Inertial Effects on the Flow of Capsules in Cylindrical Channels

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Abstract

A front-tracking method was used to study moderate to large-sized capsules flowing in cylindrical channels at Reynolds numbers ranging from 0.1 to 225. Two different constitutive equations, the Neo-Hookean and Skalak laws were considered to describe the mechanics of the thin membrane. The effect of capsule size, elastic capillary number, and Reynolds number on the shape, migration velocity, and extra pressure loss were determined. The deformation of the capsules was strongly tied to the size of the capsule compared with the channel diameter with larger capsules deforming more due to the confining effect of the wall. As the Reynolds number was increased, capsules were more elongated in the direction of flow. The effect of Reynolds number was more apparent as the elastic capillary number was increased. Both the migration velocity and extra pressure loss were seen to depend primarily on the size of the capsule with deformation playing a secondary role. The Neo-Hookean membrane showed a larger deformation than the Skalak law due to its strain softening nature. The Neo-Hookean membrane also displayed a failure phenomenon of continuous deformation at large enough elastic capillary numbers not seen in the Skalak law membranes. This limiting elastic capillary number was shown to decrease as Reynolds number became larger. The membrane strain was largest at the front of the capsule indicating the most likely region where the capsule would fail.

Keywords: capsule; pressure-driven; tube flow; inertia; Neo-Hookean law; Skalak law

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1. Introduction

Capsules consist of liquids or gels enclosed by a thin walled elastic membrane typically used to protect sensitive chemicals such as drugs or flavoring compounds for controlled release (Duncanson, et al., 2012; Nazzaro, et al., 2012; Zhang, et al., 2013). During capsule formation and use it is important to keep the membrane deformation below a critical level or it can rupture and prematurely release its contents (Chang & Olbricht, 1993b; Li, et al., 1988). The level of strain within the membrane can be predicted using a continuum model in which the capsule consists of a liquid drop surrounded by a two dimensional elastic membrane (Pozrikidis, 2003). Human red blood cells (RBC), in particular have received a lot of attention as they have a relatively simple non-nucleated interior which can be modeled as a Newtonian liquid (Fung & Zweifach, 1971; Skalak, et al., 1973). The flow and deformation of RBCs in small capillaries has been studied by a variety of authors to better understand human microcirculation (Secomb, 1993; Secomb & Hsu, 1996; Pozrikidis, 2005b; Chien, et al., 1971).

As capsules are often formed and processed in liquids it is of interest to study the flow induced deformation of capsules. Barthès-Biesel (1980) provided a small deformation analysis for the shape of a thin walled capsule in general linear flows. This work has been used to estimate elastic properties of artificial capsules based on their deformation by Chang and Olbricht (1993a) and by Walter et al. (2000). The analytical solutions are limited to small deformation studies in unbounded domains. For larger deformations, there have been many numerical simulations of capsules in shear flow which have elucidated the effects of different membrane constitutive equations (Barthes-Biesel, et al., 2002), membrane bending rigidity (Pozrikidis, 2001a), and the unstressed shape of the capsule (Bagchi & Kalluri, 2009). The continuum model of a capsule has also been used to understand the mechanical properties of biological cells (Lim, et al., 2006; Evans & Skalak, 1980). In addition to shearing flows, a lot of attention has been given to the flow of capsules in channels. Early research on channel flow was conducted by Lee and Fung (1969) who used thin walled rubber capsules flowing in cylindrical channels as model for blood flow. Leyrat-Maurin and Barthès-Biesel (1994) used a boundary integral technique to study the motion of a capsule through a channel with a constriction. They showed that as the capsule moved through the narrowest portion of the channel it significantly increased the flow resistance and could sometimes plug the channel. Numerical simulations of capsule flow have been performed in cylindrical channels (Lefebvre & Barthes-Biesel, 2007; Pozrikidis, 2005a; Queguiner & Barthes-Biesel, 1997), and square channels (Hu, et al., 2012; Kuriakose & Dimitrakopoulos, 2011; Doddi & Bagchi, 2009) by several authors in the Stokes flow limit. These studies have elucidated the effects of varying the elastic properties of the membrane and the size and shape of the capsules. Hu, Salsac, and Barthès-Biesel (2012) performed fully three dimensional studies of capsule flow in cylindrical and square channels and showed that the capsules are less deformed in square channels at similar flow conditions. The predictions of capsule shapes in the numerical simulations have been used to calculate material properties of artificial capsules in channel flow (Chu, et al., 2013; Lefebvre, et al., 2008; Dimitrakopoulos & Kuriakose, 2015).

