - 1$ are plotted both for the Oldroyd-B and FENE-CR models. As can be seen, the Oldroyd-B model results in a large build up of polymer extensions along the droplet centerline (Fig. 2.29a) whereas the polymer extension is moderate in the FENE-CR model case (Fig. 2.29b). This is a direct result of the finitely extensible nature of the FENE-CR model and is the main reason that the Oldroyd-B model presents a considerable challenge to numerical simulations especially at high Weissenberg numbers. The present results demonstrate that the front-tracking method is robust and successfully simulates viscoelastic two-phase systems at high Weissenberg numbers, i.e., as high as $Wi = 100$ for Oldroyd-B model.

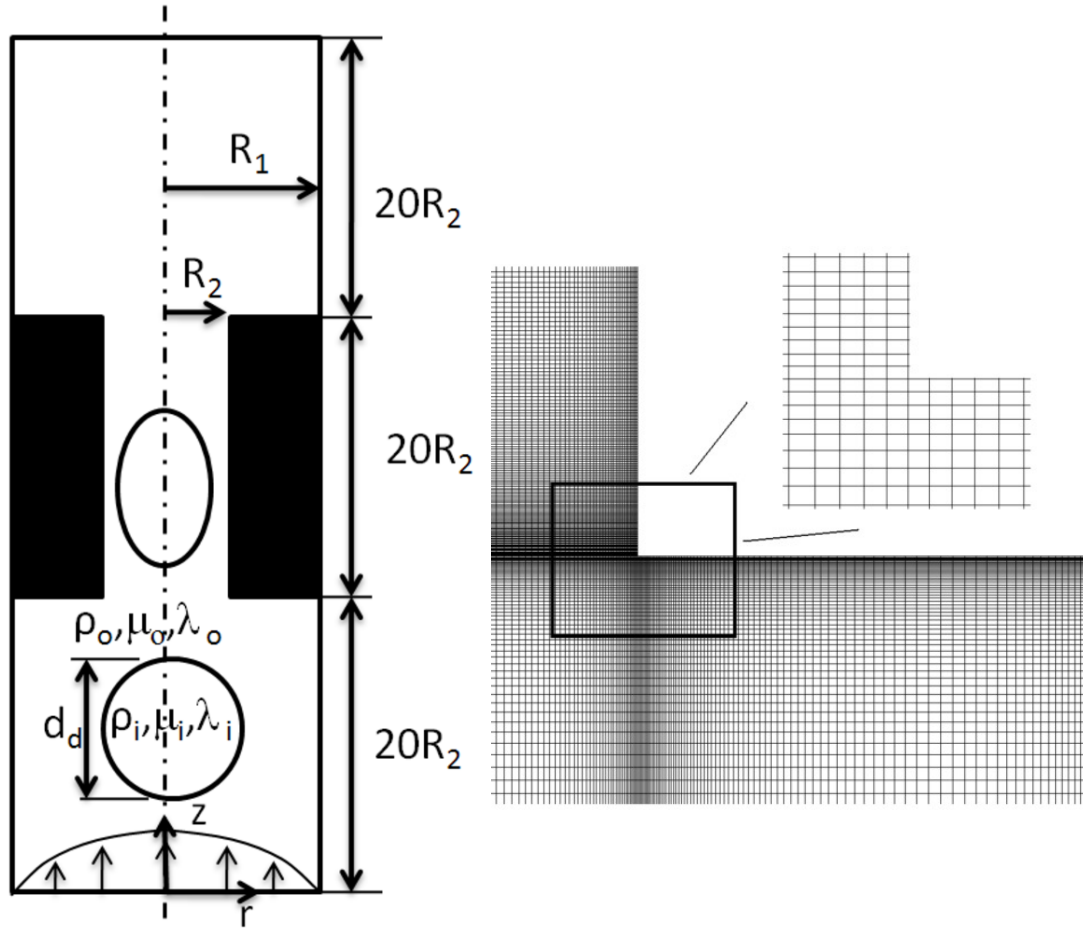


Figure 2.17: (a) Schematic illustration of a pressure-driven viscoelastic two phase system. (b) Mesh near the re-entrant corner.

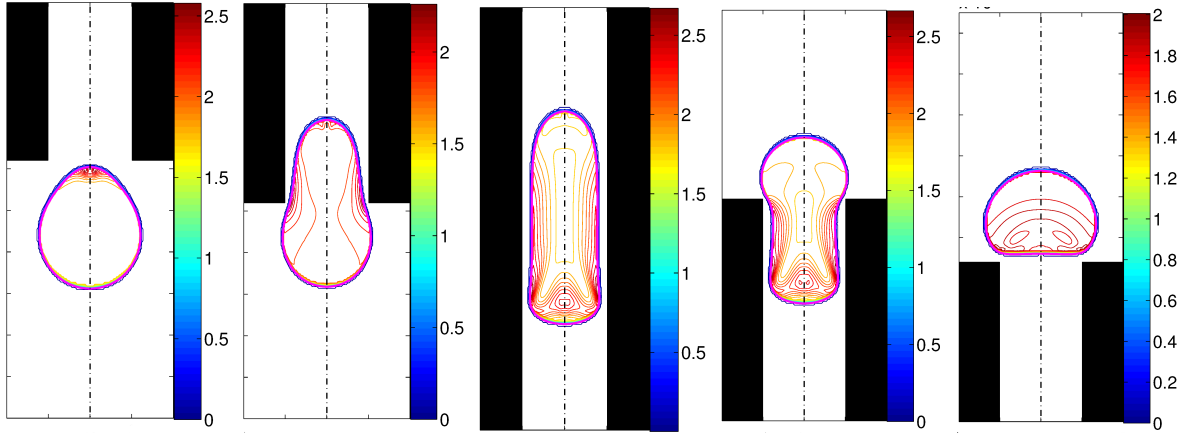


Figure 2.18: An Oldroyd-B droplet moving through a Newtonian ambient fluid in a pressure driven constriction/expansion tube for $Wi = 0.4$. The constant contours represent the average polymer extension defined as $\sqrt{\text{trace}(\mathbf{A})}$. From left to right, the snapshots are taken at times $t/t^* = 0.70, 0.71, 77, 83$ and 0.85 . Simulations are performed using the LCM on a 96×1152 grid ($Ca = 0.1, Re = 1$).

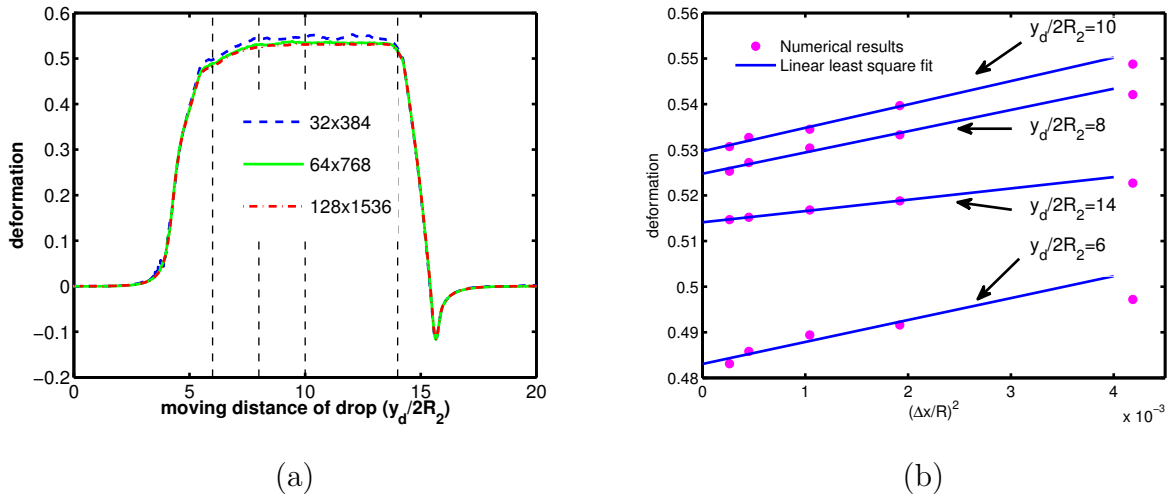


Figure 2.19: Grid convergence for the VN case. The results are obtained using various grid resolutions ranging between 32×384 and 128×1536 . (a) Drop deformation versus the moving distance of the drop centroid. (b) Variation of drop deformation with the square of the non-dimensional grid size $(\Delta x/R)^2$ at the axial locations $y_d/2R_2 = 6, 8, 10$ and 14 . The solid lines are the linear least squares fits to the computational results indicating the expected second-order accuracy of the method. ($Wi = 0.4, Ca = 0.1, Re = 1$).

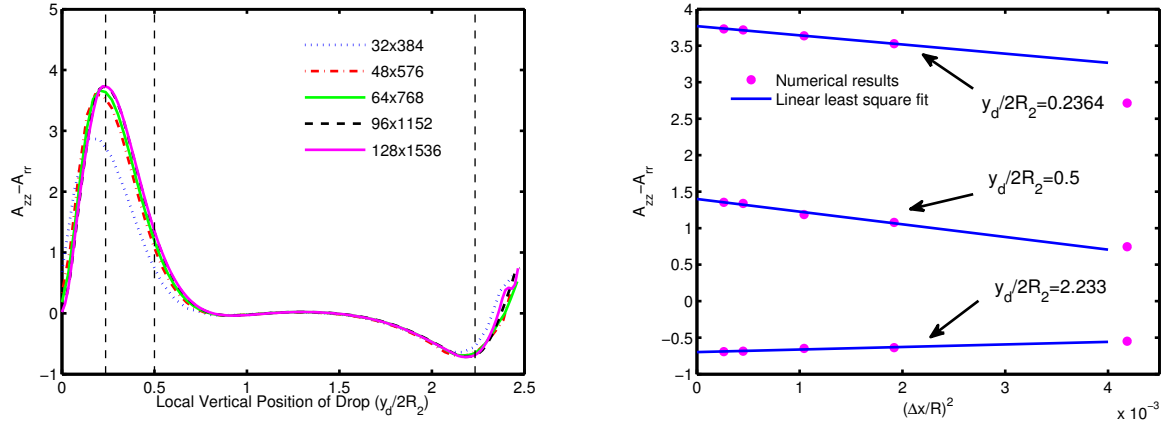


Figure 2.20: Grid convergence for the VN case. The results are obtained using various grid resolutions ranging between 32×384 and 128×1536 . (a) Steady distribution of $A_{zz} - A_{rr}$ along the drop centerline. (b) Variation of $A_{zz} - A_{rr}$ with the square of the non-dimensional grid size $(\Delta x/R)^2$ at the axial locations $y_d/2R_2 = 0.2364, 0.5, 2.233$. The solid lines are the linear least squares fits to the computational results indicating the expected second-order accuracy of the method. ($Wi = 0.4, Ca = 0.1, Re = 1$).

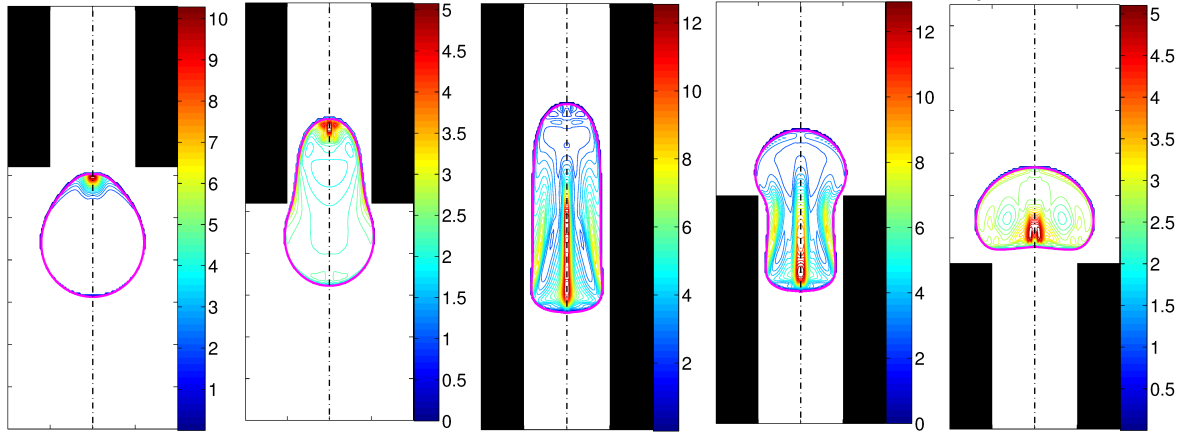


Figure 2.21: An Oldroyd-B droplet moving through a Newtonian ambient fluid in a pressure driven constriction/expansion tube for $Wi = 2$. The constant contours represent the average polymer extension defined as $\sqrt{\text{trace}(\mathbf{A})}$. From left to right, the snapshots are taken at times $t/t^* = 0.70, 0.71, 77, 83$ and 0.85 . Simulations are performed using the LCM on a 96×1152 grid ($Ca = 0.1, Re = 1$).

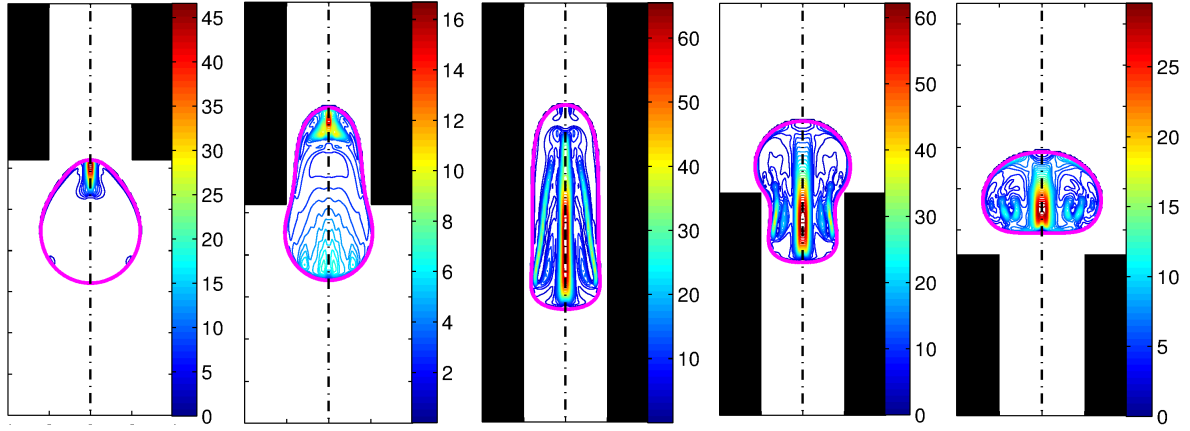


Figure 2.22: An Oldroyd-B droplet moving through a Newtonian ambient fluid in a pressure driven constriction/expansion tube for $Wi = 50$. The constant contours represent the average polymer extension defined as $\sqrt{\text{trace}(\mathbf{A})}$. From left to right, the snapshots are taken at times $t/t^* = 0.70, 0.71, 77, 83$ and 0.85 . Simulations are performed using the LCM on a 96×1152 grid ($Ca = 0.1, Re = 1$).

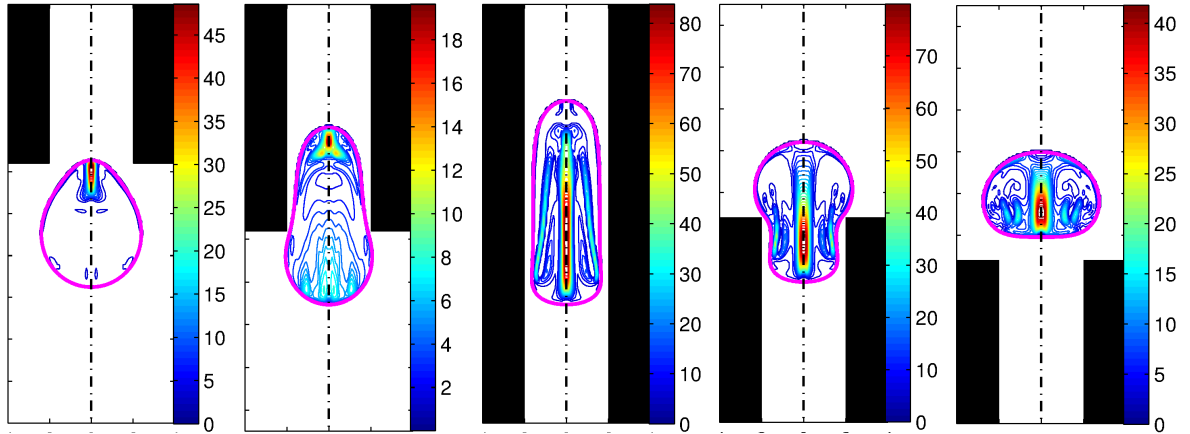


Figure 2.23: An Oldroyd-B droplet moving through a Newtonian ambient fluid in a pressure driven constriction/expansion tube for $Wi = 100$. The constant contours represent the average polymer extension defined as $\sqrt{\text{trace}(\mathbf{A})}$. From left to right, the snapshots are taken at times $t/t^* = 0.70, 0.71, 77, 83$ and 0.85 . Simulations are performed using the LCM on a 96×1152 grid ($Ca = 0.1, Re = 1$).

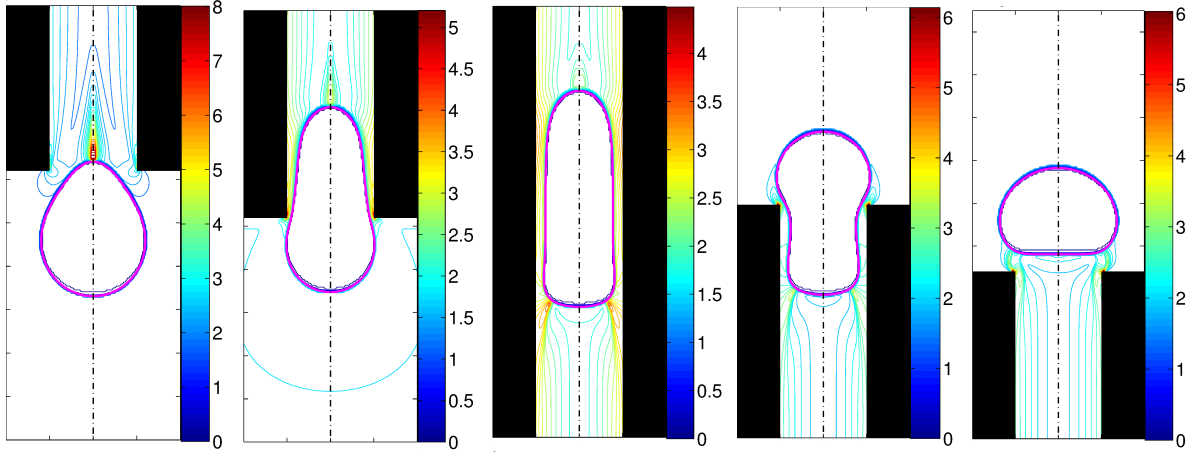


Figure 2.24: A Newtonian droplet moving through an Oldroyd-B fluid in a pressure driven constriction/expansion tube for $Wi = 0.4$. The constant contours represent the average polymer extension defined as $\sqrt{\text{trace}(\mathbf{A})}$. From left to right, the snapshots are taken at times $t/t^* = 0.70, 0.71, 77, 83$ and 0.85 . Simulations are performed using the LCM on a 96×1152 grid ($Ca = 0.1, Re = 1$).

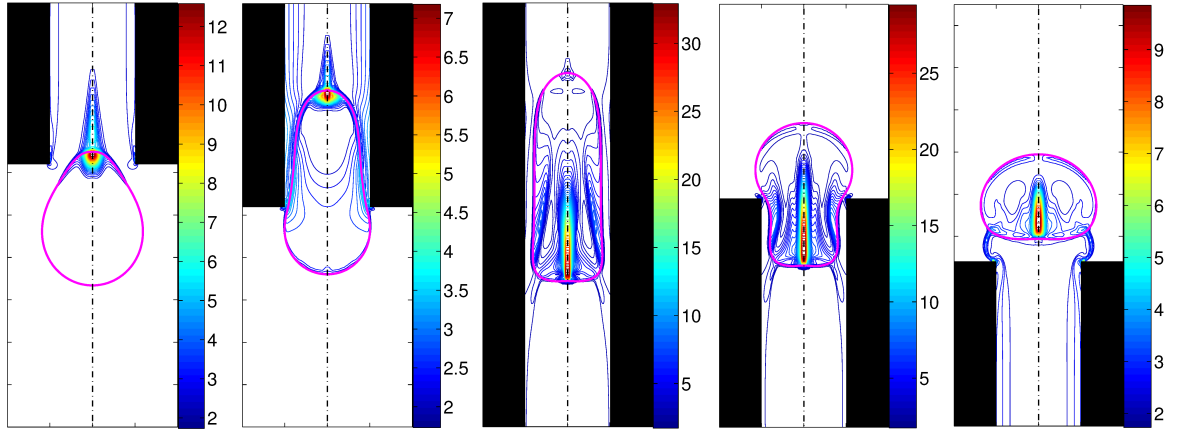


Figure 2.25: An Oldroyd-B droplet moving through another Oldroyd-B fluid in a pressure-driven constriction/expansion tube for $Wi_i = 2$ and $Wi_o = 0.4$. The constant contours represent the average polymer extension defined as $\sqrt{\text{trace}(\mathbf{A})}$. From left to right, the snapshots are taken at times $t/t^* = 0.70, 0.71, 77, 83$ and 0.85 . Simulations are performed using the LCM on a 96×1152 grid ($Ca = 0.1, Re = 1$).

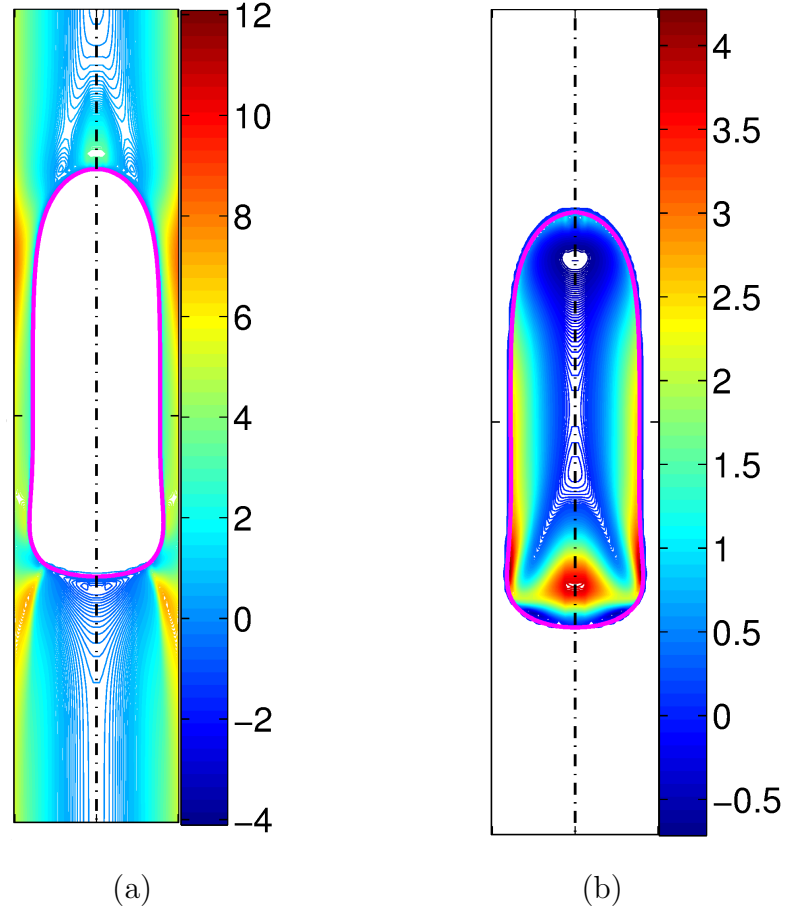


Figure 2.26: The constant contours of the difference between the normal components of the conformation tensor $A_{zz} - A_{rr}$ in the vicinity of the droplet in the constriction. (a) NV system and (b) VN system. ($Ca = 0.1$, $Re = 1$, $Wi = 0.4$ and Grid: 96×1152 .)

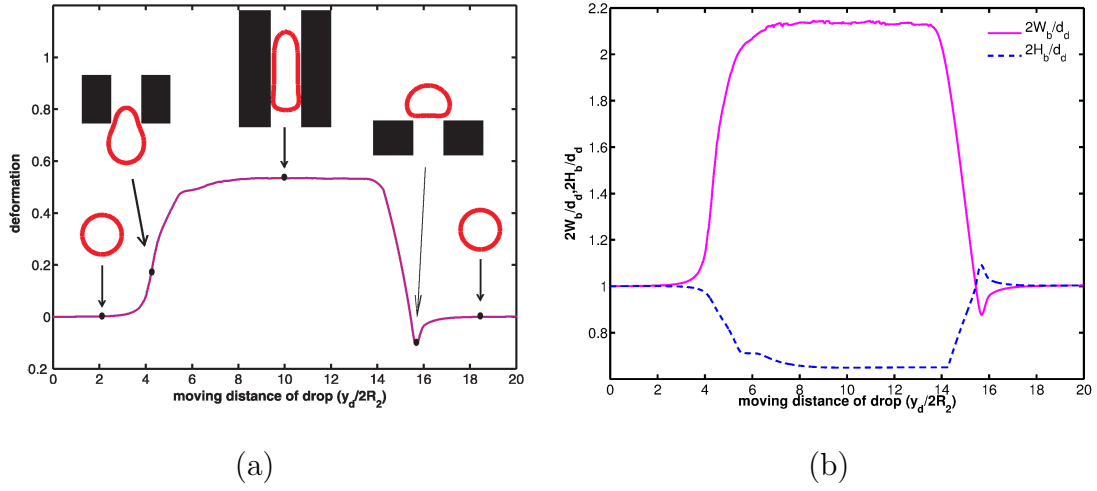


Figure 2.27: Drop deformation versus the moving distance of the drop centroid for the Newtonian-Newtonian system (NN). (a) The drop deformation and the corresponding drop shapes. (b) The drop deformation in the axial (solid line) and the radial (dashed line) directions, respectively. ($Wi = 0$, $Re = 1$, $Ca = 0.1$ and Grid: 96×1152).

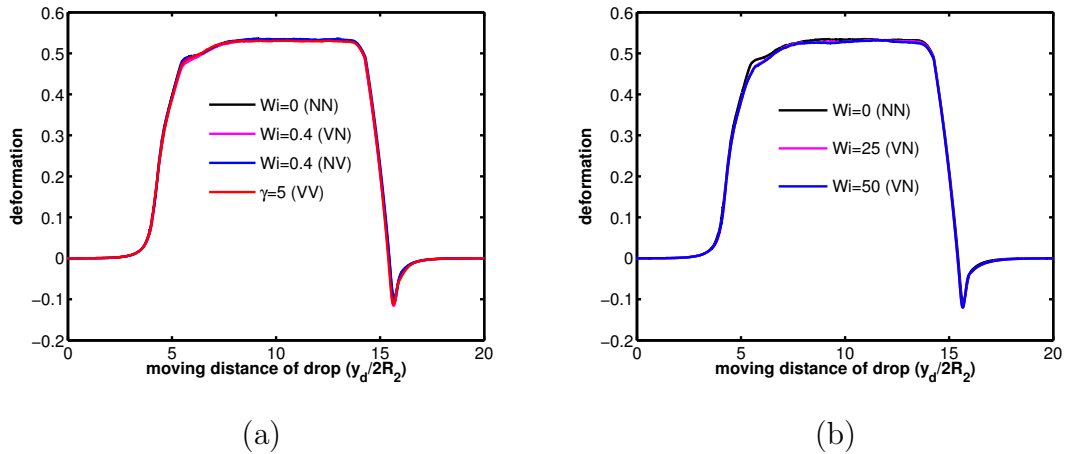


Figure 2.28: Effects of fluid elasticity on drop deformation. The simulations are performed using a 96×1152 grid for $Re = 1$ and $Ca = 0.1$. (a) Oldroyd-B model ($Wi_i = 2$, $Wi_o = 0.4$ for VV), (b) FENE-CR model ($L = 5$).

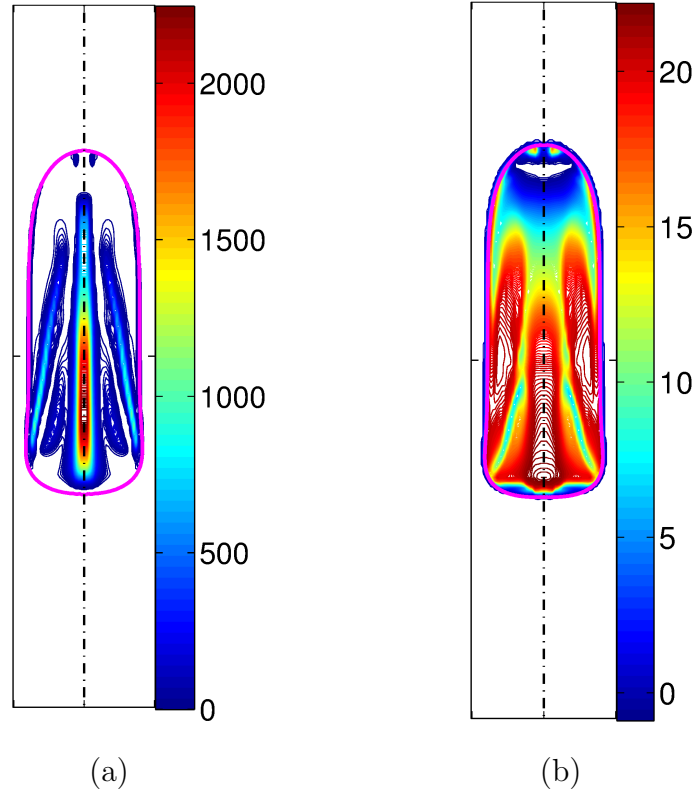


Figure 2.29: The constant contours of $A_{zz} - 1$ for a viscoelastic drop in a Newtonian fluid for $Wi = 25$, $Re = 1$, $Ca = 0.1$. The simulations are performed on a 96×1152 grid. (a) Oldroyd-B model. (b) FENE-CR model ($L = 5$).

2.5 Conclusions

A front-tracking method is developed for direct numerical simulations of viscoelastic interfacial flows. The method is general and applicable to two-phase systems in which either phase or both phases can be viscoelastic. It can accommodate virtually any viscoelastic model for each phase. Moreover, the method is readily extendible for simulation of multiphase systems in which more than two-phases may exist.

Semi-analytical and log-conformation schemes are used to integrate the viscoelastic constitutive equations in time. The log-conformation method is found to be in a good agreement with the semi-analytical method and very robust for a wide range of Weissenberg numbers. A fifth-order upwinded WENO-Z scheme is used to discretize the convective terms in the viscoelastic model equations and found to be crucially important for resolving thin viscoelastic boundary layers near the interface.

The method is first validated for single-phase viscoelastic flows including a start up flow in a circular channel and a pressure-driven flow through a 4:1 constriction. Then it is applied to buoyancy-driven motion of viscoelastic two-phase systems encompassing a viscoelastic droplet in Newtonian medium, a Newtonian droplet in a viscoelastic medium and a viscoelastic droplet in another viscoelastic medium. The results are compared and found to be in good qualitative and quantitative agreement with the computational simulations of You et al. [142]. Moreover, the present method is found to be stable and very robust for very low solvent viscosity ratios, i.e., as low as $\beta = 10^{-4}$. It is also verified that the results obtained using the log-conformation and semi-analytical methods are consistent. Finally, the method is applied to study the dynamics of viscoelastic droplet systems in a pressure-driven contraction/expansion channel. It is found that the log-conformation method is stable and preserves positive definiteness of conformation tensor for a wide range of Weissenberg numbers whereas the semi-analytical method remains stable only for small or moderate Weissenberg numbers, i.e., up to $Wi = 2$ for this case. However the semi-analytical method has advantage of requiring lower computational time and implementation complexity compared to the log-conformation method. Thus the semi-analytical method is an optimal choice for computation of viscoelastic flows at small or moderate Weissenberg numbers. It is also worth to note that the log-conformation

method can provide stable simulations at large Weissenberg numbers, but it cannot guarantee accuracy at arbitrarily high Weissenberg numbers as discussed by Fattal and Kupferman [41].

2.6 Acknowledgement

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Chapter 3

A COMPUTATIONAL STUDY OF TWO-PHASE VISCOELASTIC SYSTEMS IN A CAPILLARY TUBE WITH A SUDDEN CONTRACTION/EXPANSION²

3.1 Introduction

Confined multiphase fluid dynamics is of fundamental importance in a wide range of engineering applications and natural processes such as the droplet-based microfluidics [117, 118], enhanced oil recovery [95], blood cells in microcirculation [43, 136, 63, 145], polymer blends and polymer processing [54]. Viscoelastic effects play a significant role in all these applications often in the presence of confinement. Viscoelastic liquids exhibit a range of exotic behaviors that can be utilized to perform useful functions especially in microfluidic applications. For instance, microfluidic memory and control device [50], microfluidic rectifier [51], nonlinear viscoelastic flow resistor [50], synthesis of non-spherical particles [35] and enhanced mixing in microchannels [49] rely on viscoelasticity of working fluids. With the rapidly growing popularity of droplet-based microfluidic devices, there has been significant interest recently in viscoelastic two-phase systems in confined geometries [52, 21, 59, 36]. It is thus crucially important to understand viscoelastic effects on drop dynamics in confined geometries for development of various lab-on-a-chip devices.

Unlike viscous systems, understanding of viscoelasticity is severely limited, and yet of great importance for flow modeling and simulation. The difficulty is due to complex rheological behavior of the fluids which often leads to controversies [42, 39, 82, 83, 139]. For instance, there were contradictory observations about the effects of viscoelasticity on drop deformation, i.e., whether viscoelasticity increases or decreases drop deformation

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in a shear flow [42, 39]. Numerical simulations of Yue et al. [139] and Aggarwal and Sarkar [2] recently resolved this issue and found a non-monotonic dependence of deformation on viscoelasticity with an initially decreasing followed by an increasing trend. In a uniform extensional flow, reduced deformation is predicted for a viscoelastic drop in a viscous medium and the enhanced deformation otherwise [105, 106]. This is consistent with the heuristic idea that viscoelasticity in the drop phase opposes deformation, while in the matrix facilitates it. Also there were contradictory results about the effects of fluid elasticity on drop deformation in a converging conical channel [26, 82, 73]. Experimental works of Chin and Han [26] and Mighri et al. [82] demonstrated similar droplet deformation and dynamics in this geometry as are for a uniform extensional flow. On the contrary, the numerical study of Khayat [73] showed that viscoelastic effects in the drop assist deformation while in the matrix impede it. A more recent computational study of Zhou et al. [148] demonstrated a more complex picture, in which viscoelasticity in either phase may suppress or promote drop deformation depending on the capillary number and the drop-to-matrix viscosity ratio.

Confined multiphase flows have recently received a special attention due to the growing interest in microfluidic technologies [32, 78, 43]. There have been a few experimental studies [61, 93, 74] on confined motion of viscoelastic two-phase systems, e.g., motion of neutrally/non-neutrally buoyant drops suspended in a Newtonian/viscoelastic Stokes flow. Ho and Leal [61] and Olbricht and Leal [93] demonstrated that viscoelasticity of the suspending fluid significantly influences the droplet dynamics in straight and constricted capillary tubes. Recently, Khobdeh [74] studied deformation and breakup of viscoelastic two-phase systems in capillaries of different cross-sections. For cylindrical and rectangular channels, an increase in elasticity of drop phase inhibits deformation, while in suspending fluid, has non-monotonic effect: a decrease followed by an increase. Khobdeh [74] also investigated drop dynamics in periodically constricted capillary tubes and found that drop deformation is enhanced by viscoelasticity irrespective of which phase is elastic. Wu [135] numerically investigated both buoyancy-driven and pressure-driven motion of viscoelastic drop in a capillary tube. He found that elasticity in the drop phase suppresses drop deformation. You et al. [142] conducted numerical simulations for a confined buoyancy-driven drop in various viscoelastic two-phase systems.

They concluded that viscoelasticity in the interior phase pulls the trailing end inward, while in the exterior fluid, pulls it out.

Unlike single phase case, viscoelastic multiphase flows through a contraction/expansion geometry have received less attention. When a drop passes through a contraction it experiences regions of strong shearing near the walls: non-homogeneous uniaxial extension along the centerline upstream of the contraction plane and non-homogeneous biaxial expansion downstream of the expansion. Extensive simulations have been done by Harvie and co-workers [56, 57, 58] to understand a Newtonian and a generalized non-Newtonian drop dynamics in an axisymmetric 4:1:4 contraction/expansion geometry. Viscoelastic effects on drop deformation have been also investigated by several other groups in axisymmetric [147] and planar [59, 30, 31] configurations for similar geometries. Zhou et al. [147] simulated the deformation of an axisymmetric viscoelastic/Newtonian droplet to model fluid dynamics of a neutrophil moving through a constriction in a Newtonian environment. However their simulations were restricted to low Reynolds number (creeping) flows with viscoelasticity contained only in the drop phase and a capillary tube without any expansion region. Harvie et al. [59] considered a viscoelastic drop moving in a Newtonian medium in a planar channel with a sudden contraction/expansion. They demonstrated qualitative agreement between computational results and experimental observations. In particular, they observed the forked tail formation in the contraction region. Chung et al. [31] investigated two-phase systems in a planar channel with a 5:1:5 constriction/expansion region and considered cases in which either droplet or ambient fluid is viscoelastic. They found that viscoelasticity significantly enhances drop deformation especially at high viscosity ratios for a Newtonian drop in a viscoelastic medium while it has much less effects on drop deformation for the case of a viscoelastic droplet in a Newtonian fluid. Note that they considered relatively low Weissenberg number cases, i.e., up to $Wi = \mathcal{O}(1)$.

The inertial effects on drop deformation have been often neglected in previous studies. However, in spite of the common wisdom that inertia is negligible in microfluidic systems, recent studies have shown that a variety of inertial effects can be utilized for various applications in microchannels including enhanced mixing, particle separation, and bioparticle focusing [38, 3]. Amini et al. [3] reviewed a variety of mechanisms by

which inertia and asymmetry in channel or particle geometry can be used to control particles and flows in microfluidic platforms. Moreover, inertia can significantly promote the deformation of microdroplets for the Reynolds number in the range of $Re = 1 - 100$ [111, 22]. To our knowledge, there has been no numerical study to investigate the effects of viscoelasticity and inertia on drop dynamics in an axisymmetric tube with a sudden contraction/expansion.

In the present study, extensive direct numerical simulations are carried out to examine the effects of viscoelasticity on drop dynamics in various two-phase systems in a pressure-driven tube with a 4:1:4 sudden contraction/expansion. The inertial effects are fully taken into account by solving the Navier-Stokes and viscoelastic model equations in the entire computational domain using the front-tracking method [130, 67]. We consider the cases of a Newtonian droplet in a viscoelastic medium (NV), a viscoelastic droplet in a Newtonian medium (VN) and a viscoelastic droplet in another viscoelastic medium (VV). The fluid viscoelasticity is accounted for using the FENE-CR model of Chilcott and Rallison [25]. Simulations are performed to investigate drop deformation and dynamics for the NV, VN and VV systems in a contraction/expansion geometry for a wide range of parameters including the relative droplet size (κ), the capillary number (Ca), Reynolds number (Re), viscosity ratio (θ) and the viscoelasticity characterized by the Weissenberg number (Wi), solvent viscosity ratio (β) and the extensibility parameter (L^2). In addition, the effects of the inner and outer Weissenberg numbers (Wi_i and Wi_o) as well as their ratio (k) are also examined for the VV system.

The main contributions of the present work can be summarised as follows:

1. This is the first direct numerical simulation study of pressure-driven viscoelastic two-phase flow systems in an axisymmetric channel with a sudden contraction and expansion at finite Reynolds and Weissenberg numbers. The previous computational studies were restricted to planar two-dimensional geometries [59, 30, 31], the only exception being the numerical study by Zhou et al. [147] who considered an axisymmetric channel with only a smooth constriction but without an expansion region.
2. Combined inertial and viscoelastic effects on drop dynamics are studied for the

Weissenberg and Reynolds numbers up to $Wi = 100$ and $Re = 100$. The previous computational studies were limited to low Reynolds number flows ($Re = \mathcal{O}(1)$ or smaller) in the VN system [147, 59] or to low Weissenberg numbers (i.e., $Wi = \mathcal{O}(1)$) [30, 31]. It is found that a drop undergoes a large deformation in the narrow pipe followed by strong shape oscillations in the expansion region at high Re numbers and these oscillations interact strongly with the viscoelasticity in a non-monotonic and complicated way.

3. Combined viscous and viscoelastic effects on drop dynamics are also investigated for the NV and VN systems. It is found that a highly viscous drop may develop a re-entrant cavity at the trailing edge which eventually leads to encapsulation of ambient fluid into main droplet in some cases. This phenomenon is highly influenced by viscoelasticity non-monotonically in a complicated and somewhat unexpected way. Compared to the corresponding straight channel case, the effects of viscoelasticity are reversed in the constricted channel: Viscoelasticity in drop/continuous phase hinders/enhances formation of the re-entrant cavity and entrainment of ambient fluid into main drop. This result may indicate that the viscoelasticity can be used to create a compound droplet with a precise volume of the inner and outer droplets.
4. The FENE-CR model employed in the present study is more realistic than the commonly used Oldroyd-B model since it accounts for the finite polymer extensibility. Thus the present results are expected to better represent the physics of two-phase viscoelastic fluid systems.

The rest of this paper is organized as follows: In the next section, we briefly describe the governing equations including the constitutive model for viscoelasticity and numerical method. The physical problem and flow geometry are described in Sec. 3.3. The results are presented and discussed in Sec. 3.4. Conclusions are drawn in Sec. 3.5. An extensive grid convergence study is also presented in the Appendix.

3.2 Formulation and Numerical Method

The governing equations are described in the framework of the finite difference/front tracking method. The flow is assumed to be incompressible. Following Unverdi and Tryggvason [130] and Izbassarov and Muradoglu [67], a single set of governing equations can be written for the entire computational domain provided that the jumps in the material properties such as density, viscosity and relaxation time are taken into account and the effects of the interfacial surface tension are treated appropriately.

The continuity and momentum equations can be written as follows:

$$\nabla \cdot \mathbf{u} = 0, \quad (3.1)$$

$$\begin{aligned} \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot \mu_s (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \nabla \cdot \boldsymbol{\tau} + \Delta \rho g + \\ &\int_A \sigma \kappa \mathbf{n} \delta(\mathbf{x} - \mathbf{x}_f) dA, \end{aligned} \quad (3.2)$$

where μ_s , ρ , p , $\mathbf{u}$ and $\boldsymbol{\tau}$ denote the solvent viscosity and the density of the fluid, the pressure, the velocity vector and the viscoelastic extra stress tensor, respectively. The last term in Eq. (3.2) represents the body force due to surface tension where σ is the surface tension coefficient, κ is twice the mean curvature, and $\mathbf{n}$ is the unit vector normal to the interface. 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 points at which the equation is being evaluated and a point at the interface, respectively.

The FENE-CR model is adopted as the constitutive equation for the viscoelastic extra stresses. This model can be written as

$$\begin{aligned} \frac{\partial \mathbf{A}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{A}) - (\nabla \mathbf{u})^T \cdot \mathbf{A} - \mathbf{A} \cdot \nabla \mathbf{u} &= -\frac{F_A}{\lambda} (\mathbf{A} - \mathbf{I}), \\ F_A &= \frac{L^2}{L^2 - \text{trace}(\mathbf{A})}, \end{aligned} \quad (3.3)$$

where $\mathbf{A}$, λ , L , F_A and $\mathbf{I}$ are the conformation tensor, the relaxation time, the extensibility parameter defined as the ratio of the length of a fully extended polymer dumbbell to its equilibrium length, the stretch function and the identity tensor, respectively. The extra stress tensor $\boldsymbol{\tau}$ is related to the conformation tensor as

$$\boldsymbol{\tau} = \frac{F_A \mu_p}{\lambda} (\mathbf{A} - \mathbf{I}), \quad (3.4)$$

where μ_p is the polymeric viscosity.

It is also assumed that the material properties remain constant following a fluid particle, i.e.,

$$\frac{D\rho}{Dt} = 0; \frac{D\mu_s}{Dt} = 0; \frac{D\mu_p}{Dt} = 0; \frac{D\lambda}{Dt} = 0, \quad (3.5)$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$ is the material derivative. The density, polymeric and solvent viscosities, and the relaxation time vary discontinuously across the fluid interface and are given by

$$\begin{aligned} \mu_p &= \mu_{p,i}\phi + \mu_{p,o}(1 - \phi); \quad \mu_s = \mu_{s,i}\phi + \mu_{s,o}(1 - \phi); \\ \rho &= \rho_i\phi + \rho_o(1 - \phi); \quad \lambda = \lambda_i\phi + \lambda_o(1 - \phi), \end{aligned} \quad (3.6)$$

where the subscripts i and o denote the properties of the drop and the bulk fluids, respectively. The indicator function ϕ is defined such that it is unity inside the droplet and zero outside.

The flow equations (Eqs. 3.1 and 3.2) are solved fully coupled with the viscoelastic model equations (Eq. 3.3) by the finite-difference/front-tracking method developed by Izbassarov and Muradoglu [67]. The flow and viscoelastic model equations are solved on a staggered Eulerian grid using a projection method[29]. The log-conformation method (LCM) of Fattal and Kupferman [41] is employed to enhance numerical stability in solving the viscoelastic model equations at high Weissenberg numbers. A fifth-order upwinded WENO-Z [17] scheme is used to discretize the convective terms in the viscoelastic constitutive equations while all the other spatial derivatives are approximated using central differences. Time integration is achieved using a first order explicit Euler method both for the flow and viscoelastic model equations. Although it is straightforward to make the present numerical method second order accurate in time, a first order method is used here since the time stepping error is generally found to be negligibly small compared to the spatial error mainly due to a small time step imposed by the numerical stability of the present explicit scheme [67].

A separate Lagrangian grid is used to explicitly track the fluid-fluid interface. The Lagrangian grid consists of linked marker points (the front) moving with the local flow velocity interpolated from the stationary Eulerian grid. The piece of the Lagrangian grid

between two marker points is called a front element. The surface tension is computed on the Lagrangian grid and then distributed onto the Eulerian grid points near the interface to be added to the momentum equations in the form of body forces as described by Tryggvason et al. [127]. The indicator function is computed at each time step based on the location of the interface using the standard procedure [127] and is then used to set the fluid properties in each phase. The Lagrangian grid is restructured at every time step by deleting the front elements that are smaller than a prespecified lower limit and by splitting the front elements that are larger than a prespecified upper limit in the same way as described by Tryggvason et al. [127] to keep the front element size nearly uniform and comparable to the Eulerian grid size. It is critically important to restructure the Lagrangian grid since it avoids unresolved wiggles due to small elements and lack of resolution due to large elements. A complete description of the front-tracking method can be found in Tryggvason et al. [127] and the treatment of the viscoelasticity in Izbassarov and Muradoglu [67].