In the current paper we examine the flow of capsules in cylindrical channels when inertial effects are important, such as flow through ventricular assist devices (Fraser, et al., 2011) or through syringes (Aguado, et al., 2011). Microfluidic devices have been created that rely on inertial forces to sort cells emphasizing the need for a better understanding on the role of inertia in these flows (Mach & Di Carlo, 2010; Zhang, et al., 2013). To date most of the work on inertial effects on capsule deformation has been limited to the case of capsules in shear flow (Bai, et al., 2013;

Salac & Miksis, 2012; Sui, et al., 2008; Doddi & Bagchi, 2008) with a few studies on capsule flow in channels (Kilimnik, et al., 2011; Shin & Sung, 2012). Bai *et al.* (2013) showed that the deformation and the time scale for deformation increased with the Reynolds number. Doddi and Bagchi (2008) made a phase diagram of the different pairwise interactions seen between capsules in shear flow at finite Re . The few numerical studies on inertial effects in channel flow have looked at lateral migrations (Kilimnik, et al., 2011) and tumbling motions of oblate capsules (Shin & Sung, 2012). Kilimnik, Mao, and Alexeev (2011) showed that the capsules deformation increased and the equilibrium position changed with the Reynolds number. However, to date there have been no studies that examine the effects of inertia on the deformation of confined capsules in channels.

In the current study we focus on the inertial effects of an axisymmetric capsule flowing in Poiseuille flow in a cylindrical channel. A front-tracking method, previously used to study droplet flow in channels (Carroll & Gupta, 2014), was modified to include an elastic membrane that provides a more localized treatment of the elastic tension and bending moments along the membrane. The numerical method is first validated against the test case of a capsule in an extensional flow field. Simulations were performed with channel Reynolds number ranging from 0.1 to 225. We examine the deformation of capsules with increases in Re and relate the deformation to changes in the capsules velocity and extra pressure loss.

2. Problem Formulation

We consider a single, thin walled, initially spherical, capsule flowing through a cylindrical channel as seen Figure 1. The capsule is taken to be neutrally buoyant with the density of the fluid inside ρ_c and outside of the capsule ρ_b , set equal and the mass of the capsule membrane considered to be negligible. The non-dimensional capsule size $\kappa = a / R$, where a is the undeformed capsule radius and R is the channel radius, is taken to be large enough that hydrodynamic forces keep the capsule on the channel centerline. The flow is therefore axially symmetric and we only consider the motion in the r - z plane. Fluid enters the channel at a constant flow rate Q , giving an average velocity $U = Q / (\pi R^2)$. The suspending fluid and the capsule's internal fluid are taken to be incompressible and Newtonian with equal viscosities, $\mu_c = \mu_b$. The location of the capsule membrane separating the two fluid is denoted by $\mathbf{x}_s$.

Figure 1. Description of capsule geometry and surface vectors. The flow is from the left to the right with the arc length starting from the rear of the capsule where $s = 0$.

The capsule is placed at the center of a long channel of length L , where the inlet and outlet boundaries are sufficiently far from the capsule that the flow is undisturbed. As the Reynolds number increases the flow disturbances from the capsule take longer to decay away requiring channels up to $L = 20R$. The capsule is set in a non-inertial reference frame $\mathbf{u}_{\text{ref}}$, which tracks the center of mass of the capsule. As we are interested in inertial effects on the capsule motion we solve the full Navier-Stokes equations written in conservative form as

$$Re \left[\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) \right] = -\nabla P + \nabla \cdot \boldsymbol{\tau} - Re \frac{\partial \mathbf{u}_{\text{ref}}}{\partial t}, \quad (1)$$

$$\nabla \cdot \mathbf{u}, \quad (2)$$

with the viscous stress tensor given as $\boldsymbol{\tau} = [(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T]$ and the channel Reynolds number based on the bulk fluid properties $Re = \rho_b UR / u_b$.

The no slip condition is imposed on the rigid walls of the tube and the inlet flow is specified to be parabolic, Poiseuille flow. The velocity field is assumed to be continuous at the interface and the membrane moves and deforms with the local velocity

$$\frac{d\mathbf{x}_s}{dt} = \mathbf{u}(\mathbf{x}_s). \quad (3)$$

Because we have assumed the interface to be massless the difference in stress of the two fluids exerts a load on the interface $\mathbf{f}$,

$$\mathbf{f} = [\boldsymbol{\Pi}_c(\mathbf{x}_s) - \boldsymbol{\Pi}_b(\mathbf{x}_s)] \cdot \mathbf{n}, \quad (4)$$