3.3 Problem Statement

The physical problem and computational domain are sketched in Fig. 3.1. The flow is assumed to be axisymmetric so only one half is used as the computational domain. The capillary tube contains a 4:1:4 contraction/expansion section. The radii of the main channel and the contraction are R_1 and R_2 , respectively. The total length of the tube is varied depending on the Reynolds number (Re). At higher Re , due to oscillation of the drop in the expansion region, longer tube is required to reach a steady-state. The tube has a total length of $60R_2$ and $130R_2$ for the range of $2 \leq Re < 10$ and $10 \leq Re \leq 100$, respectively. A sudden constriction of length $20R_2$ is located at $20R_2$ from the upstream as shown in Fig. 3.1. A spherical droplet of diameter d_d is placed instantly in a distance of $10R_2$ from the inlet. The flow is initiated instantaneously by imposing a fully-developed steady flow at the inlet and keeping the pressure constant at the outlet. Symmetry and no-slip boundary conditions are applied at the centerline and at the wall of the tube, respectively. The viscoelastic stress tensor at the inlet is specified based on the analytical solution assuming a fully developed pipe flow. The

Neumann boundary conditions are used for all viscoelastic stress components at the other boundaries. The governing equations are solved in their dimensional forms but the results are expressed in terms of relevant non-dimensional quantities. Using the average flow velocity V and the channel radius R_2 in the narrow part of channel as the velocity and length scales, respectively, and the time scale R_2/V , the governing non-dimensional numbers are defined as

$$\begin{aligned} Ca &= \frac{\mu_o V}{\sigma}, Re = \frac{\rho_o V R_2}{\mu_o}, Wi = \frac{\lambda V}{R_2}, \theta = \frac{\mu_i}{\mu_o}, \alpha = \frac{\rho_i}{\rho_o}, k = \frac{\lambda_i}{\lambda_o}, \beta = \frac{\mu_s}{\mu_p + \mu_s}, \\ \kappa &= \frac{d_d}{2R_2}, \end{aligned} \quad (3.7)$$

where Ca , Re and Wi are the capillary, Reynolds and Weissenberg numbers, respectively. The other parameters θ , α , k and β denote the total viscosity, density, relaxation time and solvent viscosity ratios, respectively. The relative droplet size κ is used as a measure for the confinement. The drop deformation is defined as

$$\text{deformation} = \frac{d_a - d_r}{d_a + d_r}, \quad (3.8)$$

where d_a and d_r are the maximum droplet dimensions in the axial and radial directions, respectively. The density ratio α is fixed to be unity, i.e., $\rho_i = \rho_o$, in all the results presented in this paper. Simulations are performed by varying only one parameter while keeping all the others constant in order to demonstrate the sole effects of the parameter on the flow. To facilitate this, we define a base case as $\theta = 1$, $\kappa = 1.25$, $Re = 2$, $Ca = 0.1$, $Wi = 1$, $L^2 = 25$ and $\beta = 0.5$. Note that the base case is selected to be consistent with the range of parameters used by Chung et al. [30, 31]

3.4 Results and Discussions

Extensive simulations are carried out to study the dynamics of viscoelastic two-phase systems in a pressure driven axisymmetric contraction/expansion capillary tube. A non-uniform Cartesian grid (Fig. 3.1) is employed in the computations. The grid is stretched near the contraction and expansion regions, where the largest stress gradients occur. A comprehensive grid convergence study is performed to determine the minimum grid size required to reduce the spatial discretization error below a threshold value. As detailed

in the Appendix, for $Re < 10$, a grid with 64 cells in the radial direction is sufficient to reduce the numerical error below 4% for all the flow quantities and thus this grid is used in all relevant computations presented in this paper. A finer grid containing 96 cells in the radial direction is used for $Re > 10$ and found to reduce the spatial error below 2% for all the flow quantities except for the case of the VN system at very high Weissenberg numbers (i.e., $Wi = 100$) for which the maximum error becomes as large as 9% in the vicinity of the expansion. Note that, although not shown here, the drop volume is preserved within 2% for all the cases considered in this study.

Simulations are first performed to examine the effects of various flow parameters on the drop dynamics in the NV, VN and VV systems at a low Reynolds number, i.e., $Re = 2$. Note that the Reynolds number is set to $Re = \mathcal{O}(1)$ to relax the restriction on time step due to numerical stability and thus to facilitate extensive numerical simulations. Then further simulations are performed to demonstrate the combined effects of inertia and viscoelasticity for the Reynolds and Weissenberg numbers up to $Re = 100$ and $Wi = 100$.

3.4.1 Computations at a Low Reynolds Number ($Re = 2$)

Effects of Confinement (κ)

First the effects of confinement on the drop dynamics are examined in the constriction region. The confinement is characterized by the relative droplet size κ and it is varied between $0.5 \leq \kappa \leq 1.75$ while keeping all other parameters fixed at their values in the base case. The results are shown in Fig. 3.2 for the VN case. The square root of the trace of conformation tensor ($\sqrt{\text{trace}(\mathbf{A})}$) is plotted as a measure of average polymer length. The enlarged version of the droplet in the middle of the constriction is also illustrated on the right side of each case in Fig. 3.2 to better show the details of drop deformation and viscoelastic stress distribution. Similar to the all Newtonian case [81], the drop shape is asymmetric, i.e., the curvature at the fore is higher than that at the aft, due to the pressure gradient in the axial direction. Large viscoelastic stresses are generated at the sides of the drop due to high shear stresses exerted by the continuous fluid, and then these stresses are convected by the internal circulation to create a stress

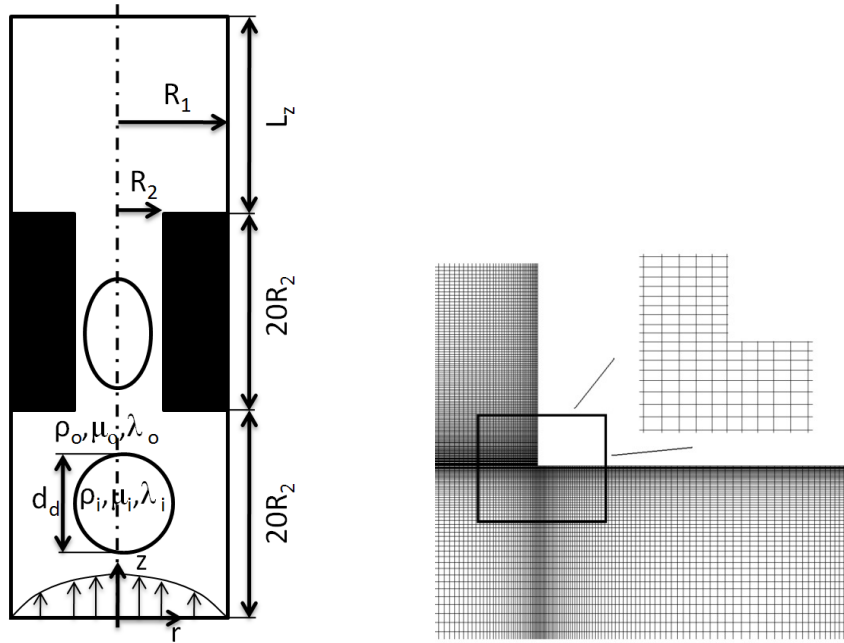


Figure 3.1: (left) Schematic illustration of a pressure-driven viscoelastic two phase system. (right) Mesh near the re-entrant corner.

concentration near the rear stagnation point, as shown in Fig. 3.2. Similar to the planar case studied by Chung et al. [30], the droplet takes a bullet like shape at low confinement and becomes more elongated as κ increases. The drop deformation is plotted in Fig. 3.3 against the dimensionless moving distance of the drop centroid defined as $z_d/2R_2$ where z_d is the axial distance of the drop centroid from its initial location. Note that the narrow pipe is located between $z_d/2R_2 = 5$ and $z_d/2R_2 = 15$. The drop undergoes a significant deformation for $\kappa \geq 0.8$ and the deformation grows rapidly as κ is further increased. In the entrance region, there is an overshoot in the drop deformation, which is more pronounced for smaller droplets. This overshoot is caused by the retraction of droplet after it enters the constriction. All the droplets reach a steady shape except for the largest one (i.e., $\kappa = 1.75$) in the narrow channel. In the expansion region, all drops swell towards the cross-stream direction making the deformation parameter negative and eventually reach a nearly spherical shape in the further downstream.

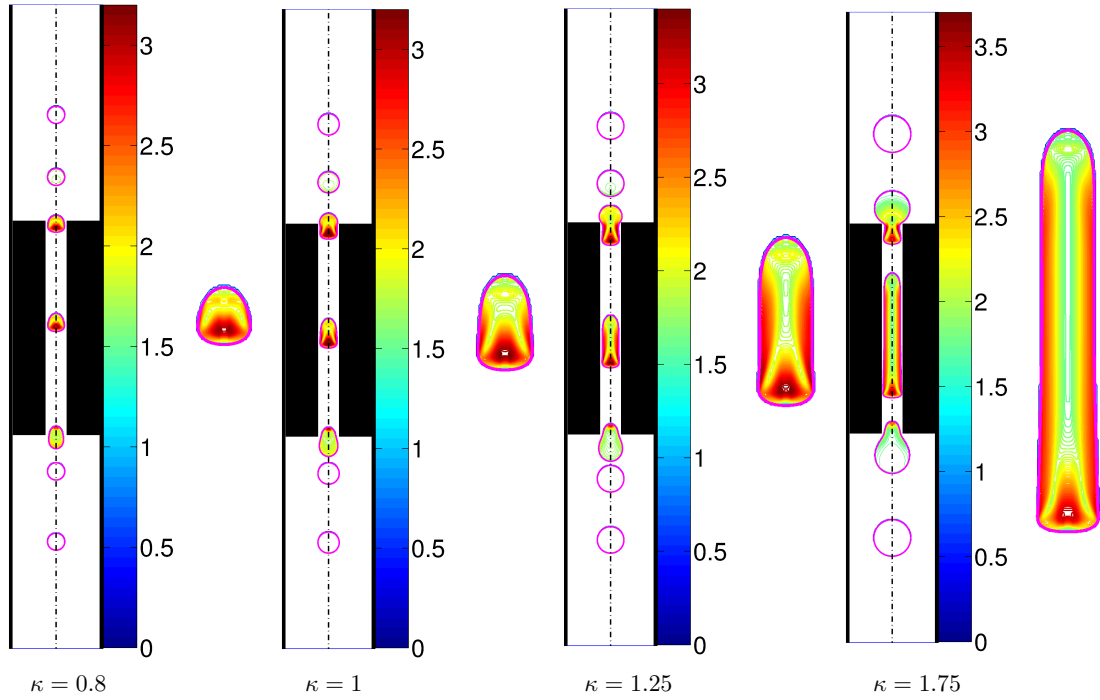


Figure 3.2: The effects of the relative drop size (κ) for the VN case. The evolution of droplet shape and contours of average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$ are plotted for a FENE-CR droplet moving in a Newtonian fluid. The enlarged version of the drop in the middle of the constriction is also shown on the right side of each case. ($Ca = 0.1, Re = 2, Wi = 1, Grid : 64 \times 768$).

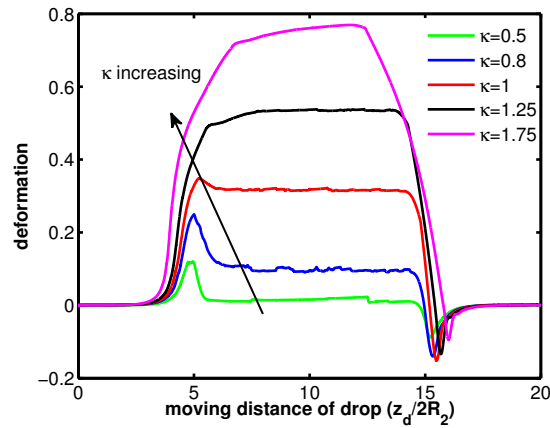


Figure 3.3: The effects of the relative drop size (κ) for the VN case. Drop deformation is plotted against the moving distance of the drop centroid for various κ ranging between $\kappa = 0.5$ and $\kappa = 1.75$. ($Ca = 0.1, Re = 2, Wi = 1, Grid : 64 \times 768$).

Effects of Weissenberg Number (Wi)

Next, we investigate the viscoelastic effects on drop dynamics at $Re = 2$. For low Re , viscoelastic effects are especially pronounced in the constriction region. It is known that the drop shape is strongly influenced by viscoelastic normal stress difference $A_{zz} - A_{rr}$ [30, 31, 67]. The drop shapes together with the contours of constant normal stress differences are shown in Figs. 3.4 and 3.5 for the VN and NV cases, respectively, for various combinations of Ca and Wi numbers. Since a steady droplet shape is not attained by the end of the constriction for high Ca and Wi number cases, the results are shown when the droplets are approximately at the middle of the constriction. For the VN case (Fig. 3.4), as Wi increases, the viscoelastic stresses increase in magnitude and penetrate further into the bulk of the drop. It is worth noting that, in contrast with the Oldroyd-B model, the FENE-CR model bounds the growth of normal stress difference. Therefore the increase in the maximum normal stress difference gets smaller when Wi exceeds a threshold value as can be seen in Fig. 3.4. Furthermore, decreasing surface tension enhances drop deformation and reduces strain rate inside the droplet. Thus, for higher Ca , the viscoelastic stresses inside the drop grow more slowly. This effect is more pronounced for $Wi < 10$. For up to a moderate Ca number (i.e., $0.05 \leq Ca \leq 0.2$), drop deformation is affected far less by the viscoelasticity than the capillary forces. Viscoelastic stresses inside the drop at the rear stagnation point pull the interface inwards resulting in a slight indentation at the trailing edge. As Ca increases, the droplet becomes more elongated and its leading edge bulges. The bulge formation is caused by the surface tension that increases the pressure inside the high curvature at the tip of the interface and in turn pulls the tip towards the main body of droplet [56]. As can be seen in Figs. 3.4 and 3.5 bulge formation occurs at $Ca = 0.5$. The bulge formation is more pronounced in the VN case since the viscoelastic stresses accumulate in the vicinity of neck region of the bulge (Fig. 3.4), which in turn enhances bulge formation by pulling the interface towards the front tip.

For the NV case, when the drop is in the constriction, large normal stress differences develop in the film region as well as the regions around rear and front stagnation points (Fig. 3.5). For low to moderate Ca ($0.05 \leq Ca \leq 0.1$), the drop occupies major width of

the constriction while, at high Ca ($Ca = 0.5$), the drop forms a thin extended filament with a pointed end, occupying only a small portion of the constriction width. A notable difference with the VN case is that the trailing end of the drop is stretched out when $Ca = 0.5$ and Wi increases up to $Wi = 10$. This is mainly due to the stretching of the interface by polymer stresses concentrated around the rear stagnation point. For a higher Wi number ($Wi > 10$), the viscoelastic stresses become stronger but penetrate over the entire cross-section to make the stress distribution more uniform, which dramatically changes the drop deformation. The most striking effect is that the trailing end is not extended anymore at high Wi numbers even for $Ca = 0.5$. The non-monotonic droplet deformation has been also observed for a NV system in a shear flow by Yue et al. [139] as well as Aggarwal and Sarkar [2], and in a converging pipe flow by Zhou et al. [148]. The deformation is plotted in Fig. 3.6 against the moving distance of the drop centroid for both the VN and NV systems. It is generally observed that the viscoelasticity has a weaker effect on drop deformation in the VN case than that in the NV case. In the NV case, the viscoelastic effects are non-monotonic, i.e., the deformation first increases and then decreases with Wi . Although not shown here, an increase in the elasticity ratio k in the VV system decreases drop deformation resulting in a consistent pattern with that shown in Fig. 3.6.

Effects of Total Viscosity Ratio (θ)

We next examine the effects of drop-to-matrix viscosity ratio θ . The droplet shapes and the constant contours of normal stress differences are plotted in Figs. 3.7 and 3.8 for the VN and NV cases, respectively, in the middle of the constriction. These figures clearly show great sensitivity of drop deformation to θ . As θ increases, the viscous normal stresses grow and eventually dominate over the combination of viscoelastic normal stresses and surface tension, leading to development of a re-entrant cavity. In a straight capillary tube, the viscoelasticity in drop/matrix fluid generally opposes/enhances drop deformation. However, as seen in Figs. 3.7 and 3.8, the re-entrant cavity occurs at a lower value of θ in the NV case compared to the VN system in the constricted channel. For instance, the re-entrant cavity forms in the NV system at $\theta = 20$ (Fig. 3.8) while the drop remains intact for the VN system for the same viscosity ratio (Fig. 3.7). This

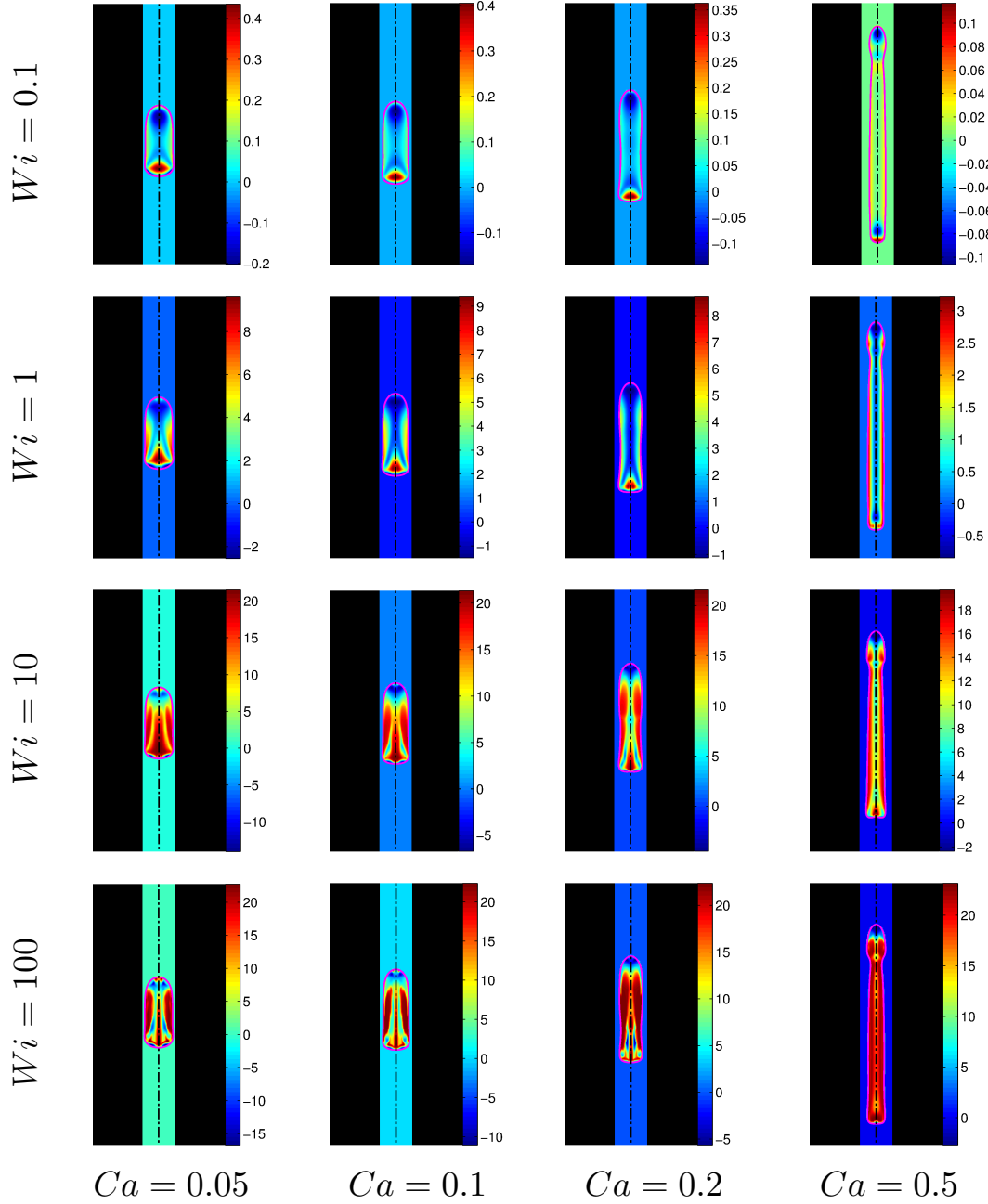


Figure 3.4: The effects of the capillary and Weissenberg numbers for the VN case. The droplet shapes and the constant contours of the difference between the normal components of the conformation tensor $A_{zz} - A_{rr}$ in the vicinity of the droplet in the middle of the constriction. ($Re = 2, \kappa = 1.25, Grid : 64 \times 768$).

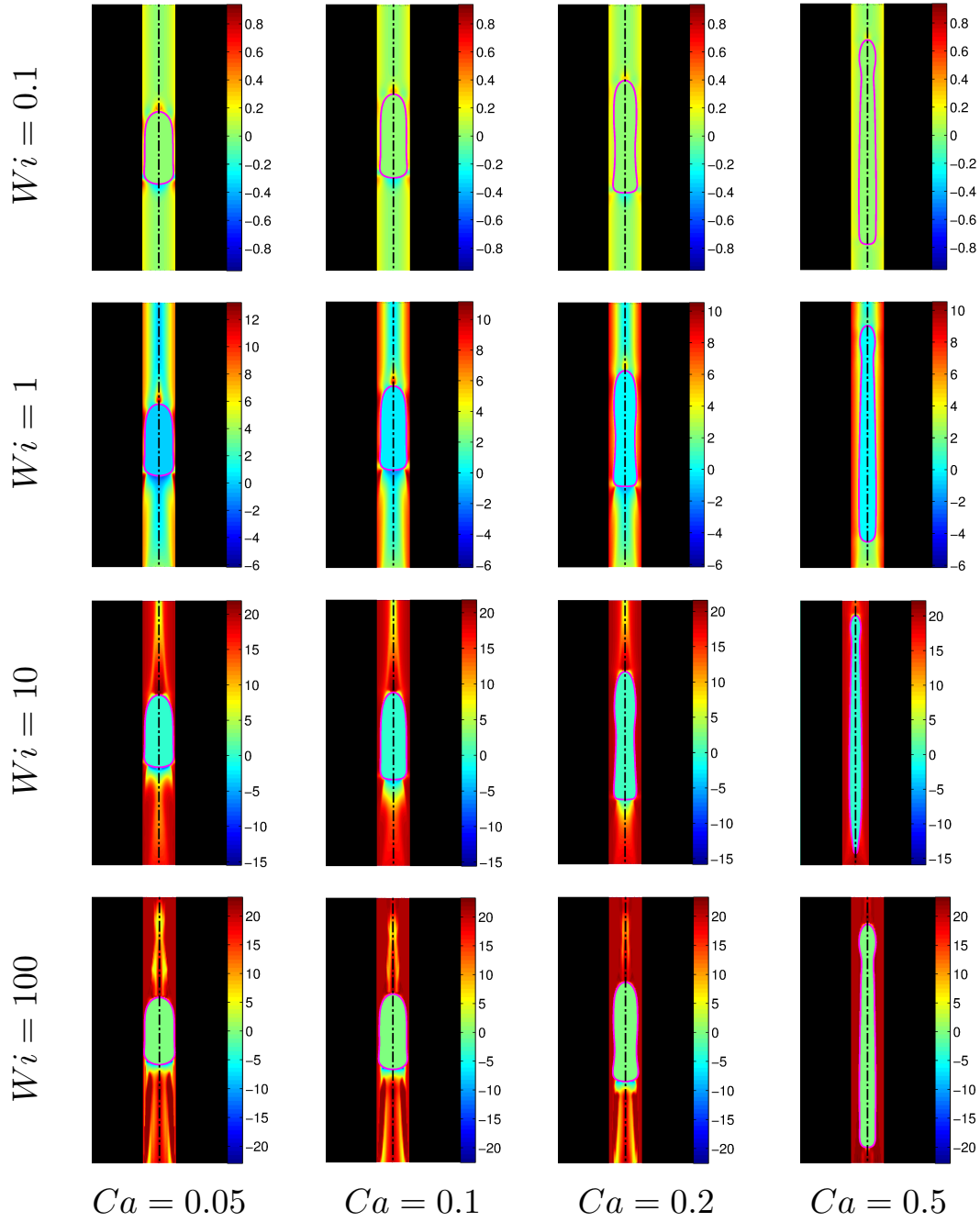


Figure 3.5: The effects of the capillary and Weissenberg numbers for the NV case. The droplet shapes and the constant contours of the difference between the normal components of the conformation tensor $A_{zz} - A_{rr}$ in the vicinity of the droplet in the middle of the constriction. Note that $Wi = 10$ and $Ca = 0.5$ case is not in the same scale with the other snapshots. ($Re = 2, \kappa = 1.25, Grid : 64 \times 768$).