where $\boldsymbol{\Pi}_c$ and $\boldsymbol{\Pi}_b$ are the total stress tensors in the capsule and bulk fluids, and $\mathbf{n}$ is the outward pointing normal vector. Force equilibrium within the membrane requires a balance between the in-plane elastic tensions $\mathbf{T}$, and transverse shear tension $\mathbf{q}$, with the external load $\mathbf{f}$ as

$$\mathbf{f} = \frac{1}{Ea} \nabla_s \cdot (\mathbf{T} + \mathbf{q}\mathbf{n}), \quad (5)$$

where $\nabla_s = (\mathbf{I} - \mathbf{n}\mathbf{n}) \cdot \nabla$ is the surface gradient operator and $Ea = \mu_b U / G_s$ is the elastic capillary number based on the shear modulus G_s of the capsule membrane. The shear tension is calculated from the bending moment $\mathbf{m}$, within the membrane as

$$\mathbf{q} = \nabla_s \cdot \mathbf{m} \cdot (\mathbf{I} - \mathbf{n}\mathbf{n}). \quad (6)$$

The neo-Hookean law (Barthes-Biesel, et al., 2002) and the Skalak law (Skalak, et al., 1973) are used as constitutive equations in this paper. The derivation of the membrane mechanics has been reported previously by (Barthes-Biesel, 1980; Evans & Skalak, 1980; Pozrikidis, 2001b), and is only briefly summarized here. For axisymmetric capsules the deformation tensor can be represented by its two principal strain ratios: the meridional strain ratio λ_m , and the azimuthal

strain ratio λ_θ . Consequently, the tension in the membrane can also be represented by the two principal components, T_{mm} and $T_{\theta\theta}$. The strain ratios are calculated from the capsule's deformation as

$$\lambda_m = \frac{ds}{ds_r}, \lambda_\theta = \frac{r}{r_r}, \quad (7)$$

where ds and ds_r are the differential arc lengths in the deformed and reference shape and r and r_r are the radial positions of the membrane in the deformed and reference shape.

The two dimensional Neo-Hookean law is derived from a model of a thin sheet of a volume incompressible rubber like material. At large strains this material displays strain-softening behavior. The tension is related to the deformation through the principal strain ratios as

$$T_{mm} = \frac{G_s}{\lambda_m \lambda_\theta} \left(\lambda_m^2 - \frac{1}{\lambda_m \lambda_\theta} \right), \quad (8)$$

where G_s is the membrane shear modulus and $T_{\theta\theta}$ is found by interchanging the indices. The Skalak law was originally introduced to model red blood cells membranes (Skalak, et al., 1973), and has the following relationship between the principal strain and the principal tensions,

$$T_{mm} = \frac{G_s}{\lambda_m \lambda_\theta} \left(\lambda_m^2 (\lambda_m^2 - 1) + C (\lambda_m^2 \lambda_\theta^2) [(\lambda_m^2 \lambda_\theta^2) - 1] \right). \quad (9)$$

The Skalak law has a material parameter C , which describes the resistance to area dilation. For red blood cells the ratio C/G_s can be as large as 10^5 (Guido & Tomaiuolo, 2009), however $O(1)$ values of C/G_s have been used to describe alginate membranes (Lefebvre & Barthes-Biesel, 2007). At larger deformations the Skalak law displays strain-hardening behavior.

A simple linear constitutive equation (Pozrikidis, 2003), is used to relate the bending moments to changes in curvature from a reference state

$$M_{mm} = E_b (\kappa_m - \kappa_{m_r}), M_{\theta\theta} = E_b (\kappa_\theta - \kappa_{\theta_r}), \quad (10)$$

where E_b is a bending modulus, κ_m and κ_θ are the two principal curvatures, and κ_{m_r} and κ_{θ_r} are the reference curvatures for the membrane in an unstressed state. In the current problem we chose the reference curvatures to be that of the capsule in a spherical shape, $\kappa_{m_r} = \kappa_{\theta_r} = 1/a$.

The membrane that comprises the shell of the capsule is often permeable to water and small ions while retaining larger compounds. In previous studies on alginate capsules (Lefebvre & Barthes-Biesel, 2007; Risso, et al., 2006) it was theorized that part of the alginate capsule had dissolved into the internal fluid leading to an osmotically driven flow of water into the capsule. For spherical, isotropic membranes this osmotic swelling will lead to an isotropic increase in the capsule strain. We define this pre-strain as the ratio between the deformed and initial radius

$$\lambda_{mo} = \lambda_{\theta\theta} = \frac{a}{a_r} = 1 + \alpha. \quad (11)$$

Here λ_{mo} is the strain ratio at the start of the simulation, α represent the amount of extra initial strain in the membrane, and a_r is the radius of the capsule before osmotic swelling. In the current simulations we use a small pre-strain to ensure the capsule is in tension everywhere to avoid surface instabilities and surface wrinkling (Chu, et al., 2013). When an initial strain is applied to a capsule we characterize its size and reference curvature using the deformed radius a , not the un-swelled radius a_r .

3. Numerical Method

A hybrid Volume-Of-Fluid (VOF)-front tracking scheme was implemented to study the dynamics of pressure-driven capsules in a flow as it combines the volume conservation property of the VOF method and the accuracy of interfacial force description of the front tracking method (Popinet & Zaleski, 1999; Agresar, et al., 1998; Carroll & Gupta, 2014). In the VOF method, the capsule and bulk fluids are treated as a single phase with varying properties (Hirt & Nichols, 1981) and the interfacial stress condition is converted to a volume force using the continuum surface force method of Brackbill et al. (Brackbill, et al., 1992). The interfacial forces are only applied to cells on the Cartesian grid that are intersected by the capsule interface.

The membrane is located by materials points that are connected with a cubic spline that allows for accurate computation of surface normal and curvatures. In the axisymmetric formulation the stress jump at the interface is separated in normal $\mathbf{n}$, and tangential $\mathbf{t}_m$ components as

$$\mathbf{f} = \frac{1}{Ea} \left[\left(\kappa_m T_{mm} + \kappa_\theta T_{\theta\theta} - Br \frac{1}{r} \frac{\partial(rq)}{\partial s} \right) \mathbf{n} - \left(\frac{\partial T_{mm}}{\partial s} - \frac{(T_{mm} - T_{\theta\theta})}{r} \frac{\partial r}{\partial s} - Br (\kappa_m q) \right) \mathbf{t}_m \right], \quad (12)$$

where $\partial/\partial s$ is a derivative along the meridian of the capsule and $Br = E_b / G_s R^2$ is the reduced bending modulus. The transverse shear tension is calculated from the bending moments as

$$q = \frac{1}{r} \left(\frac{\partial(rM_{mm})}{\partial s} - M_{\theta\theta} \frac{\partial r}{\partial s} \right). \quad (13)$$

The strain ratios are updated at the end of each time step with the meridional strain at a given node taken to be the average of the strain in the neighboring line segments and the azimuthal strain coming directly from the change in radial position of the node. The meridional strain in the neighboring line segments is calculated from the distance between material points and becomes more accurate as the spacing between the material points decreases. The stress jump at the interface is converted into a body force $\mathbf{F}$, by integrating the stress jump over a given Eulerian grid cell as

$$\mathbf{F} = \int \mathbf{f} \delta(\mathbf{x}_s - \mathbf{x}) dV = \int \mathbf{f} ds \quad (14)$$

where δ is the Dirac delta function, dV is the volume associated with a velocity node and ds is the interface arc length within the volume. The delta function reduces the volume integral to a line integral over the intersection of the interface and the cell. The total stress within the cell is

then divided by the cell volume to give an average forcing term that can be incorporated into a finite difference method. The momentum equation is then written in a form valid in the entire domain with the extra forcing term only being non-zero on cells intersected by the interface

$$Re \left[\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) \right] = -\nabla P + \nabla \cdot \boldsymbol{\tau} + \mathbf{F} - Re \frac{\partial \mathbf{u}_{\text{ref}}}{\partial t}. \quad (15)$$

The Navier-Stokes equations are solved using a projection method for the time stepping and a multigrid preconditioned Krylov subspace method as a linear solver. A more thorough description of the solver can be found in previous paper on droplet flow (Carroll & Gupta, 2014).

The simulations are run with on an equally spaced grid with a grid resolution $\Delta r = \Delta z = 0.006125$ and time step at or below 10^{-4} . Two extra numerical procedures are used at the end of each time step. The first procedure is a volume conservation step that adjusts the position of the interface to ensure that the volume of the capsule is exactly conserved over the simulation. To test the impact of the volume conservation step, a simulation was run for a capsule without the volume conservation adjustment for $\kappa = 0.9$, $Re = 100$, $Ea = 0.10$, $\alpha = 0.10$, and $Br = 10^{-4}$. The simulation was run with a grid resolution of $\Delta r = \Delta z = 0.006125$ for 50 non-dimensional time units which was twice the time required to reach steady state for that simulation and is long enough for most simulations reported here to reach steady state. The capsule volume was found to decrease by less than 1% over the course of the run. The error tends to grow as the elastic capillary number decreases. While the volume conservation steps are not required for most of the simulations, they are maintained for consistency throughout this paper. The second procedure is a surface smoothing step. The inclusion of bending moments in the simulation requires the calculation of the fourth derivate of the interface position. Small numerical noise inherent to this simulations is greatly amplified when numerical derivatives are taken, so a Savitsky-Golay smoothing procedure is used at the end of each time step (Savitzky & Golay, 1964). As excess smoothing can alter the solution, the smallest amount of smoothing that maintains a stable solution is used.