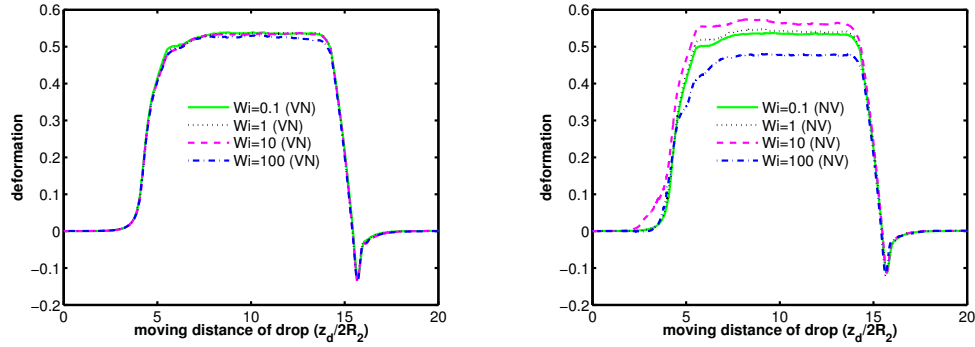


Figure 3.6: Effects of fluid elasticity on drop deformation for the VN (left) and NV (right) cases. The deformation parameter is plotted against the moving distance of the drop centroid for various Wi ranging between $Wi = 0.1$ and $Wi = 100$. ($Ca = 0.1$, $Re = 2$, $\kappa = 1.25$, $Grid : 64 \times 768$).

is a direct result of the viscoelastic stress distribution at the back of the droplet when it enters the constriction as shown in Figs. 3.9 and 3.10 where the transient motion of a droplet is shown for the NV and VN cases, respectively. Note that the Weissenberg number is increased in these figures to better demonstrate the stress distribution in the vicinity of the droplet. As seen, just before entering the constriction, a viscoelastic stress concentration occurs at the back of the droplet pushing the trailing edge to cause an indentation and subsequently a re-entrant cavity formation in the NV case. On the other hand, in the VN case, the viscoelastic stress concentration occurs at the shoulder of the droplet that acts against the viscous stresses to restore the indentation of the trailing edge. The re-entrant cavity grows continuously while the droplet is in the narrow channel and the entrained ambient fluid is eventually encapsulated within the main drop to form a bigger compound drop. The re-entrant cavity formation has been previously observed for all Newtonian[94, 129, 47] and viscoelastic [59] systems in circular tubes[94, 129] as well as in planar channels[59, 47]. Note that Harvie et al. [59] reported only a few cases and only for a VN system in a similar constricted but a planar configuration. Once the indentation occurs at the entrance, the overall features of the re-entrant cavity formation and encapsulation are similar for both the VN and NV systems. The dorsal filaments created at the rear edge of the droplet excessively elongate especially for the NV system,

which may even lead to a breakup. Note that the breakup is allowed only along the channel centerline in the present implementation of the numerical method and thus long posterior threads are not allowed to rupture. The dorsal filaments of the drop are thicker and shorter in the VN case than that in the NV case, so a posterior thread rupture is more likely to occur in the NV system. It is emphasized that, in spite of its great importance in applications, the drop breakup is not studied in details here since it is out of the scope of the present study.

It is evident that viscoelastic effects are important for the development of a puckered end and a re-entrant cavity. Therefore, further simulations are performed for the VN case for various Wi numbers, and the results are shown in Fig. 3.11. The viscosity ratio is fixed at $\theta = 40$. It is interesting to observe that the viscoelasticity has a non-monotonic effect on the drop deformation, i.e., the size of the re-entrant cavity and resulting inner droplet first decrease and then increase with Wi . This behavior is mainly attributed to the fact that the polymer stresses take a finite time ($T_{elas} \sim \lambda$) to react to the flow. As mentioned before, the re-entrant cavity is essentially created in the entrance region. Since the flow time scale is proportional to the time required for the droplet to fully enter into the narrow channel, the relevant flow time scale is $T_{flow} \sim 2R_2/V$. Thus the flow time scale is much smaller than the viscoelastic response time, i.e., $T_{flow} \ll T_{elas}$ when $Wi \gg 1$. As a result, the viscoelastic droplet behaves more like a Newtonian droplet in the entrance region for a sufficiently large Wi number.

The effects of viscosity ratio on drop deformation are quantified in Fig. 3.12 both for the VN and NV cases. The drop deformation increases with the viscosity ratio in the both systems with a similar trend but a drop undergoes larger deformation in the NV system than that in the VN system. In the constriction region, a less viscous drop reaches a steady state very quickly while a more viscous drop continuously elongates and exits the constriction without reaching a steady motion. As demonstrated by Hooper et al. [62], a more viscous drop reacts the exterior flow more slowly so its initial deformation lags that of a less viscous drop. However, it eventually attains larger deformation provided that the capillary number is below the critical value for a breakup and the narrow section is sufficiently long. The slower initial reaction is due to a longer emulsion time (i.e., $T_{emulsion} = \mu_i d_d / \sigma$) [112] and the greater steady-state deformation is due to the fact that

more viscous interior sustains higher internal stresses [148]. Similarly, the experimental study of Olbricht and Kung [94] showed that the time scale for reaching a steady drop deformation increases with θ . We finally note that the computational time is highly increased with θ due to time step restriction as well as the finer grid required to resolve very large drop deformations.

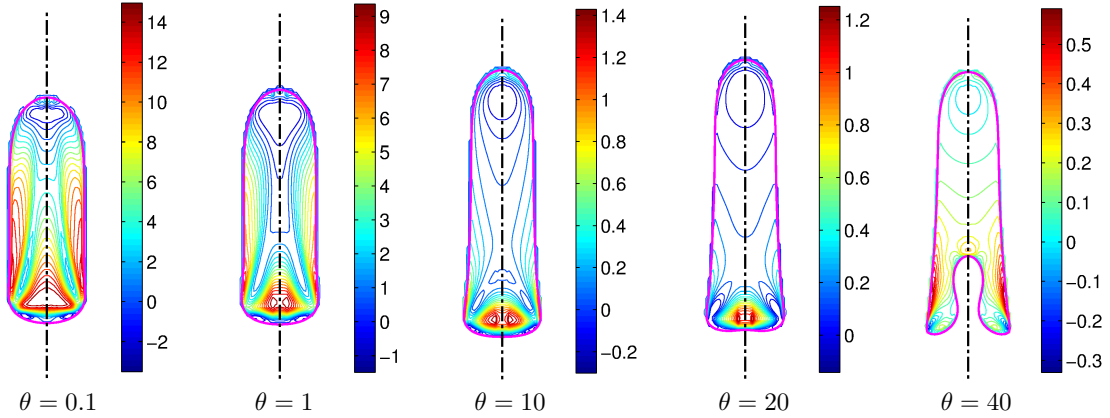


Figure 3.7: The effects of viscosity ratio (θ) for the VN case. The droplet shapes and the constant contours of the difference between the normal components of the conformation tensor $A_{zz} - A_{rr}$ in the vicinity of the droplet in the constriction. ($Ca = 0.1, Re = 2, Wi = 1, \kappa = 1.25, Grid : 64 \times 768$).

Effects of Extensibility (L^2) and Solvent Viscosity Ratio (β)

Further simulations are carried out to examine the effects of solvent viscosity ratio and the extensibility parameter in the range of $0.1 \leq \beta \leq 0.9$ and $25 \leq L^2 \leq 400$, respectively. Although not shown here due to space considerations, it is found that the effects of β and L^2 are negligible for the VN case, so results are presented only for the NV system. The drop deformation is plotted in Fig. 3.13 for $Wi = 10$ and $\beta = 0.1, 0.5$ and 0.9 while keeping the other parameters the same as the base case. In fact, the solvent viscosity ratio essentially modifies the effective Weissenberg number defined as $Wi' = Wi(1 - \beta)$, see for instance, Aggarwal and Sarkar [2]. Thus increasing β has a similar effect as decreasing the Weissenberg number. The drop deformation generally increases as β decreases and the effects of β are moderate for $Wi = 10$. Note that, although not shown here, β has

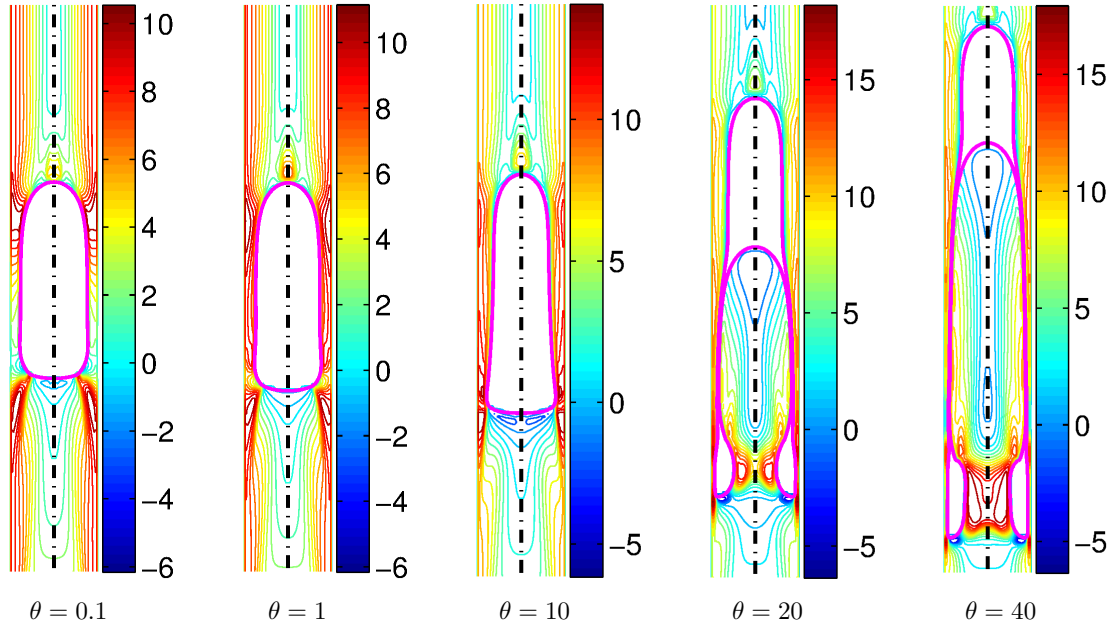


Figure 3.8: The effects of viscosity ratio (θ) for the NV case. The droplet shapes and the constant contours of the difference between the normal components of the conformation tensor $A_{zz} - A_{rr}$ in the vicinity of the droplet in the constriction. ($Ca = 0.1$, $Re = 2$, $Wi = 1$, $\kappa = 1.25$, $Grid : 64 \times 768$).

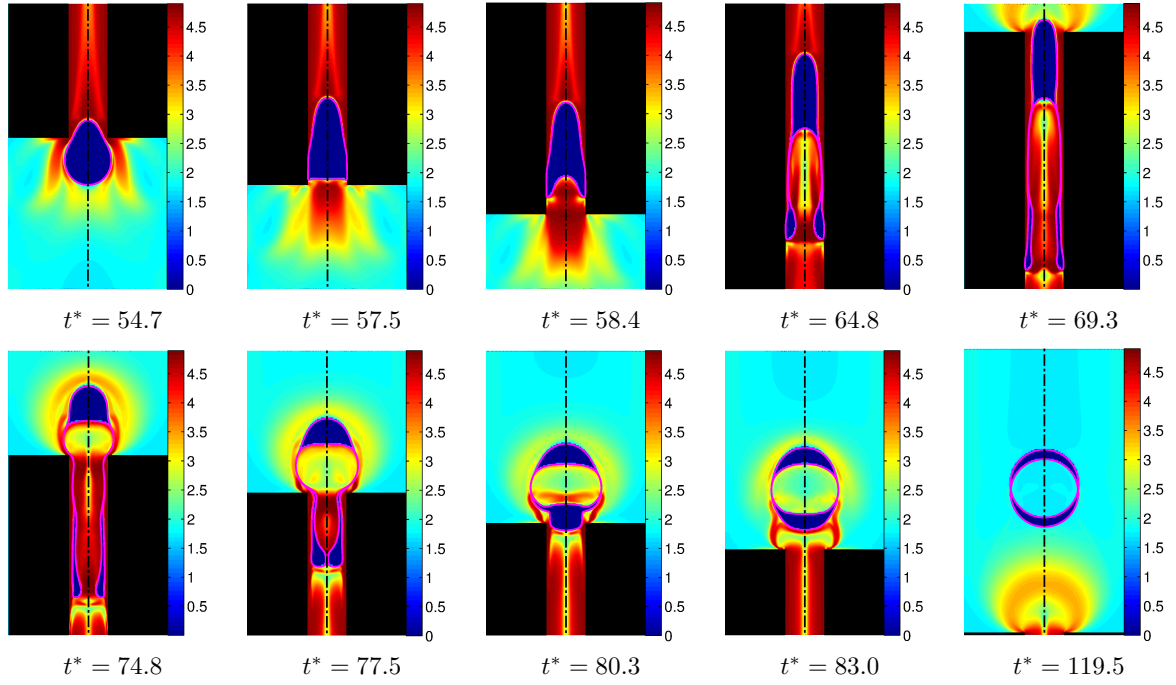


Figure 3.9: A Newtonian droplet moving through a FENE-CR fluid in a pressure driven contraction/expansion capillary tube. The contours represent the average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$. ($Ca = 0.1, Re = 2, Wi = 10, \theta = 20, Grid : 64 \times 768$).

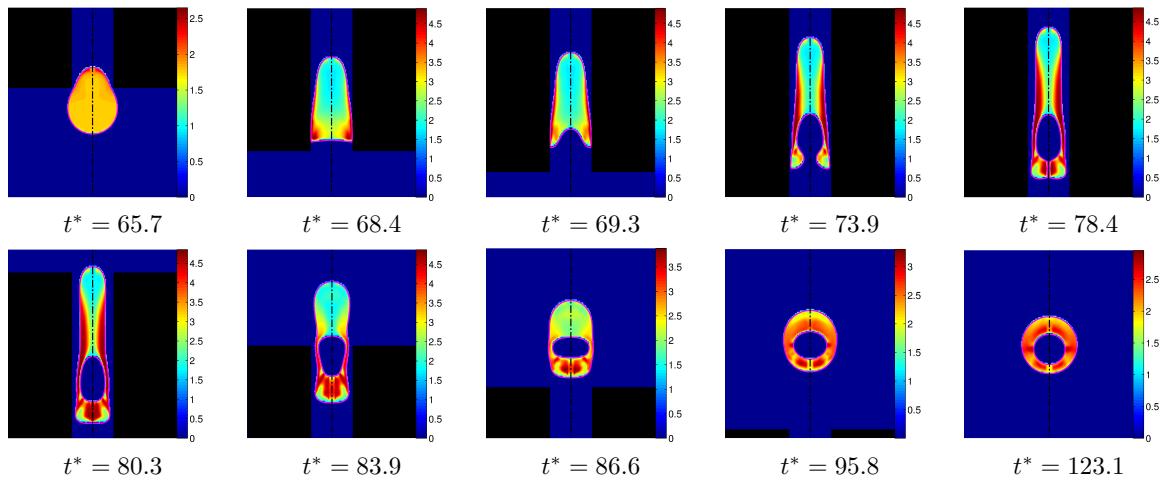


Figure 3.10: A FENE-CR droplet moving through a Newtonian fluid in a pressure driven contraction/expansion capillary tube. The contours represent the average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$. ($Ca = 0.1, Re = 2, Wi = 100, \theta = 40, Grid : 64 \times 768$).

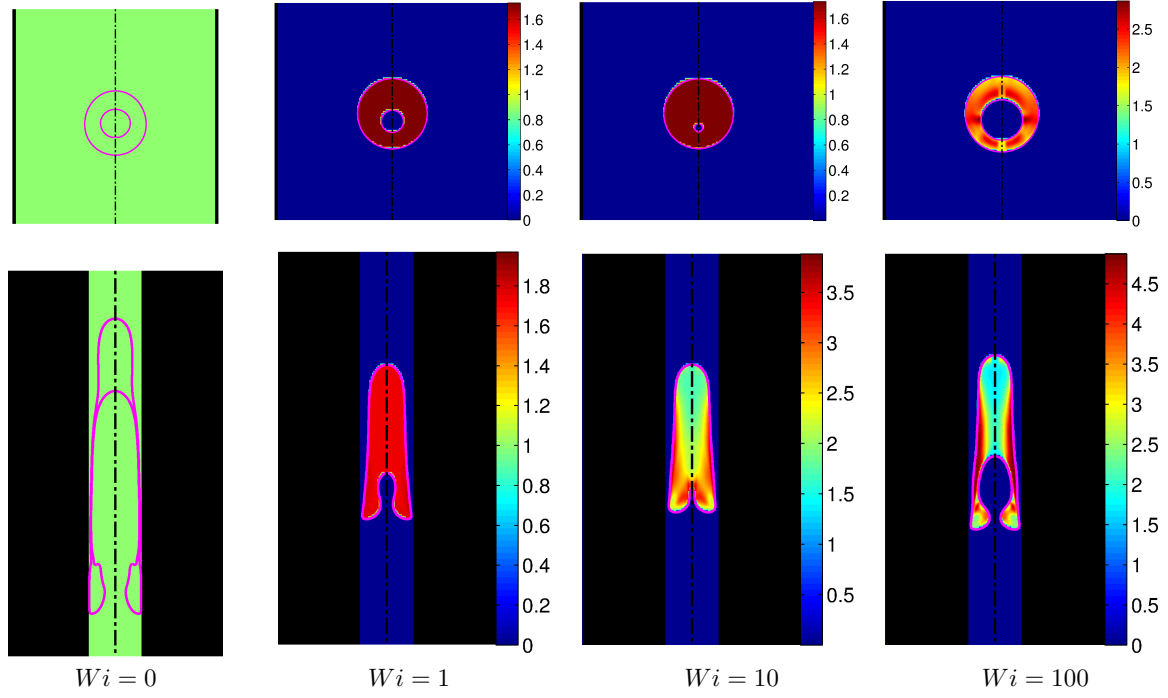


Figure 3.11: The effects of fluid elasticity on drop deformation at a high viscosity ratio of $\theta = 40$ for the NN and VN cases. The droplet shapes and the constant contours of the average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$ are plotted in the vicinity of the droplet in the middle of the constriction (bottom plots) and in the further downstream of the expansion region (top plots). ($Ca = 0.1, Re = 2, \kappa = 1.25, Grid : 64 \times 768$).

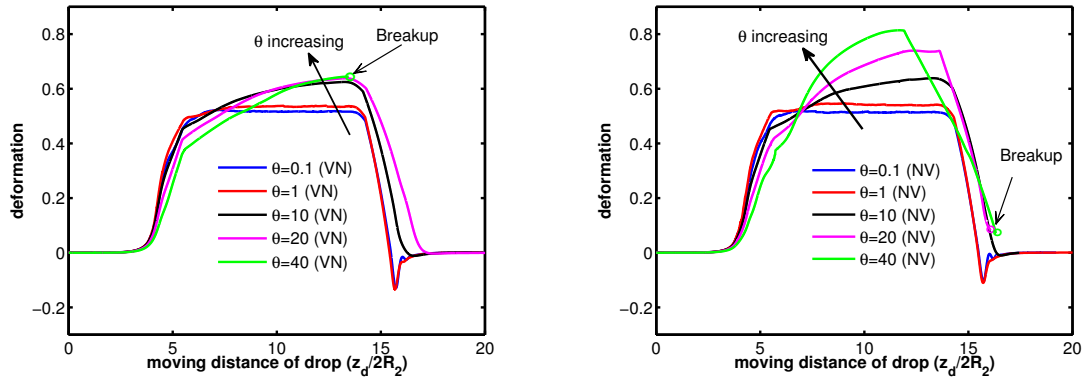


Figure 3.12: The effects of viscosity ratio (θ) on drop deformation for the VN and NV cases. The deformation parameter is plotted against the moving distance of the drop centroid for various θ ranging between $\theta = 0.1$ and $\theta = 40$. ($Ca = 0.1, Re = 2, Wi = 1, \kappa = 1.25$).

negligible influence on drop deformation for $Wi = 1$. Since the effective Weissenberg number increases with decreasing β and the drop deformation is not very sensitive to Wi around $Wi = 1$, these results are consistent with the effects of Wi number (see, e.g., Fig. 3.6). Similar results are also found for the effects of L^2 on drop deformation as shown in Figs. 3.13 and 3.14. The larger L^2 , the more the molecule can be extended leading to enhanced viscoelastic effects. Viscoelastic stresses significantly increase with L^2 which in turn increase the deformation of the drop as shown in Figs. 3.13 and 3.14. A particular case is an infinite extension ($L^2 \rightarrow \infty$) which corresponds to the well-known Oldroyd-B model. These results are consistent with the fact that the viscoelasticity in the continuous phase enhances drop deformation as discussed before.

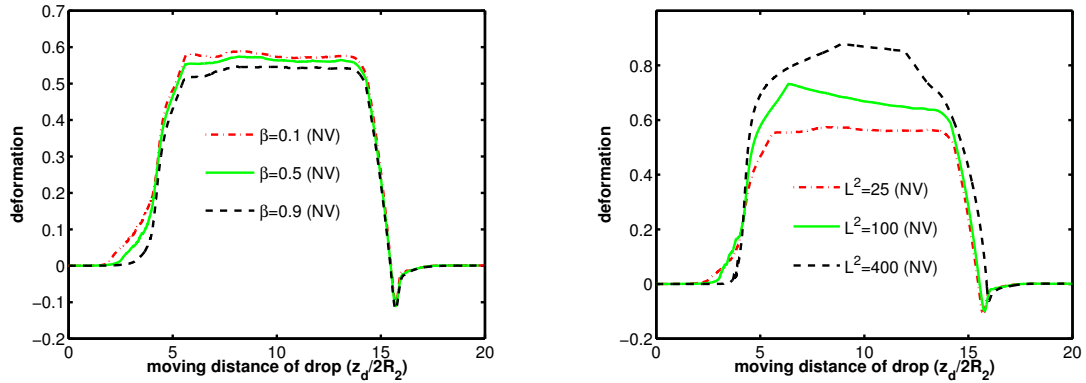


Figure 3.13: The effects of solvent viscosity ratio (β) (left plot) and extensibility (L^2) (right plot) on drop deformation for the NV case. The deformation parameter is plotted against the moving distance of the drop centroid for various β ranging between $\beta = 0.1$ and $\beta = 0.9$ and L^2 ranging between $L^2 = 25$ and $L^2 = 400$. ($Ca = 0.1$, $Re = 2$, $Wi = 10$, $\kappa = 1.25$, $Grid : 64 \times 768$).

3.4.2 Computations at High Reynolds Numbers

Finally, simulations are performed to study the role of viscoelasticity at high Re for the VN, NV and VV systems. Sample results are shown in Figs. 3.15 and 3.16 to show the overall droplet shape evolution together with the contours of average polymer extension for two different VV cases. The Reynolds number and fluid elasticity ratio are fixed at

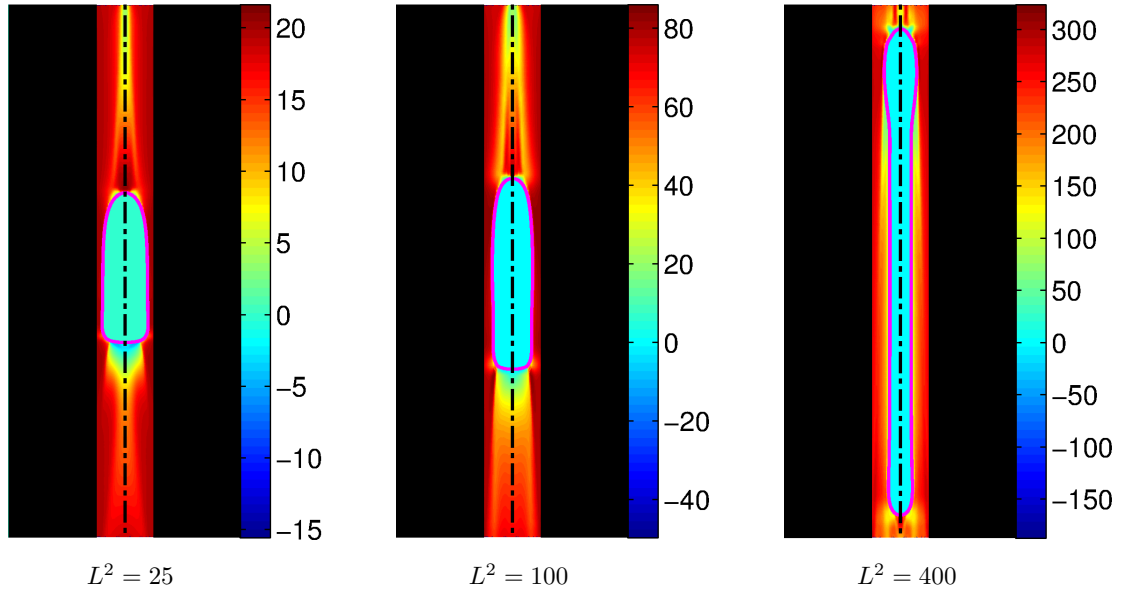


Figure 3.14: The effects of extensibility (L^2) on drop deformation for the NV case. The droplet shapes and the constant contours of the difference between the normal components of the conformation tensor $A_{zz} - A_{rr}$ are plotted in the vicinity of the droplet in the middle of the constriction. ($Ca = 0.1$, $Re = 2$, $Wi = 10$, $\kappa = 1.25$, $Grid : 64 \times 768$).

$Re = 100$ and $k = 0.1$ for both cases while the inner and outer Weissenberg numbers are selected differently to demonstrate the effects of viscoelasticity, i.e., $(Wi_i, Wi_o) = (1, 10)$ and $(10, 100)$ in Figs. 3.15 and 3.16, respectively. In both cases, as the droplet moves into the constriction, it first elongates and then retracts slowly. After entering the narrow channel, its leading edge bulges. The elongation is mainly due to the fact that the inertial forces become dominant over the other forces. The bulge formation occurs more severely at high Re numbers as seen in Figs. 3.15 and 3.16. In addition, a bulge also forms at the trailing edge at high Wi numbers. At the trailing tip, the surface tension and viscoelastic stresses inside the droplet act in the same direction to increase the radius of the tip and thus to enhance the bulge formation. The stability of the bulge is determined by the competition between four forces: The viscous and the viscoelastic stresses in the ambient fluid are directed away from the bulk of the droplet promoting a breakup while viscoelastic stresses in the drop fluid and the surface tension act to pull the bulge back towards the bulk of the droplet and thus suppressing the breakup. Depending on the net resultant force, the bulge at the trailing edge may break up in some cases (Fig. 3.16).

Strong interactions between the inertia, surface tension and viscoelastic stresses result in very rich and highly complicated dynamics both in the constriction and expansion regions. The droplet undergoes large deformation in the narrow channel followed by shape oscillations in the expansion region. These oscillations sustain for a long time in the downstream of the expansion, and thus require a long expansion pipe to reach a steady state. Similar oscillations were also observed by Carroll [22] for an all-Newtonian drop system in a capillary tube with a sudden expansion at high Re numbers, i.e., up to $Re = 200$. However, Carroll [22] considered a relatively small droplet size (e.g., $\kappa = 0.7$) so the magnitude of shape oscillations were significantly smaller than those in the present study. Drop breakup is also observed in the narrow channel near the expansion in some cases, see e.g., Fig. 3.16.

The effects of viscoelasticity on drop deformation at a high Reynolds number are further studied for the VN, NV and VV systems. First simulations are carried out for the VN and NV cases at $Re = 50$ and the Weissenberg number ranging between $Wi = 0$ (all Newtonian) and $Wi = 100$. Comparing Figs. 3.17 and 3.6 reveals that the inertia significantly enhances drop deformation especially in the constriction and expansion

regions both for the VN and NV cases. Similar to the low Re case, the effects of Wi on drop deformation are non-monotonic and more pronounced for the NV case in the narrow channel. However, unlike the low Re cases, drop deformation increases rapidly, reaches a maximum close to the entrance of the constriction and then decreases continuously until it exits the narrow channel. The droplet undergoes large damped oscillations in the expansion region and reaches a steady motion after about $50R_2$ in the downstream of the expansion. Wi has a non-monotonic effect on the shape oscillations in both the VN and NV cases. For the VN case, the amplitude of oscillation first increases and then decreases with Wi while it is just opposite for the NV case.

We next consider the VV case. For this purpose, first the Weissenberg number of the outer fluid is fixed at $Wi_o = 1$ and the simulations are performed for the Weissenberg numbers of the inner fluid $Wi_i = 0.1, 1$ and 10 , which correspond to the elasticity ratio of $k = 0.1, 1$ and 10 , respectively. The Reynolds number is set to $Re = 100$ and the results are shown in Fig. 3.18. The overall deformation pattern resembles the VN case for moderate Weissenberg numbers, see e.g., Fig. 3.17. This is not surprising since the viscoelasticity of the outer fluid is kept fixed similar to the VN case with only difference being a non-zero value of the Weissenberg number. As k increases, the amplitude of the oscillations in the expansion region increases. The drop deformation exceeds a critical value leading to a drop breakup in the constriction near the expansion region. Then simulations are also performed by fixing the inner Weissenberg number at $Wi_i = 1$ and varying the outer Weissenberg number as $Wi_o = 0.1, 1$ and 10 (Fig. 3.18). This case resembles the NV system. The effects of k on overall drop dynamics and deformation are similar to the previous case, i.e., the amplitude of surface oscillation in the expansion region increases as k increases. Note that, for the same value of k , the drop undergoes a larger deformation for the case in which Wi_o is kept constant. Therefore we can conclude that the values of Wi_i and Wi_o as well as their ratio k are important for the VV case.

Finally the sole effects of Reynolds number are examined both for the VN and NV cases. For this purpose, the Reynolds number is varied in the range $2 \leq Re \leq 100$ while fixing all other parameters at their values in the base case. The results are shown in Fig. 3.19 for the VN and NV cases. As can be seen in these figures, the drop deformation and amplitude of surface oscillations generally increase with Re . The surface oscillations

exhibit a transition from an over damped regime for up to $Re = \mathcal{O}(1)$ to an under damped regime for $Re > 10$. Similar observations have also been made by Carroll [22] for an all Newtonian case. In the expansion region, maximum amplitude of oscillation increases monotonically with a phase shift as Re increases both for the VN and NV cases. Eventually a drop breakup occurs in the constriction for $Re = 100$ and $Wi = 1$ in the VN case as indicated by a circle in Fig. 3.19. It can be seen that the trend is the same for all the systems but oscillations are more pronounced for the VN case.

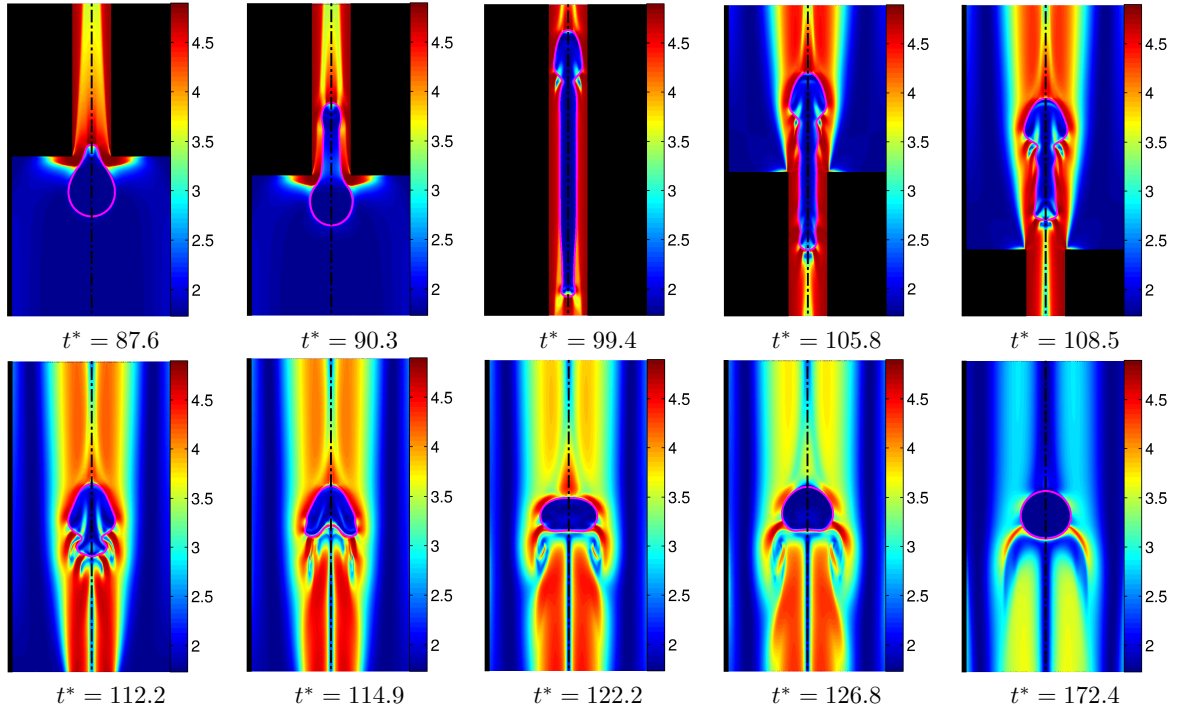


Figure 3.15: A FENE-CR droplet moving through another FENE-CR fluid in a pressure driven contraction/expansion capillary tube at $Wi_i = 1$ and $Wi_o = 10$. The contours represent the average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$. ($Ca = 0.1$, $Re = 100$, $Grid : 96 \times 2496$).

3.5 Conclusions

The effects of viscoelasticity on drop dynamics and deformation in a pressure-driven capillary tube with a sudden contraction/expansion are studied computationally using

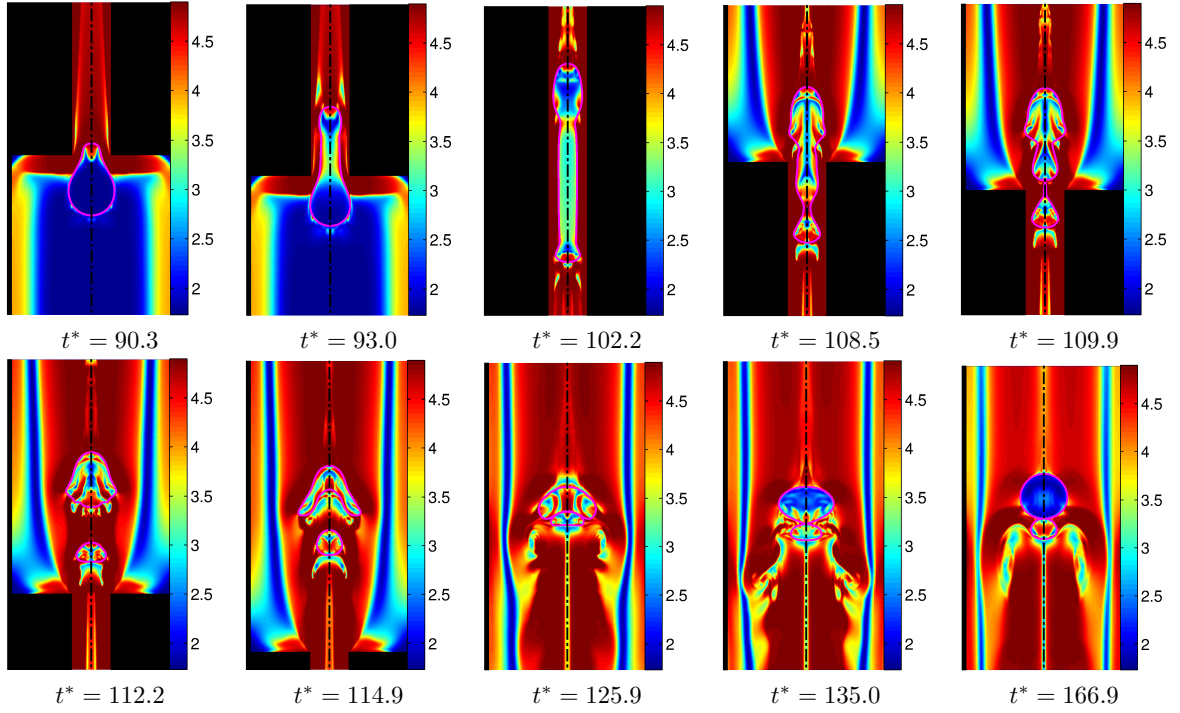


Figure 3.16: A FENE-CR droplet moving through another FENE-CR fluid in a pressure driven contraction/expansion capillary tube at $Wi_i = 10$ and $Wi_o = 100$. The contours represent the average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$. ($Ca = 0.1, Re = 100, Grid : 96 \times 2496$).

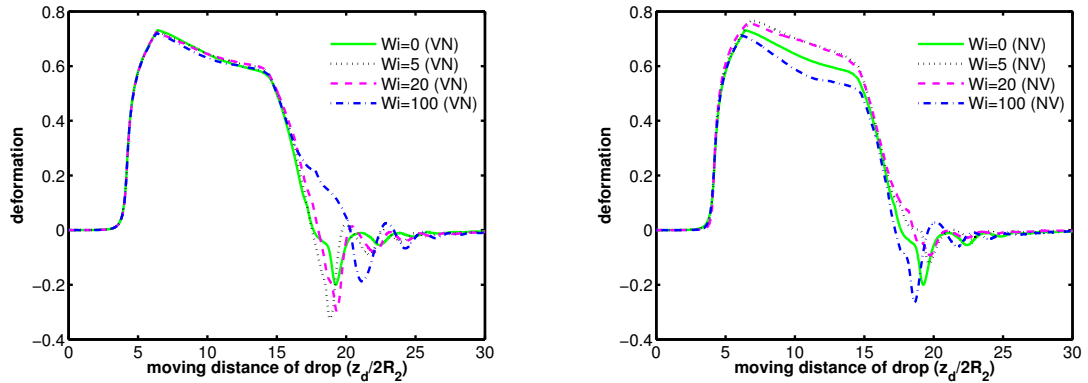


Figure 3.17: The effects of fluid elasticity on drop deformation at a high Reynolds number $Re = 50$ for the VN and NV cases. The deformation parameter is plotted against the moving distance of the drop centroid for various Wi numbers ranging between $Wi = 0$ (Newtonian) and $Wi = 100$. ($Ca = 0.1, \kappa = 1.25, Grid : 96 \times 2496$).

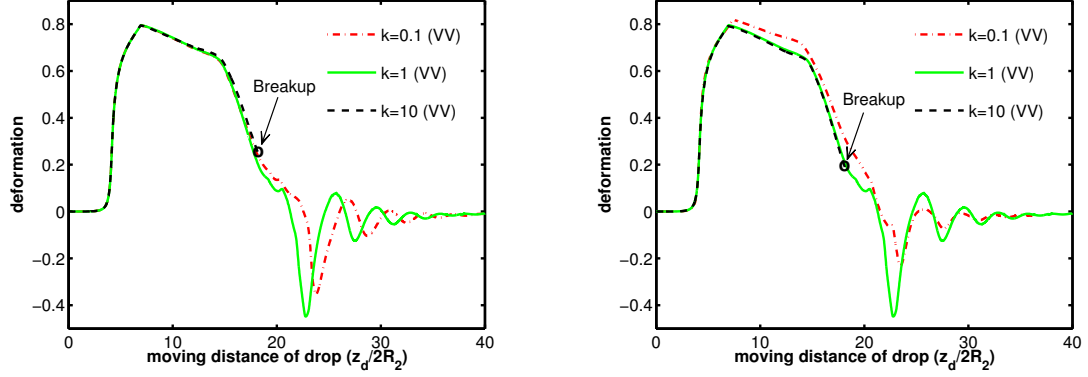


Figure 3.18: Effects of fluid elasticity ratio (k) on drop deformation. The inner and outer Weissenberg numbers are set to $Wi_o = 1$ and $Wi_i = 0.1, 1, 10$ (left) and $Wi_i = 1$ and $Wi_o = 0.1, 1, 10$ (right) for the VV cases. The deformation parameter is plotted against the moving distance of the drop centroid for various k ranging between $k = 0.1$ and $k = 10$. ($Ca = 0.1$, $Re = 100$, $\kappa = 1.25$, $Grid : 96 \times 2496$)

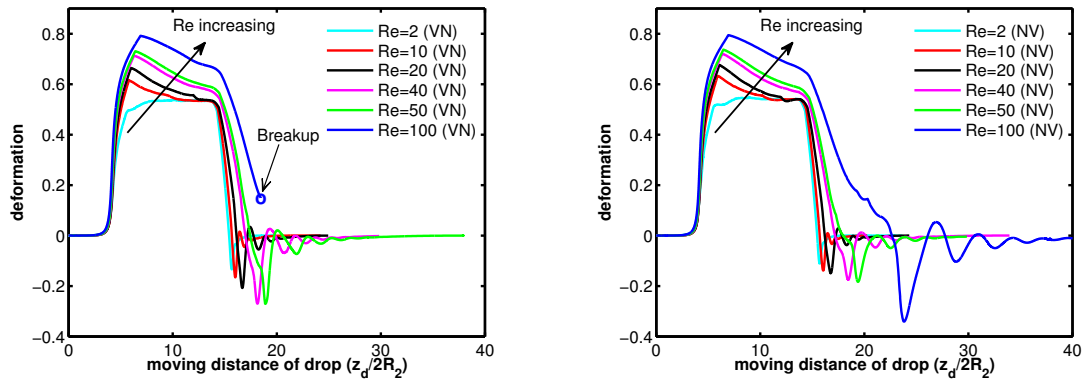


Figure 3.19: Effects of inertia on drop deformation for the VN (left) and NV (right) cases. The deformation parameter is plotted against the moving distance of the drop centroid for various Re ranging between $Re = 2$ and $Re = 100$. ($Ca = 0.1$, $\kappa = 1.25$, $Wi = 1$, $Grid : 96 \times 2496$).

a front-tracking method. A Newtonian drop in a viscoelastic medium (NV), a viscoelastic drop in a Newtonian medium (VN) and a viscoelastic drop in another viscoelastic medium (VV) cases are considered. The FENE-CR model is employed to account for viscoelasticity of inner and outer fluids. Extensive simulations are performed to examine the effects of relevant dimensionless parameters including the viscosity ratio (θ), the relative droplet size (κ), the Reynolds number (Re) and the capillary number (Ca) as well as the fluid elasticity characterized by the Weissenberg number (Wi), solvent viscosity ratio (β) and the extensibility parameter (L^2). In the VV case, the effects of the inner and outer Weissenberg numbers (Wi_i and Wi_o) as well as their ratio (k) are also examined.

At a low Reynolds number ($Re = 2$), it is found that the drop deformation generally increases as the relative droplet size and capillary number increase similar to the all Newtonian system. The Weissenberg number is found to have a non-monotonic influence on drop dynamics for both the VN and NV systems. At a low to moderate Reynolds number ($Re < 10$), the drop deformation first increases/decreases as Wi increases up to $Wi = \mathcal{O}(10)$ and decreases/increases as Wi increases further for the NV/VN case. At small Wi , the viscoelastic stresses are mainly generated near the interface at the side of the drop and convected towards the trailing edge by the external/internal flow for the NV/VN cases, leading to a stress concentration in the vicinity of the rear stagnation point. This stress concentration pulls out/in the drop interface to cause a pointed/rounded trailing edge in the NV/VN case. As Wi is further increased, e.g., $Wi = 100$, the viscoelastic stresses become more uniform in the dispersed/continuous phase and thus reduce the overall viscoelastic effects on drop deformation in the VN/NV system. We found that L^2 and $1 - \beta$ have a similar effect and both increase drop deformation for the NV case. The effects of these parameters are found not to be very significant for the VN case. It is found that the viscosity ratio has a significant influence and generally increases drop deformation. A re-entrant cavity may develop at the back of the droplet as the viscosity ratio increases. In contrast with the straight channel case, the viscoelasticity in the drop phase hinders whereas in the continuous phase enhances the formation of a re-entrant cavity in the constricted channel. It is found that this unexpected behavior is primarily due to the viscoelastic stress distribution at the back

of the droplet when the droplet enters the constriction. However, at sufficiently high Wi , the droplet enters the narrow channel before the viscoelastic stresses are fully developed, so the droplet behaves more like a Newtonian droplet in the entrance region. The viscoelastic stresses then develop in the narrow channel and the viscoelastic effects resemble those in the two-phase viscoelastic systems in a straight tube.

At high Re , the droplet exhibits very rich dynamics with highly complicated deformation and stress distribution patterns. In particular, the droplet undergoes large deformation in the constriction followed by damped surface oscillations in the expansion region. Similar to the low Re case, Wi also has a non-monotonic effect on drop deformation at high Re numbers. In the expansion region, the magnitude of surface oscillation first increases/decreases and then decreases/increases with Wi for the VN/NV case. The large deformation may even lead to a drop breakup in some cases, especially at high Re and Wi numbers. The drop breakup occurs near the end of the narrow channel. The surface oscillations are generally more pronounced for the VN case. In the VV case, the surface oscillations generally increase with the elasticity ratio (k) but the values of the inner and outer Weissenberg numbers are also found to be important for drop dynamics.

3.6 Acknowledgement

The authors are grateful to the Scientific and Technical Research Council of Turkey (TUBITAK) for the support of this research through Grant 112M181 and Turkish Academy of Sciences (TUBA). The authors are grateful for the use of the computing facilities at TUBITAK-ULAKBIM, High Performance and Grid Computing Center.

3.7 Appendix: Grid Convergence

Extensive computational simulations are performed to determine the minimum grid size required to reduce the spatial discretization error below a threshold value. Sample results are presented here for the low and high Reynolds numbers flows. For this purpose, first simulations are performed at low Re for the VN and NV systems shown in Fig. 3.20 using various grid resolutions ranging between 32×384 and 128×1536 . The evolution of drop deformation is plotted in Fig. 3.20. As can be seen in this figure, differences between

successive grid resolutions decrease as grid is refined indicating grid convergence. The relative spatial error is also plotted in Fig. 3.20 at selected locations. For the grid size of Δx , the relative error is defined as

$$\text{Error} = \left| \frac{\text{deformation}_{\Delta x \rightarrow 0} - \text{deformation}_{\Delta x}}{\text{deformation}_{\Delta x \rightarrow 0}} \right|, \quad (3.9)$$

where $\text{deformation}_{\Delta x}$ is the computed value and $\text{deformation}_{\Delta x \rightarrow 0}$ is the spatial error free value predicted using the Richardson's extrapolation. Note that, although not shown here, the drop volume is preserved within 2% for all the cases considered in this study. The approximate linear relationship confirms the expected second order spatial accuracy of the method. These figures show that a 64×768 grid is required to reduce the maximum spatial error below 2% in the drop deformation. Note that the results for low Re presented in this paper are obtained using a 64×768 grid for which the maximum spatial error is reduced below 4% in all the flow quantities of interest. Finally, the mesh convergence analysis is also done for high Re flows both for VN and NV cases using various grid resolutions ranging between 32×832 and 128×3328 . The results are shown in Fig. 3.21. It is found that a grid convergence is achieved with expected second order accuracy and a 96×2496 grid is sufficient to reduce the spatial error below 2% in all the flow quantities except for the VN system at high Wi numbers, i.e., in the extreme case of $Wi = 100$, the relative error becomes as large as 9% in the vicinity of the expansion.

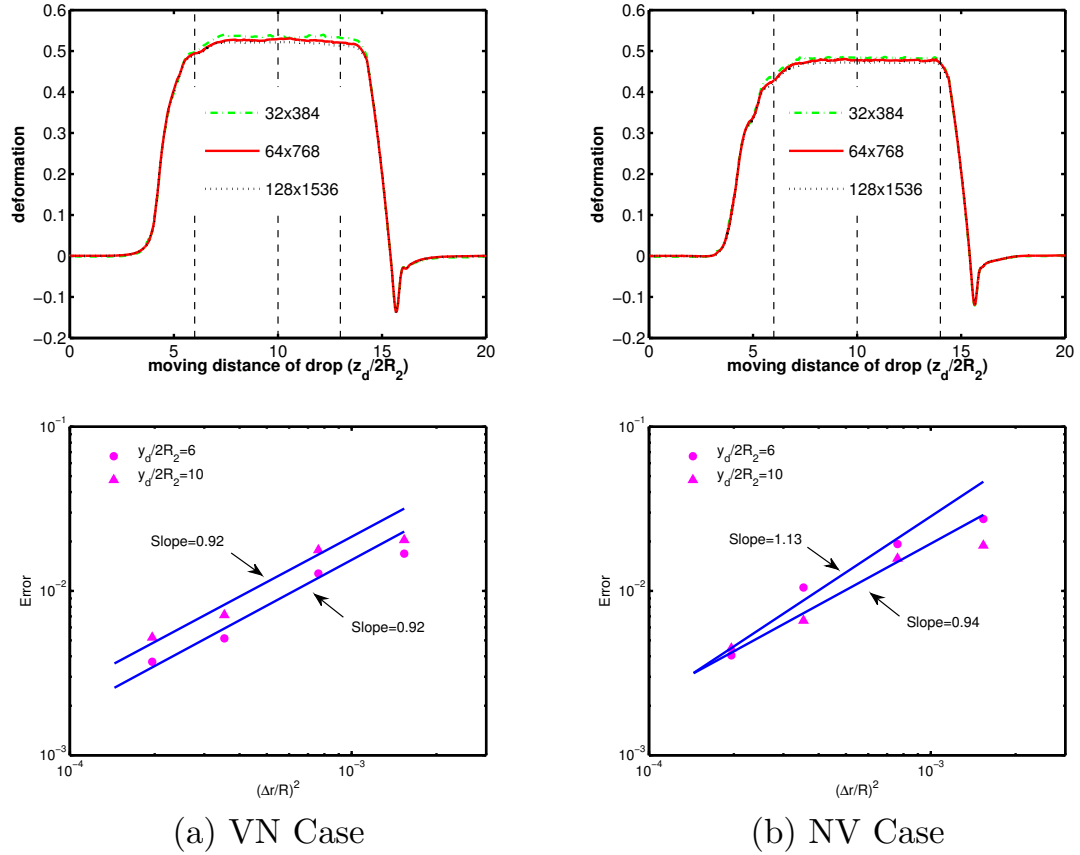


Figure 3.20: Grid convergence for the VN and NV cases at $Re = 2$. The results are obtained using various grid resolutions ranging between 32×384 and 128×1536 . The drop deformation versus the moving distance of the drop centroid (top row) and the variation of error in drop deformation with the square of the non-dimensional grid size $(\Delta r/R)^2$ at the axial locations $y_d/2R_2 = 6, 10, 13$ and $y_d/2R_2 = 6, 10, 14$ (bottom row) for (a) the VN and (b) the NV cases, respectively. The solid lines are the linear least squares fits to the computational results indicating the expected second-order accuracy of the method. ($Ca = 0.1, Wi = 100$).

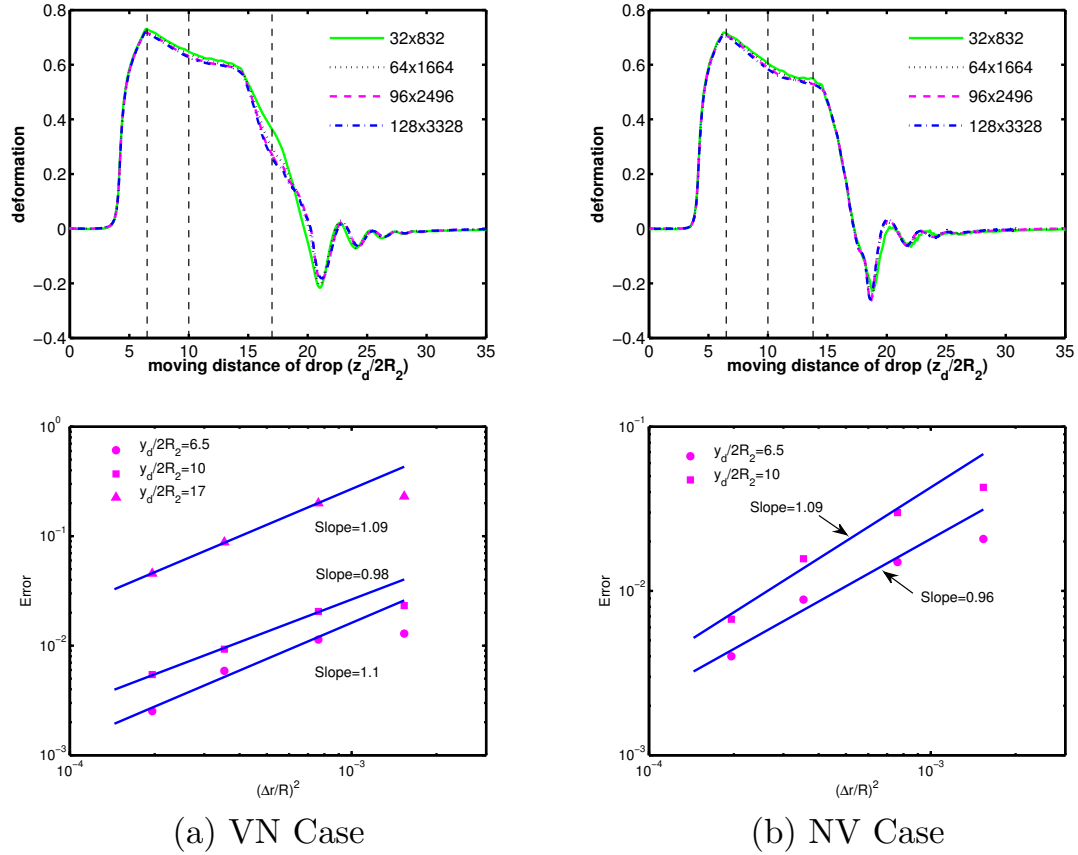


Figure 3.21: Grid convergence for the VN and NV cases at $Re = 50$. The results are obtained using various grid resolutions ranging between 32×832 and 128×3328 . The drop deformation versus the moving distance of the drop centroid (top row) and the variation of error in drop deformation with the square of the non-dimensional grid size $(\Delta r/R)^2$ at the axial locations $y_d/2R_2 = 6.5, 10, 17$ and $y_d/2R_2 = 6.5, 10, 13.8$ (bottom row) for (a) the VN and (b) the NV cases, respectively. The solid lines are the linear least squares fits to the computational results indicating the expected second-order accuracy of the method. ($Ca = 0.1, Wi = 100$).

Chapter 4

EFFECTS OF VISCOELASTICITY ON DROP IMPACT AND SPREADING ON A SOLID SURFACE ³

4.1 Introduction

Controlled deposition of a droplet on a flat substrate is an important problem in many applications including pesticide deposition[8], spray coating [5], ink jet printing [116], additive manufacturing [138], tissue engineering and single cell epitaxy [34, 122]. It is particularly important to know whether a droplet will deposit or rebound after the impact, thus it is required to investigate full drop impact dynamics. In the literature, a Newtonian droplet impacting on a flat substrate has been extensively investigated [107, 138]. The influence of viscoelasticity on the impact and spreading of a droplet on a substrate has received growing attention in the recent years particularly due to the discovery of the anti-rebound effects of polymer additives [8, 11].

Unlike the Newtonian systems, understanding of the impact dynamics of a viscoelastic droplet is severely limited, and yet of great importance for a wide range of applications. It has been reported that a tiny amount of polymer such as polyethylene oxide (POE) added to water can dramatically affect drop dynamics, suppressing the rebounding of a drop on a hydrophobic substrate. Based on the experimental observations, several hypotheses have been proposed to explain this interesting behavior, which often led to controversies. Initially, the anti-rebound effect was thought to be due to large energy dissipation caused by the elongational viscosity of the polymers [8]. However, further studies have detected some flaws in this hypothesis. Bertola [10] and Rozhkov et al. [109] examined the influence of the substrate on the retraction of polymeric drops using a hot surface (Leidenfrost drops) and small targets, respectively. They both found that

³TO BE SUBMITTED AS A PAPER UNDER THE SAME TITLE IN PHYSICAL REVIEW FLUIDS (2016)

the polymer additives do not change the retraction velocity and thus concluded that the anti-rebound effect can not be explained by the elongational viscosity of the fluid. Bartolo et al. [7] proposed an alternative hypothesis based on their own experimental observations and suggested that the polymer additives generate high normal stresses near the moving contact line of the drop that counter the capillary force and in turn prevent rebound of the drop. However, Bertola [11] has recently raised questions about this hypothesis and asserted that the slow retraction observed in the experiments might be simply due to a higher shear viscosity of the solution. Moreover, he also argued that dilute polymer solutions do not exhibit appreciable normal stresses in the range of shear rates that occur during the receding phase. Recent experimental studies have provided evidence that the anti-rebound effect might be due to the modification of dynamic wetting properties by the polymers deposited on the substrate rather than the change in the bulk fluid properties. Smith and Bertola [114] observed that polymer molecules that are left behind the contact line produce a resistant force during the retraction and act to prevent a drop from rebounding. Zang et al. [143] investigated impact dynamics of droplets containing nanoparticles and polymers. They concluded that drop rebound is inhibited by enhanced friction due to interaction of particles and polymers with the substrate. Later, Zang et al. [144] demonstrated that the rebounding of a non-Newtonian droplet can be restored via nanoparticle enwrapping, and thus concluded that the anti-rebound effect is related to the drop-substrate friction rather than the bulk rheological properties. Smith and Sharp [115] provided a further evidence that polymers deposited on the substrate result in a velocity-dependent friction force at the contact line during droplet retraction phase. Bertola and Wang [12] have also confirmed the existence of the polymer-induced friction and showed that the receding contact angle in polymer solution drops is significantly smaller than that in the case of pure water drops. They also observed that the minimum contact angle decreases with respect to both increasing polymer concentration and the Weber number. In addition, Huh et al. [64] have also shown that energy dissipation is significantly increased during the retraction phase due to polymeric residues left on the substrate. They found that the energy dissipation increases with the molecular weight and concentration of the polymer. Based on these experimental findings, they proposed a semiempirical model to estimate the rebounding

tendency of a polymer solution drop. The impact and spreading of polymeric drops on solid surfaces have been recently reviewed by Bertola [11].

On the computational side, various numerical techniques have been used to model a viscoelastic drop impacting on a solid surface. The smoothed particle hydrodynamics (SPH) method has been used by several groups for this purpose including Fang et al. [40], Jiang et al. [69, 70, 71]. In these studies, the effects of surface tension have been ignored and the focus has been placed mainly on the numerical method rather than examination of flow physics. Fang et al. [40] simulated impact of an Oldroyd-B fluid droplet on a rigid plate using a SPH method. They found that the viscoelasticity enhances both spreading and contraction. Jiang et al. [69] studied impact and spreading of an Oldroyd-B fluid droplet on an inclined surface. They found that the viscoelastic droplet spreads faster than the Newtonian counterpart. Jiang et al. [70] simulated the impact of a highly viscous extended Pom-Pom (XPP) fluid droplet at high Weissenberg numbers. They found that the viscoelasticity increases spreading rate but decreases the tendency to contraction. Jiang et al. [71] investigated spreading process of two XPP model droplets impacting on a plate in a sequence at a low Reynolds number. Their results revealed that model parameters have significant influence on the deformation process of the XPP droplets. They also confirmed the enhancement of drop spreading with the Weissenberg number. Grid-based methods have been also used to study the drop impact problem. For instance, Tomé et al. [124], Oishi et al [92] and Paulo et al [100] investigated a viscoelastic drop impacting on a flat solid substrate using a marker-and-cell (MAC) method with various viscoelastic models including the Oldroyd-B [124], XPP [92] and FENE-CR[100] models. The problem has been simplified by assuming a non-wetting substrate and neglecting the effects of the surface tension. In addition, these works have all assumed a planar 2D configuration. Tomé et al. [124] simulated impact of an Oldroyd-B drop on a rigid plate and found that a viscoelastic droplet exhibits a greater tendency for spreading compared to the Newtonian one. They also found that only the viscoelastic droplet undergoes a significant contraction. Oishi et al [92] studied XPP drop impact problem for a wide range of flow conditions. They found that the drop spreading increases with increasing Weissenberg number and decreasing solvent viscosity ratio. Paulo et al [100] simulated impact of a FENE-CR droplet and reported that the

viscoelasticity favors drop spreading. More recently, Wang et al. [133] have investigated the dynamic wetting of viscoelastic droplets on a solid substrate using a phase-field method. They ignored the inertial effects but accounted for the surface tension. They also found that the viscoelastic droplets spread faster than the Newtonian counterparts.

In this paper, we computationally study the effects of viscoelasticity on drop impact, spreading and rebound on a solid surface. We fully account for the effects of surface tension and treat the partially wetting cases with a dynamic contact angle. The Navier-Stokes and the viscoelastic model equations (FENE-CR) are solved in the entire computational domain using a front tracking method [130, 90, 67]. The fluid viscoelasticity is characterized by the Weissenberg number (Wi), polymeric viscosity ratio (β), the concentration parameter defined as the ratio of polymeric viscosity to solvent viscosity (c) and the extensibility parameter (L^2). We first examined the effects of drop viscoelasticity without the polymer-induced contact angle hysteresis and found that the drop viscoelasticity enhances the rebounding tendency, which is in contrast with the experimental observations. To remedy this deficiency, we propose a model that mimics the hysteresis of the contact angle observed experimentally by Bertola and Wang [12]. The simulations with the contact line hysteresis result in good qualitative agreement with the experimental results [12] supporting the hypothesis that the anti-rebound effect is mainly due to the modification of surface wetting properties by the deposited polymer molecules rather than the drop viscoelasticity. Although the emphasis is placed on the effects of the viscoelasticity in the present study, further simulations are also carried out to examine the effects of the Weber number (We), the Reynolds number (Re) and the equilibrium contact angle (θ_e).

4.2 Formulation and Numerical Method

The governing equations are described in the framework of the finite-difference/front-tracking method. The flow is assumed to be incompressible. Following Unverdi and Tryggvason [130] and Izbassarov and Muradoglu [67], Izbassarov and Muradoglu [68], a single set of governing equations can be written for the entire computational domain provided that the jumps in the material properties such as density, viscosity and relax-

ation time are taken into account and the effects of the interfacial surface tension are treated appropriately.

The continuity and momentum equations can be written as follows:

$$\nabla \cdot \mathbf{u} = 0, \quad (4.1)$$

$$\begin{aligned} \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot \mu_s (\nabla \mathbf{u} + \nabla \mathbf{u}^T) + \nabla \cdot \boldsymbol{\sigma} + \Delta \rho g + \\ &\int_A \gamma \kappa \mathbf{n} \delta(\mathbf{x} - \mathbf{x}_f) dA, \end{aligned} \quad (4.2)$$

where μ_s , ρ , p , $\mathbf{u}$ and $\boldsymbol{\sigma}$ denote the solvent viscosity and the density of the fluid, the pressure, the velocity vector and the viscoelastic extra stress tensor, respectively. The last term in Eq. (4.2) represents the body force due to surface tension where γ is the surface tension coefficient, κ is twice the mean curvature, and $\mathbf{n}$ is the unit vector normal to the interface. 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 points at which the equation is being evaluated and a point at the interface, respectively.

The FENE-CR model [25] is adopted as the constitutive equation for the viscoelastic extra stresses. This model can be written as

$$\begin{aligned} \frac{\partial \mathbf{A}}{\partial t} + \nabla \cdot (\mathbf{u} \mathbf{A}) - (\nabla \mathbf{u})^T \cdot \mathbf{A} - \mathbf{A} \cdot \nabla \mathbf{u} &= -\frac{F_A}{\lambda} (\mathbf{A} - \mathbf{I}), \\ F_A &= \frac{L^2}{L^2 - \text{trace}(\mathbf{A})}, \end{aligned} \quad (4.3)$$

where $\mathbf{A}$, λ , L , F_A and $\mathbf{I}$ are the conformation tensor, the relaxation time, the extensibility parameter defined as the ratio of the length of a fully extended polymer dumbbell to its equilibrium length, the stretch function and the identity tensor, respectively. The extra stress tensor $\boldsymbol{\sigma}$ is related to the conformation tensor as

$$\boldsymbol{\sigma} = \frac{F_A \mu_p}{\lambda} (\mathbf{A} - \mathbf{I}), \quad (4.4)$$

where μ_p is the polymeric viscosity. The amount of polymeric viscosity is controlled by the polymeric viscosity ratio and concentration, $\beta = \frac{\mu_p}{\mu_p + \mu_s}$ and $c = \frac{\mu_p}{\mu_s}$, respectively. Note that c is related to β as $c = \frac{\beta}{1-\beta}$.

It is also assumed that the material properties remain constant following a fluid particle, i.e.,

$$\frac{D\rho}{Dt} = 0; \frac{D\mu_s}{Dt} = 0; \frac{D\mu_p}{Dt} = 0; \frac{D\lambda}{Dt} = 0, \quad (4.5)$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla$ is the material derivative. The density, polymeric and solvent viscosities, and the relaxation time vary discontinuously across the fluid interface and are given by

$$\begin{aligned}\mu_p &= \mu_{p,d}\phi + \mu_{p,a}(1 - \phi); \mu_s = \mu_{s,d}\phi + \mu_{s,a}(1 - \phi); \\ \rho &= \rho_d\phi + \rho_a(1 - \phi); \lambda = \lambda_d\phi + \lambda_a(1 - \phi),\end{aligned}\tag{4.6}$$

where the subscripts d and a denote the properties of the drop and the ambient fluids, respectively. The indicator function ϕ is defined such that it is unity inside the droplet and zero outside.

The flow equations (Eqs. 4.1 and 4.2) are solved fully coupled with the viscoelastic model equations (Eq. 4.3) by the finite-difference/front-tracking method developed by Izbassarov and Muradoglu [67]. The flow and viscoelastic model equations are solved on a staggered Eulerian grid using a projection method [29]. The log-conformation method (LCM) of Fattal and Kupferman [41] is employed to enhance numerical stability in solving the viscoelastic model equations at high Weissenberg numbers. A fifth-order upwinded WENO-Z [17] scheme is used to discretize the convective terms in the viscoelastic constitutive equations while all the other spatial derivatives are approximated using central differences. Time integration is achieved using a first-order explicit Euler method both for the flow and viscoelastic model equations. Although it is straightforward to make the present numerical method second order accurate in time, a first-order method is used here since the time stepping error is generally found to be negligibly small compared to the spatial error mainly due to a small time step imposed by the numerical stability of the present explicit scheme [67].

A separate Lagrangian grid is used to explicitly track the fluid-fluid interface. The Lagrangian grid consists of linked marker points (the front) moving with the local flow velocity interpolated from the stationary Eulerian grid. The surface tension is computed on the Lagrangian grid and then distributed onto the Eulerian grid points near the interface to be added to the momentum equations in the form of body forces as described by Tryggvason et al. [127]. The indicator function is computed at each time step based on the location of the interface using the standard procedure [127] and is then used to set the fluid properties in each phase. The Lagrangian grid is restructured at every time

step by deleting the front elements that are smaller than a prespecified lower limit and by splitting the front elements that are larger than a prespecified upper limit in the same way as described by Tryggvason et al. [127] to keep the front element size nearly uniform and comparable to the Eulerian grid size. A complete description of the front-tracking method can be found in Tryggvason et al. [127] and the treatment of the viscoelasticity and contact line in Izbassarov and Muradoglu [67], Izbassarov and Muradoglu [68] and Muradoglu and Tasoglu [90], respectively.

4.3 Problem Statement

The droplet is initially spherical and is placed near the wall with a uniform impact velocity, V_{col} , as shown in Fig. 4.1. The flow is assumed to be axisymmetric so only one half is used as the computational domain. The computational domain extends 5 drop radii both in the radial and axial directions. The surrounding air is initially quiescent. The viscosity and density ratios are set to $\rho_d/\rho_a = \mu_d/\mu_a = 20$ in all the results presented here. Note that the density and viscosity ratios are an order of magnitude larger in a typical liquid-air system than those specified here. However, it has been previously demonstrated [90, 122, 98] that a further increase in the property ratios does not affect the results significantly. Therefore the property ratios are kept small in order to enhance numerical stability and thus to reduce the computational cost.

The no-slip boundary conditions yield a stress singularity near the contact line, so require a special treatment. The slip-contact line model is essentially the same as that of Muradoglu and Tasoglu [90] so it is briefly summarized here. In the framework of the front-tracking method, the drop interface must be connected to the solid wall explicitly. To achieve this, we assume that the drop interface connects to the wall when the distance between the drop interface and solid wall gets shorter than a prespecified threshold value h_{th} as sketched in Fig. 4.1. For this purpose, the interface is monitored and the front element crossing the threshold line is detected. Then this element is connected to the solid wall such that the contact angle between the wall and droplet is equal to the apparent contact angle θ_D . In the present work, the threshold length is typically taken as $h_{th} = 3\Delta x$ where Δx is the Eulerian grid size and the apparent contact angle is

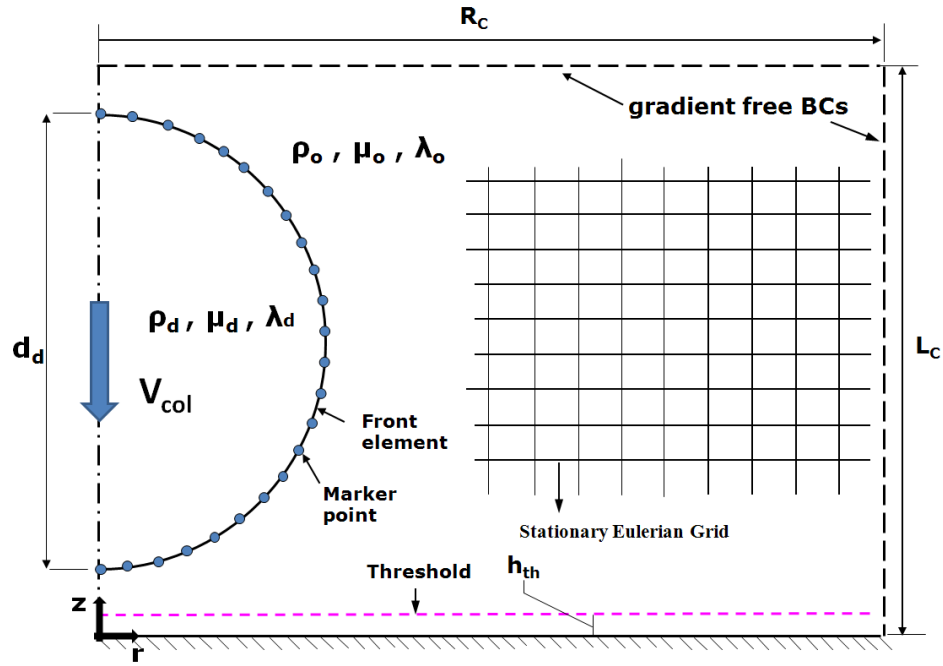


Figure 4.1: Schematic illustration of the computational setup. The interface is represented by the connected Lagrangian marker points. The flow and viscoelastic model equations are solved on a uniform Eulerian Cartesian grid. The droplet is initialized near the wall with a spherical shape and uniform collision velocity V_{col} .

specified dynamically using the Kistler's correlation [75, 113] that relates the apparent contact angle to the capillary number defined as $Ca_{cl} = \mu_d V_{cl} / \gamma$ where V_{cl} is the speed of the contact line. The dynamic contact angle is computed as

$$\theta_{D_i} = f_{\text{Hoff}}(Ca_{cl} + f_{\text{Hoff}}^{-1}(\theta_e)), \quad (4.7)$$

where f_{Hoff}^{-1} is the inverse of the Hoffman's function defined as

$$f_{\text{Hoff}}(x) = \arccos \left\{ 1 - 2 \tanh \left[5.16 \left(\frac{x}{1 + 1.31x^{0.99}} \right)^{0.706} \right] \right\}. \quad (4.8)$$

In Eq. 4.7, θ_e is the equilibrium (static) contact angle. The apparent contact angle is then computed in the advancing and receding phases as

$$\theta_D = \begin{cases} \theta_{D_i} & \text{if } V_{\text{col}} \geq 0 \quad (\text{advancing}) \\ 2\theta_e - \theta_{D_i} & \text{if } V_{\text{col}} < 0 \quad (\text{receding}). \end{cases}$$

Following Muradoglu and Tasoglu [90] the contact line velocity V_{cl} is specified as the velocity of the point where the droplet interface crosses the threshold. The details of the implementation of this slip contact line method can be found in Muradoglu and Tasoglu [90].

The governing equations are solved in their dimensional forms and the results are expressed in terms of the relevant dimensionless quantities. The length and velocity scales are defined as an initial drop diameter d_d and impact velocity V_{col} , respectively, and $T = d_d / V_{col}$ be the time scale. Then, in addition to the property ratios, the other relevant dimensionless numbers are defined as

$$Wi = \frac{\lambda V_{col}}{d_d}, We = \frac{\rho_d V_{col}^2 d_d}{\sigma}, Re = \frac{\rho_d V_{col} d_d}{\mu_d}, \quad (4.9)$$

where Wi , We and Re are the Weissenberg, Weber and Reynolds numbers, respectively.

4.4 Results and Discussion

Simulations are carried out to study effects of viscoelasticity on drop impact, spreading and rebound. The computational domain is resolved by a 1024×1024 uniform Cartesian grid in all the results presented in this paper. Since an extensive grid convergence study of

the present numerical method has been previously performed by Muradoglu and Tasoglu [90], such a study is not repeated here. However, we checked the grid convergence and ensured that the solutions are grid independent, i.e., the spatial error is below 3% for all the results presented here.

Simulations are first performed to examine the sole effects of the droplet fluid viscoelasticity without the polymer-induced contact angle hysteresis. Then a model is incorporated into the numerical method to mimic the modification of the substrate wettability due to deposition of polymer molecules and further simulations are carried out to test the performance of the model.

4.4.1 Simulations Without Polymer-Induced Hysteresis

We first designate a base case to systematically examine the effects of various flow parameters. Based on the experimental data [123] as well as the numerical stability and convergence considerations, the base case is defined as $Re = 35$, $We = 30$, $Wi = 1$, $L^2 = 225$, $\beta = 0.56$, $c = 1.27$ and $\theta_e = 145^\circ$.

The evolution of drop impact and spreading is visually depicted for the base case in Fig. 4.2 where the velocity vectors and the contours of average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$ are shown on the left and right sides, respectively. Note that the velocity vectors are plotted at every 30 grid points in both coordinate directions in all the results presented in this paper to better show the flow patterns. The square root of the trace of the conformation tensor ($\sqrt{\text{trace}(\mathbf{A})}$) is plotted here as a measure of average polymer length. Smooth interface without any artificial flow near the contact line can be considered as an indication of overall accuracy of the method. As seen in the figure, the drop spreads in the radial direction after it impacts on the surface. During the spreading phase polymers are extended due to velocity gradients in the direction parallel to the solid wall resulting in a thin viscoelastic boundary layer as can be better seen in the enlarged version of the droplet in Fig. 4.3 at time $t^* = 1.0$ for $Wi = 1$ and $Wi = 10$ cases. In the boundary layer, the polymers near the interface exert an extensional stress that pushes the contact line to increase the spreading rate. This is the main mechanism that makes the polymer droplets spread more than that of the Newtonian one as will be discussed in more details later. At the end of the spreading phase, i.e., at about $t^* = 1.3$,

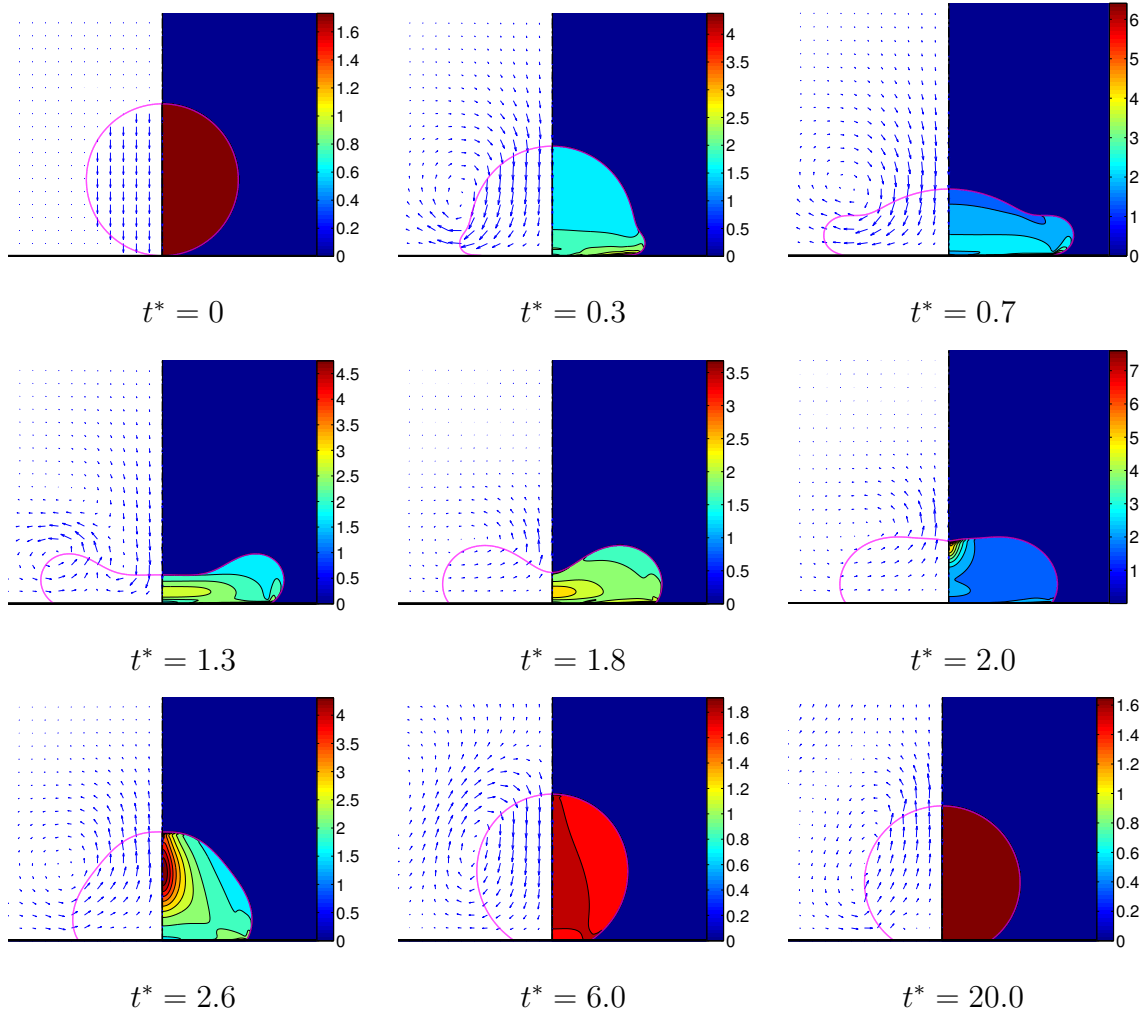


Figure 4.2: Evolution of a FENE-CR droplet after impacting on the solid surface. The velocity vectors are plotted on the left and the contours of average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$ on the right. ($Re = 35, We = 30, Wi = 1, L^2 = 225, \beta = 0.56, c = 1.27$ and $\theta_e = 145^\circ$).

the drop reaches its maximum spreading as the initial impacting kinetic energy is totally exhausted. The initial impact energy of the drop is partially dissipated, partially converted to the surface energy and partially stored as the elastic energy. As the drop reaches its maximum spreading it takes a disk like form with a thin central part (often called “lamella”), surrounded by a circular rim. At this point, the flow changes direction from spreading outward to receding inward. During the receding phase, the rim swells and moves inward until it reaches the axis of symmetry. As the droplet retracts, the viscoelastic stresses concentrate along the axis of symmetry while the stresses near the wall diminish. The stresses along the wall counter act the retraction of the contact line but this effect decreases as the polymer molecules relax due to the reversal flow. The same internal flow is also responsible for the stress concentration along the drop centerline near the apex of the droplet. As a result, the stresses along the axis of symmetry force the fluid to flow upwards and thus favor drop retraction. Depending on the remaining kinetic energy of the droplet, two different outcomes are possible: The droplet can either oscillate on the surface or rebound. In both cases, the droplet eventually reaches an equilibrium with a spherical cap shape on the substrate.

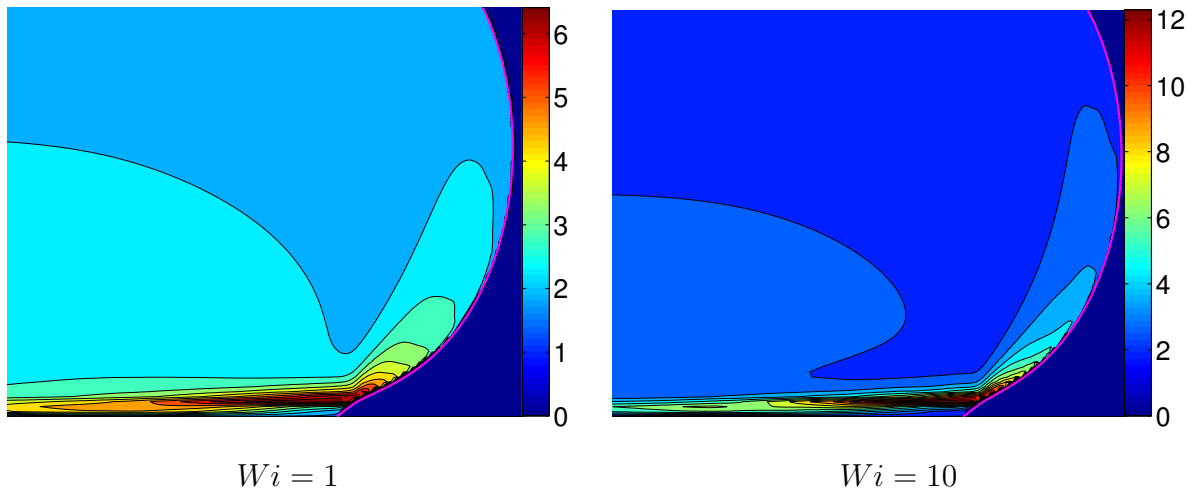


Figure 4.3: Contours of average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$ in the vicinity of contact line for $Wi = 1$ (left) and $Wi = 10$ (right). ($Re = 35, We = 30, Wi = 1, L^2 = 225, \beta = 0.56, c = 1.27$ and $\theta_e = 145^\circ$).

Next, we examine the effects of the flow parameters on the drop dynamics. For this

purpose, simulations are performed for the range of $0 \leq Wi \leq 100$ while the other parameters are the same as the base case. The evolution of drop shapes are plotted in Fig. 4.4 for $Wi = 0$ (Newtonian), $Wi = 1$ and $Wi = 10$. As seen, the magnitude of the viscoelastic stresses monotonically increases as Wi is increased. In contrast with the Oldroyd-B model, the FENE-CR model bounds the growth of viscoelastic stresses. Therefore the increase in the stresses gets smaller when Wi exceeds a threshold value, i.e., when $Wi \geq 10$ in this case. It is interesting to see that the viscoelasticity favors spreading of the droplet and the viscoelastic droplet tends to spread more than that of the Newtonian one, which is in agreement with the computational results of Tomé et al. [124] and Fang et al. [40]. Whilst, there is no significant difference between $Wi = 1$ and $Wi = 10$ cases in the advancing phase. However, in the retraction phase, the difference is more pronounced and the retraction becomes faster as Wi increases. When the retraction velocity is fast enough, the fluid rises up from the center of droplet forming a dome, which may even result in a complete rebound from the substrate, see e.g., the $Wi = 10$ case in Fig. 4.4. As it was discussed above, a part of the initial kinetic energy is stored as the elastic energy in the viscoelastic drop, which reduces the energy dissipation in the spreading phase. This elastic energy is released during the recoiling phase contributing to the drop rebound. This finding is in agreement with the experimental observation of Bertola [10]. The effects of Wi are quantified in Fig. 4.5 where the spread factor is plotted as a function of non-dimensional time. The spread factor is defined as the radius of the wetted spot normalized by the equivalent drop radius. The results obtained for a Newtonian droplet are also plotted in this figure to directly show the effects of the viscoelasticity. The viscosity in the Newtonian case is set to the total viscosity of the corresponding viscoelastic case, i.e., $\mu_{Newtonian} = \mu_s + \mu_p$. The Weissenberg number seems to have little influence on the spread factor in the spreading phase but its influence is more pronounced in the receding phase. However, the maximum spread factor slightly increases with Wi (Fig. 4.5) mainly due to the additional viscoelastic stresses which favor spreading (Fig. 4.4). More importantly, the tendency for rebound increases as Wi increases and the drop rebounds when $Wi \geq 4$ in this case.

Simulations are then carried out to examine the effects of polymeric viscosity ratio and the extensibility parameter in the range of $0.1 \leq \beta \leq 0.7$ and $9 \leq L^2 < \infty$, respectively.

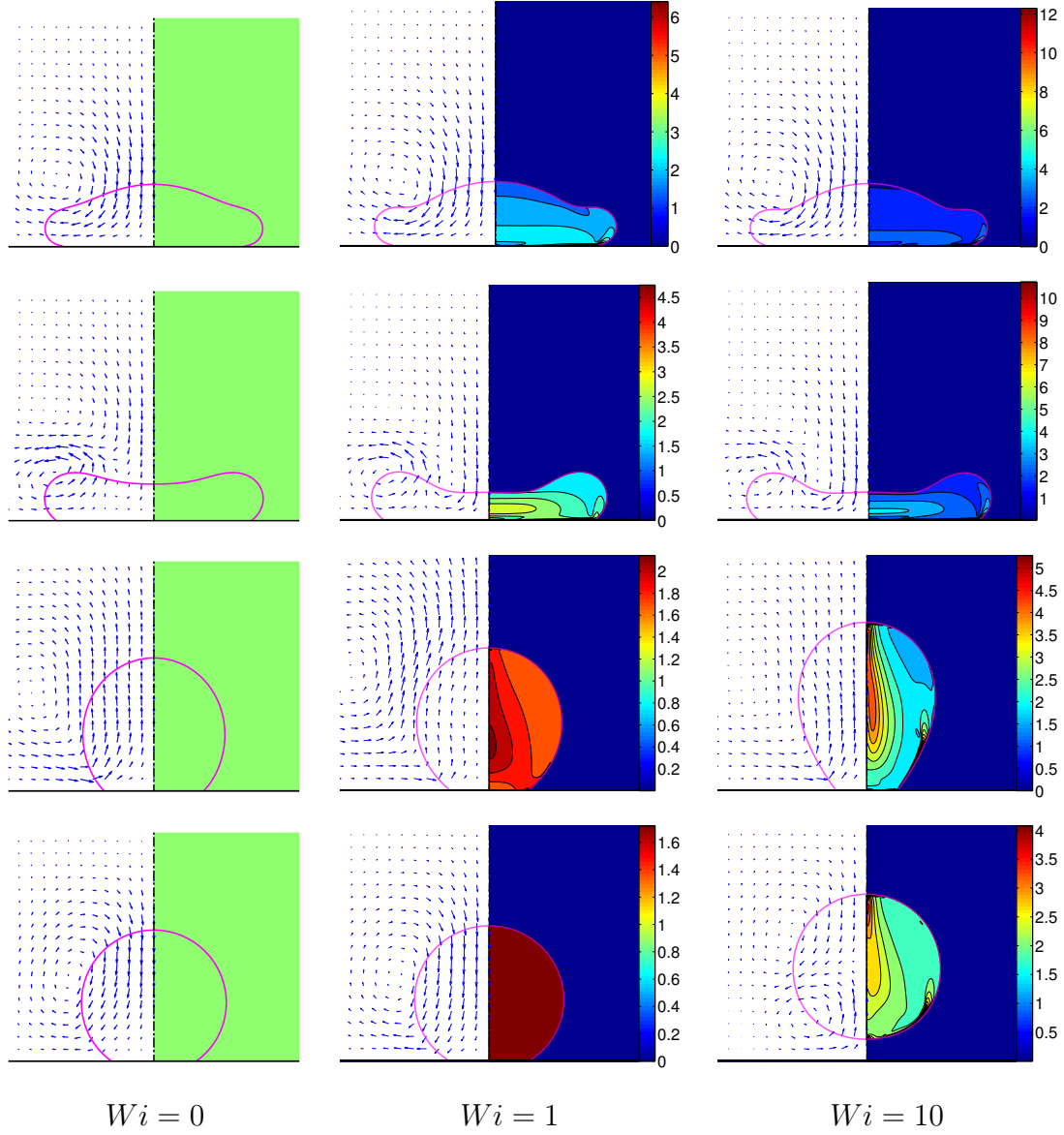


Figure 4.4: Effects of Wi on drop impact. The time evolution is from top to bottom. The velocity vectors are plotted on the left and the contours of average polymer extension $\sqrt{\text{trace}(\mathbf{A})}$ on the right. The snapshots are taken at the times $t^* = 0.7, 1.3, 5.0, 7.5$. ($Re = 35, We = 30, L^2 = 225, \beta = 0.56, c = 1.27$ and $\theta_e = 145^\circ$).

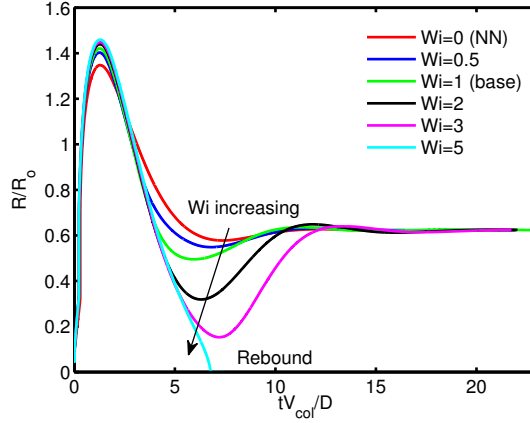


Figure 4.5: Effects of the Weissenberg number on droplet impact and spreading. Time evolution of the spread factor with Wi . ($Re = 35$, $We = 30$, $L^2 = 225$, $\beta = 0.56$, $c = 1.27$ and $\theta_e = 145^\circ$).

First, the spread factor is plotted in Fig. 4.6 for $\beta = 0.1, 0.2, 0.4, 0.56$ and 0.7 while keeping the other parameters the same as the base case. In fact, the polymeric viscosity ratio essentially modifies the effective Weissenberg number defined as $Wi' = \beta Wi$. Thus increasing β is expected to have a similar effect as increasing the Weissenberg number. This is verified in Fig. 4.6 as the maximum spread factor monotonically increases with β . The time evolution of the spread factor is plotted in Fig. 4.7 for the various values of L^2 in the range of $9 \leq L^2 < \infty$. As seen in this figure, L^2 has little influence on the spread factor and tendency of drop rebound. These results are consistent with the results plotted in Figs. 4.4 and 4.5, i.e., the viscoelastic droplet behaves like a Newtonian droplet for $Wi \leq 1$.

Obviously, these results are in contrast with the polymeric anti-rebound phenomenon. The recent studies have revealed that, when the substrate effects are removed so the hysteresis due to polymers are eliminated, the viscoelasticity in drop fluid reduces the overall energy dissipation and thus increases the tendency of the drop rebound [10, 15]. Our computational results are consistent with these findings and support the hypothesis that the anti-rebound effect results from the modification of wetting properties of the substrate due to polymer deposition. This issue will be discussed in more details in Section 4.4.2.

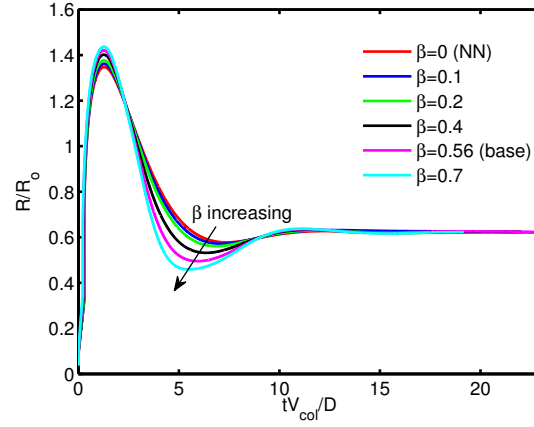


Figure 4.6: Effects of the polymeric viscosity ratio on droplet impact and spreading. Time evolution of the spread factor with the viscosity ratio β . ($Re = 35$, $We = 30$, $Wi = 1$, $L^2 = 225$ and $\theta_e = 145^\circ$).

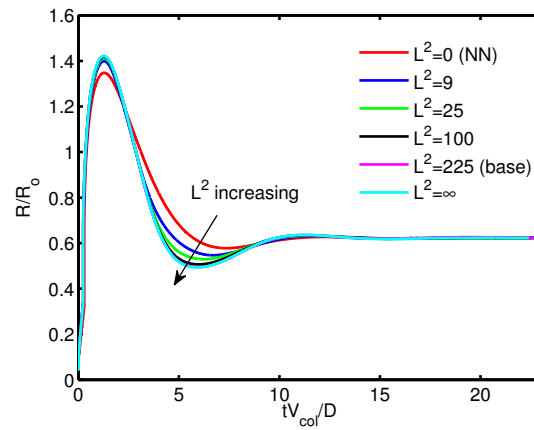


Figure 4.7: Effects of the L^2 on droplet impact and spreading. Time evolution of the spread factor with L^2 ($Re = 35$, $We = 30$, $Wi = 1$, $\beta = 0.56$, $c = 1.27$ and $\theta_e = 145^\circ$).

Next, computations are performed for a wide range of equilibrium contact angles varying between 70° and 160° and the results are plotted in Fig. 4.8. Similar to the Newtonian case [90], the equilibrium contact angle significantly influences the spreading factor and the rebound of the drop. As expected, the tendency to rebound increases as the substrate becomes more hydrophobic. We also performed simulations to examine the effects of dynamic contact angle in comparison with the fixed static contact angle. This is done because numerical simulations are often done using a static contact angle in the literature. For this purpose, we simulated a hydrophobic case, i.e., $\theta_e = 150^\circ$, using both the dynamic and static contact angle formulations. The results are shown in Fig. 4.9. This figure clearly shows a large discrepancy between two formulations: the drop rebounds in the static contact angle case while it just undergoes damped oscillations on the substrate when the dynamic contact angle is taken into account.

Then we examine the effects of the Weber number on the drop impact and spreading by varying the Weber number between 10 and 1000 while keeping the other parameters the same as the base case. The results are plotted in Fig. 4.10. Upon impact, the initial kinetic energy is partly stored as a surface energy, which is proportional to the maximum spreading diameter. Thus the maximum spread factor increases with the Weber number since the surface tension decreases making the interface more deformable. The retraction phase is governed by the balance between the surface energy, the viscous dissipation and elastic energy stored in the polymers. As the Weber number decreases, more energy is stored as the surface energy to be released during the receding phase and thus the droplet retracts faster. For the same reason, as We decreases, the droplet shifts to a rebound regime after a critical values, i.e., $We_{cr} \sim 20$ in this case. It is also observed that the viscoelastic effects are more pronounced at lower Weber numbers. For instance, the droplet rebounds in the case of $We = 20$ and $Wi = 1$ for which the Newtonian counterpart sticks to the substrate as shown in Fig 4.11.

The Reynolds number is an important parameter that measures the relative significance of the inertial forces compared to the viscous forces. The effects of the Reynolds number are examined both for a Newtonian and a viscoelastic droplet cases, and the results are shown in Fig. 4.12 where the spread factor is plotted as a function of the non-dimensional time for various Reynolds numbers ranging between $Re = 20$ and 60.

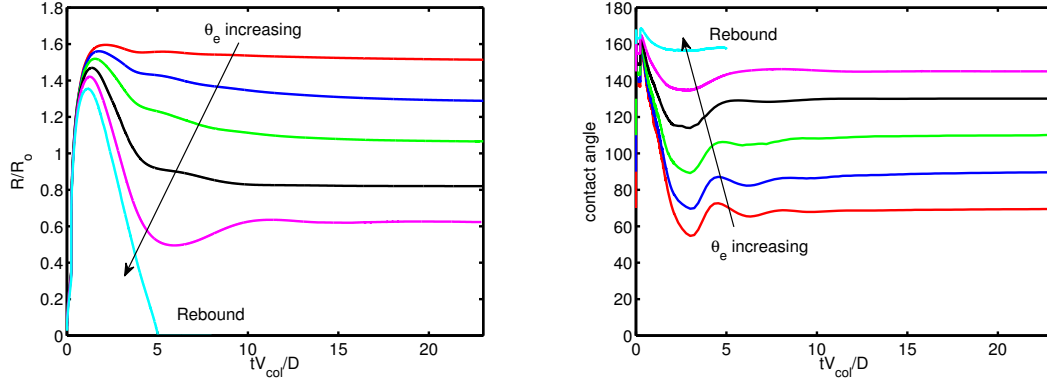


Figure 4.8: Effects of the equilibrium contact angle on droplet impact and spreading in the range $70^\circ \leq \theta_e \leq 160^\circ$. ($Re = 35, We = 30, Wi = 1, L^2 = 225, \beta = 0.56$ and $c = 1.27$).

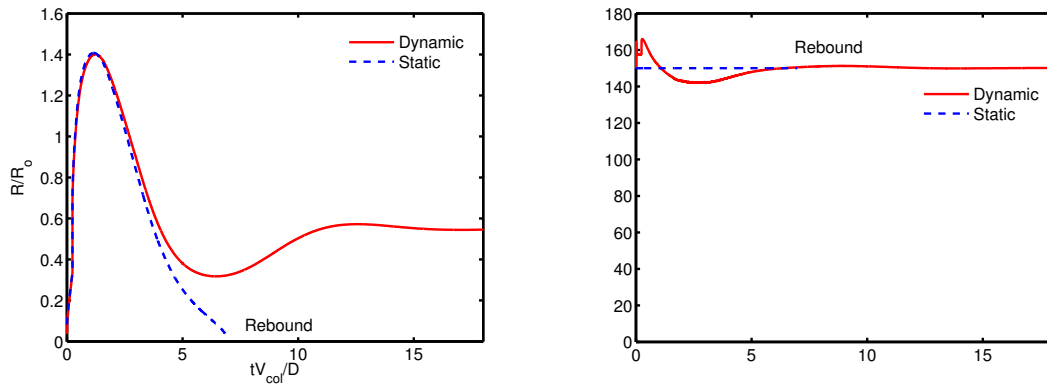


Figure 4.9: Effects of the static and dynamic contact angles on droplet impact and spreading. ($Re = 35, We = 30, Wi = 1, L^2 = 225, \beta = 0.56, c = 1.27$ and $\theta_e = 150^\circ$).

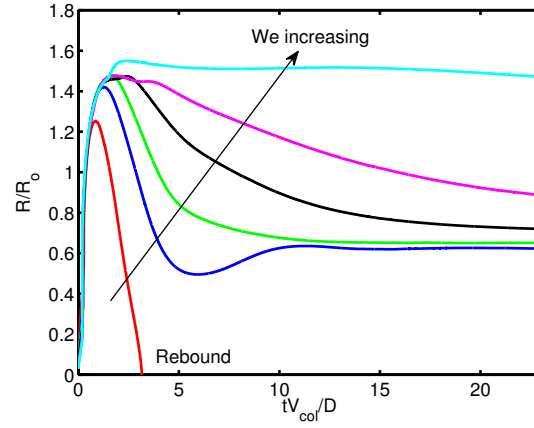


Figure 4.10: Effects of the Weber number. The evolution of spread factor is plotted for $We = 10, 30, 50, 100, 200$ and 1000 . ($Re = 35, Wi = 1, L^2 = 225, \beta = 0.56, c = 1.27$ and $\theta_e = 145^\circ$).

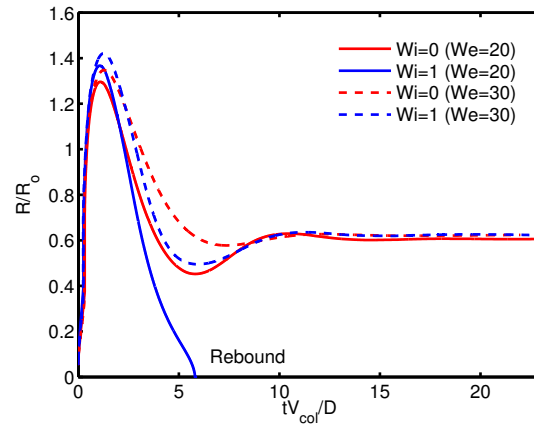


Figure 4.11: Effects of the Weber number on the impact and spreading of a Newtonian $Wi = 0$ and a viscoelastic $Wi = 1$ droplet. The solid and dashed lines denote the results obtained for $We = 20$ and $We = 30$, respectively. ($Re = 35, L^2 = 225, \beta = 0.56, c = 1.27$ and $\theta_e = 145^\circ$).

This figure shows that the maximum spreading rate and the tendency of drop rebound increase with Re for both the Newtonian and viscoelastic drop cases. This is expected since the viscous dissipation is reduced as Re increases, and thus more energy is left to be first stored as surface energy and then be released during the receding phase. It is also observed that the viscoelasticity enhances the maximum spread factor and the tendency of drop rebound since the part of the initial kinetic energy is stored as the elastic energy in the polymers that is also reversible and released contributing to the drop kinetic energy during the receding phase.

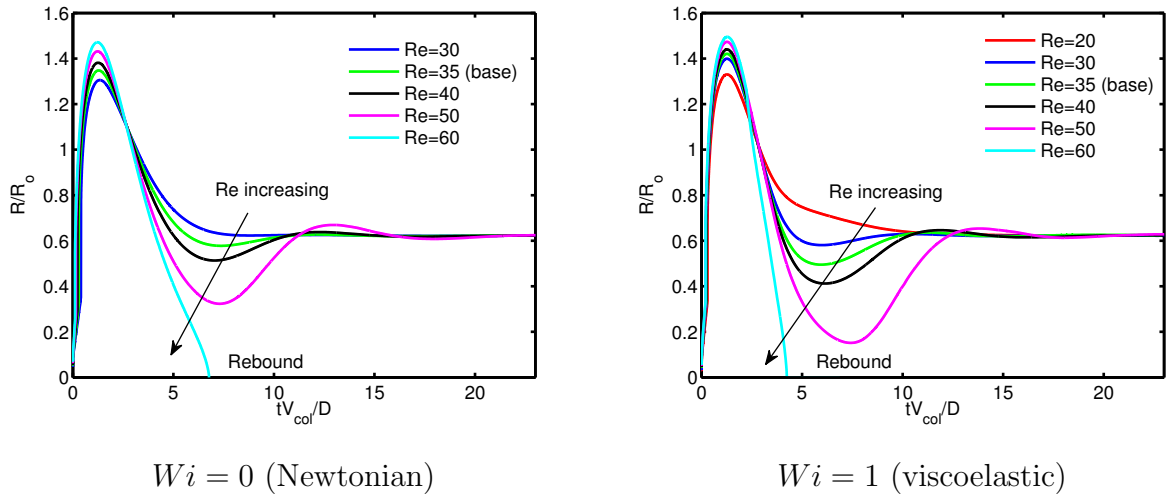


Figure 4.12: Effects of the Reynolds number for a Newtonian (left) and a viscoelastic (right) droplet in the range $Re = 20$ and $Re = 60$. ($We = 30, L^2 = 225, \beta = 0.56, c = 1.27$ and $\theta_e = 145^\circ$).

In a typical experimental study, the fluid viscoelasticity is increased by adding more polymers to the same solvent fluid. In this way, the polymeric viscosity changes while the solvent viscosity remains essentially unchanged. To mimic this, we performed simulations for a range of polymeric viscosities while keeping the other rheological properties fixed in the base case. In fact, not only the polymeric viscosity, but also the relaxation time and even L^2 change as more polymers are added to the solvent. Here, we take the advantage of the computational simulations to examine the sole effects of the polymeric viscosity. The results are shown in Fig. 4.13a where the evolution of the spread factor is plotted for $c = 0, 0.5, 0.75, 1$ and 1.27 . The concentration appears to have a large influence on

the spread factor especially in the receding phase. As c increases, both the maximum spread factor and the tendency for rebound decrease. Even though these results seem to be consistent with the anti-rebound phenomenon, it is mainly caused by the additional viscous dissipation rather than the viscoelastic effects. To verify this, further simulations are also performed for the corresponding Newtonian cases by setting the viscosity to the total viscosity of the viscoelastic counterpart, i.e., $\mu_{Newtonian} = \mu_s + \mu_p$. The results are shown in Fig. 4.13b. As seen, decreasing Reynolds number has a similar effect as increasing concentration factor. Nevertheless, a close examination of the viscoelastic and Newtonian cases reveals that the viscoelasticity favors drop rebound opposed to the experimental observations [11].

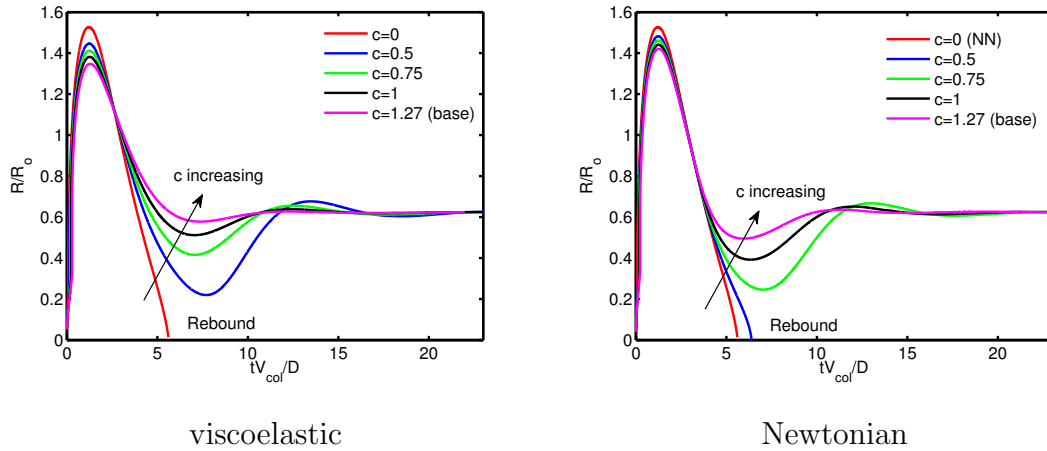


Figure 4.13: Effects of the polymer concentration on the droplet impact and spreading (left) compared to the corresponding Newtonian cases (right). The evolution of the spread factor is shown for $c = 0, 0.5, 0.75, 1.0$ and 1.27 in the left plot corresponding to $Re = 80, 53.3, 45.7, 40$ and 35 in the Newtonian case on the right plot, respectively. ($We = 30, Wi = 1, L^2 = 225$, and $\theta_e = 154^\circ$).

4.4.2 Effects of Polymer-Induced Hysteresis

The experimental studies have revealed that there is a substantial hysteresis in the contact angle in the advancing and receding phases [11]. This hysteresis is believed to be related to the deposition of the polymer molecules on the substrate during the advancing phase [12]. Smith and Sharp [115] observed that the deposited polymers outside the

drop are stretched during the receding phase, which in turn slows down the movement of the contact line. This mechanism can be interpreted as a dissipative force or an effective friction force acting in opposite direction of the contact line leading to a reduction in dynamic contact angle during the receding phase. Bertola and Wang [12] have recently shown that the contact angle may exhibit an underdamped or overdamped oscillatory behavior depending on the flow condition. However, the contact angle decays nearly exponentially during the first receding phase in both cases. To mimic this behavior, we propose a simple model for the polymer-induced hysteresis and modify the equilibrium contact angle θ_e as

$$\theta_e = \begin{cases} \theta_c & \text{if } V_{\text{col}} \geq 0 \text{ (advancing)} \\ \theta_s + (\theta_c - \theta_s)e^{-t/T_d} & \text{if } V_{\text{col}} < 0 \text{ (receding)}, \end{cases} \quad (4.10)$$

where t , T_d , θ_c and θ_s are the time, the deposition time scale, the clean and saturated equilibrium contact angles, respectively. The deposition time scale characterizes how fast the polymers deposit on the substrate. The hysteresis effect reduces as T_d increases and no-hysteresis conditions are recovered in the limit as $T_d \rightarrow \infty$.

To test the performance of this model, we slightly modify the base case so that the drop rebound occurs in the absence of the polymer-induced hysteresis. Thus the new base case is designated as $Re = 75$, $We = 30$, $Wi = 1$, $L^2 = 225$, $\beta = 0.07$, $c = 0.075$, $\theta_c = 145^\circ$ and $\theta_s = 90^\circ$. Note that the drop rebounds for this set of the parameters if $\theta_s = \theta_c$ as shown in Fig. 4.12.

Simulations are first carried out to examine the effects of the deposition time scale and the results are shown in Fig. 4.14 where the evolution of the spread factor and the dynamic contact angle is plotted for various values of the non-dimensional deposition time scale defined as $\tau = T_d V_{\text{col}} / D$ in the range $1 \leq \tau \leq 50$. As seen, the drop rebound is suppressed as τ is reduced, which qualitatively shows good agreement with the anti-rebound effect of polymer additives observed in the experimental studies. Note that the maximum spread factor is essentially unaffected by τ since the hysteresis is switched on at the beginning of the receding phase. This is also consistent with the experimental results of Bertola and Wang [12]. Further simulations are performed to examine the effects of the saturated equilibrium contact angle θ_s on drop dynamics and the results are shown in Fig. 4.15 for $\tau = 1$ and $\tau = 10$. The drop rebound is again suppressed

as θ_s decreases. Moreover the dynamic contact angle oscillates in a similar fashion as the experimental results of Bertola and Wang [12] especially for $\tau = 10$ (Fig. 4.15). These results support that the anti-rebound effect is mainly due to the modification of the surface wetting properties by the deposited polymer molecules rather than the bulk fluid properties, which is in agreement with the experimental observations of Bertola [11], Bertola and Wang [12] and Huh et al. [64].

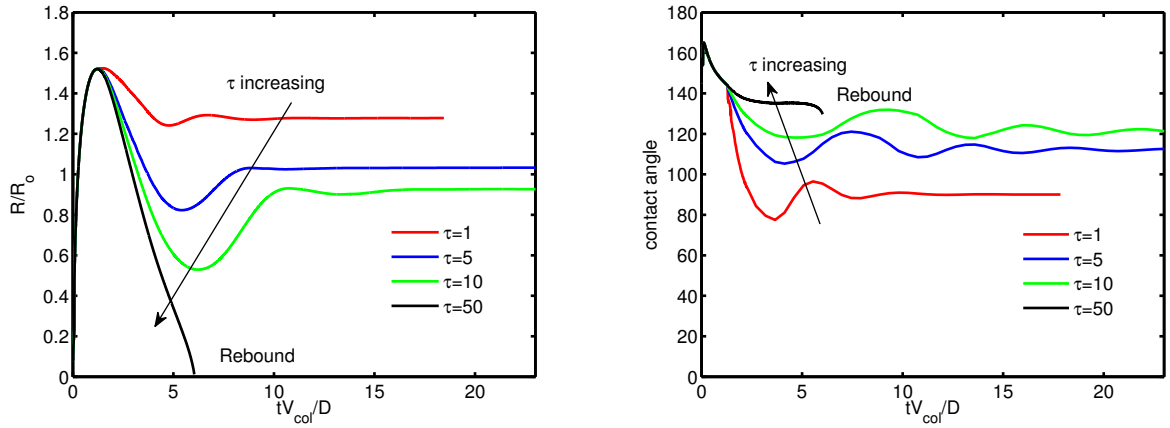


Figure 4.14: Effects of the non-dimensional deposition time scale (τ) on the droplet impact and spreading in the range $1 \leq \tau \leq 50$ ($Re = 75, We = 30, Wi = 1, L^2 = 225, \beta = 0.07, c = 0.075, \theta_c = 145^\circ$ and $\theta_s = 90^\circ$).

4.5 Conclusions

The effects of viscoelasticity on the drop impact, spreading and rebound on a solid surface are studied computationally using a front-tracking method. The FENE-CR model is employed to account for the viscoelasticity of drop fluid. Extensive simulations are performed to examine the effects of relevant dimensionless parameters including the Reynolds number (Re), the Weber number (We) as well as the fluid elasticity characterized by the Weissenberg number (Wi), polymeric viscosity ratio (β) and the extensibility parameter (L^2).

When the polymer-induced hysteresis effects are ignored, we found that the viscoelasticity favors drop rebound, which is in contrast with the well-known anti-rebound effect

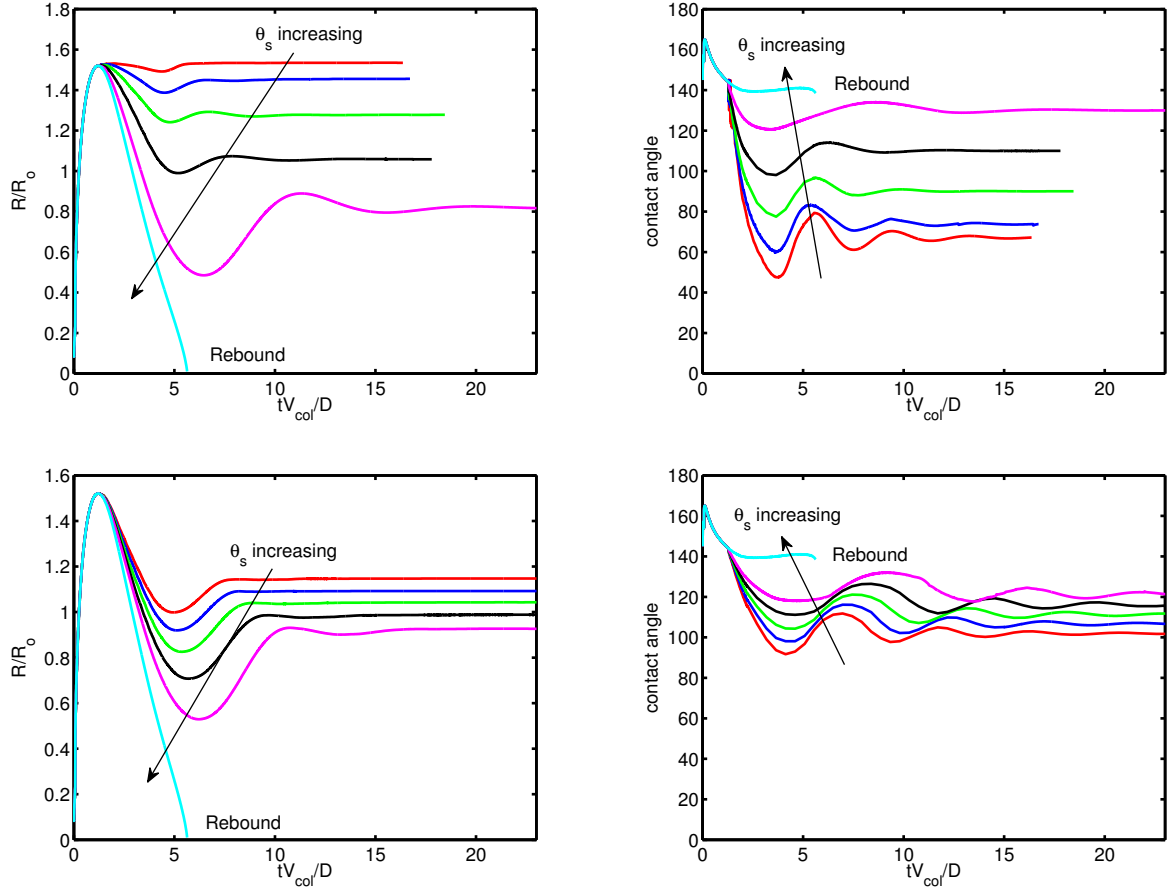


Figure 4.15: Effects of the saturated equilibrium contact angle θ_s on the drop impact and spreading for the fast deposition, $\tau = 1$, in the range $50 \leq \theta_s \leq 145$ (upper row), and the slow deposition, $\tau = 10$, in the range $10 \leq \theta_s \leq 145$ (lower row). ($Re = 75$, $We = 30$, $Wi = 1$, $L^2 = 225$, $\beta = 0.07$, $c = 0.075$ and $\theta_c = 145^\circ$).

of the polymer additives. The maximum spread factor is found to be enhanced slightly by the viscoelasticity, which is in agreement with the experimental observation and the numerical simulation results reported in the literature. These effects are pronounced as Wi is increased. It is also found that the polymeric viscosity ratio β and the extensibility parameter L^2 have a similar but weaker effect on the drop dynamics. The effects of the equilibrium contact angle θ_e , the Weber number and Reynolds number are found to be similar both for the Newtonian and viscoelastic cases: The tendency of a drop rebound strongly depends on and increases with the equilibrium contact angle θ_e and decreases with the Weber number. Similarly, the drop rebound is favored when the Reynolds number increases. The effects of viscoelasticity are found to be more pronounced at low Weber and high Reynolds numbers. Simulations are also performed to examine the effects of dynamic contact angle on the drop dynamics. As in the Newtonian case [90], the dynamic contact angle is found to be crucially important for accurate prediction of drop spreading and rebound. Further simulations are carried out by changing the polymeric viscosity while keeping the solvent viscosity unchanged. It is found that the drop rebound is suppressed as the polymeric viscosity is increased mainly due to the enhanced viscous dissipation.

Finally, the effects of polymer-induced hysteresis effects are examined. For this purpose, a simple model is developed to mimic the hysteresis due to deposition of polymer molecules on the substrate. It is found that the model is able to predict the anti-rebound effect of the polymeric additives and the results are found to be in good qualitative agreement with the experimental observations. The present results provide further evidence that the anti-rebound effect of polymer additives is related to the modification of the surface wetting properties rather than the change in the drop fluid properties.

4.6 Acknowledgement

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Chapter 5

CONCLUSION

A front-tracking method is developed for direct numerical simulations of viscoelastic interfacial flows. The method is general and applicable to two-phase systems in which either phase or both phases can be viscoelastic. It can accommodate virtually any viscoelastic model for each phase. Moreover, the method is readily extendible for simulation of multiphase systems in which more than two-phases may exist.

Semi-analytical and log-conformation schemes are used to integrate the viscoelastic constitutive equations in time. The log-conformation method is found to be very robust for a wide range of Weissenberg numbers whereas the semi-analytical method remains stable only for small or moderate Weissenberg numbers. However the semi-analytical method has advantage of requiring lower computational time and implementation complexity compared to the log-conformation method. A fifth-order upwinded WENO-Z scheme is used to discretize the convective terms in the viscoelastic model equations and found to be crucially important for resolving thin viscoelastic boundary layers near the interface. The method is first validated for single-phase viscoelastic flows. Then it is applied to buoyancy-driven motion of viscoelastic two-phase systems. The results are found to be in good qualitative and quantitative agreement with the computational simulations of You et al. [142]. Moreover, the present method is found to be stable and very robust for very low solvent viscosity ratios, i.e., as low as $\beta = 10^{-4}$.

Then, the effects of viscoelasticity on drop dynamics and deformation in a pressure-driven capillary tube with a sudden contraction/expansion are studied computationally using a front-tracking method. The FENE-CR model is employed to account for viscoelasticity of inner and outer fluids. It is found that the Weissenberg number has a non-monotonic influence on drop dynamics for both the VN and NV systems. At small Wi , the viscoelastic stresses pulls out/in the drop interface to cause a pointed/rounded trailing edge in the NV/VN case. As Wi is further increased, e.g., $Wi = 100$, the

viscoelastic stresses become more uniform in the dispersed/continuous phase and thus reduce the overall viscoelastic effects on drop deformation in the VN/NV system. It is found that the viscosity ratio has a significant influence and generally increases drop deformation. A re-entrant cavity may develop at the back of the droplet as the viscosity ratio increases. In contrast with the straight channel case, the viscoelasticity in the drop phase hinders whereas in the continuous phase enhances the formation of a re-entrant cavity in the constricted channel. At high Re , the droplet undergoes large deformation in the constriction followed by damped surface oscillations in the expansion region. Similar to the low Re case, Wi also has a non-monotonic effect on drop deformation at high Re numbers. In the expansion region, the magnitude of surface oscillation first increases/decreases and then decreases/increases with Wi for the VN/NV case. In the VV case, the surface oscillations generally increase with the elasticity ratio (k) but the values of the inner and outer Weissenberg numbers are also found to be important for drop dynamics. The large deformation may even lead to a drop breakup in some cases, especially at high Re and Wi numbers.

Finally, the effects of viscoelasticity on the dynamics of a drop impact on solid surfaces are studied computationally using a front-tracking method. The FENE-CR model is employed to account for viscoelasticity. When the hysteresis effects due to polymers are ignored, we found that viscoelasticity affects drop dynamics during both advancing and receding phases. It is found that the viscoelastic stresses favor the spreading of the droplet during advancing phase resulting in a slight increase in the maximum spreading rate. Furthermore, in the contrast with the well-known anti-rebound effects of polymeric additives, the viscoelasticity is found to enhance drop rebound during the receding phase. This finding supports the hypothesis that the anti-rebound effect is related to the resistance of polymer molecules deposited on the substrate rather than to the bulk fluid properties. This is also supported by the simple model that dynamically modifies the contact angle during the receding phase in a way to mimic the hysteresis effects observed in the experimental studies [11]. The model is able to qualitatively capture the anti-rebounding effects of the polymers.

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