4. Validation

The two phase Navier-Stokes solver was validated for droplet flow in a channel by Carroll and Gupta (2014). Here, the numerical model for membrane deformation and tension is validated for the case of an elastic capsule with a Neo-Hookean membrane in uniaxial extensional flow. The current numerical simulations are compared with the small deformation analysis of Barthes-Biesel (1980), and the boundary integral simulations of Diaz et al. (2000). The external flow field is a linear straining field given by $\mathbf{u} = \mathbf{E} \cdot \mathbf{x}$ where $E_{11} = 2$ and $E_{22} = E_{33} = -1$. A spherical capsule with zero bending modulus and no pre-strain was used for the initial configuration. The Reynolds number was set to 10^{-2} in our simulations to match the Stokes flow limit in Barthes-Biesel (1980) and Diaz et al. (2000). We consider only the extensional case as the analytical theory is only accurate to $O(Ea)$ and as such does not differentiate between uniaxial extension and compression. The capsule deformation is quantified using the Taylor deformation parameter, $D = (L - B)/(L + B)$, where L and B are the long and short axis of the capsule respectively. The steady deformation parameter as a function of the elastic capillary number is shown in Figure 2. The current results agree well with the Stokes flow simulations of Diaz et al. (2000) for large elastic capillary numbers and reduce to the small deformation theory of Barthes-Biesel (1980) in the limit as $Ea \rightarrow 0$.

Figure 2. Deformation of an initially spherical capsule in uniaxial extensional flow as a function of Ea . Comparison between the current simulations predictions and the small deformation theory of Barthes-Biesel (Barthes-Biesel, 1980) and the simulations of Diaz et al. (Diaz, et al., 2000).

5. Results and Discussion

As the steady motion of an axisymmetric capsule in a channel is characterized by a stationary inner fluid it is sufficient to only consider the case of equal fluid viscosities. The capsule motion and deformation is studied as a function of the elastic capillary number, Reynolds number, and membrane constitutive equation. The relative capsule size $\kappa = a/R$, is kept between 0.4 and 0.9. Larger capsules tend to buckle as they deform to fit into the channel destroying the symmetry of the problem and smaller capsules can migrate off the centerline.

Negative tensions tend to arise in the capsule membrane at two different locations. The confining effect of the channel forces the capsule into a narrower shape radially compressing it and the fast flow on the centerline tends to push the rear of the capsule into itself. The former leads to channel parallel wrinkles while the latter causes the rear of the capsule to change from a convex to a concave shape. The channel parallel wrinkles have been seen experimentally in capsules flowing in cylindrical channels as well as in numerical simulations (Walter, et al., 2000; Hu, et al., 2012; Lefebvre, et al., 2008), however they are not axisymmetric and cannot be captured by the current method. The inclusion of membrane pre-strain and bending rigidity ensure the capsules remain axisymmetric without forming surface wrinkles. The effect of bending rigidity on the capsule shape is shown by varying Br from 10^{-3} to 10^{-5} for a large capsule, $\kappa = 0.9$, in the absence of pre-strain and large deformations, $Ea = 0.10$ and $Re = 100$. At the small levels of Br used in the study, the capsule shape is only slightly affected as shown in

Figure 3(a). The most dramatic effects are seen near the rear of the capsule where the bending rigidity prevents the capsule from forming a cusp. In order to capture some of the physical effects of bending rigidity while still allowing for large deformations the bending ratio was set to 10^{-4} for the rest of the simulations.

Figure 3. Effect of (a) bending ratio with $\alpha = 0$ and (b) pre-strain with $Br = 10^{-4}$ on the shape of a Neo-Hookean membrane capsule with $\kappa = 0.9$, $Ea = 0.10$, and $Re = 100$.

Figure 4. Effect of initial strain on tension in the meridional (a), and azimuthal (b), direction as a function of arc length. The initial strain is shown for $\alpha = 0, 0.05, 0.10, 0.15$, for $\kappa = 0.9$, $Ea = 0.10$, $Re = 100$, and $Br = 10^{-4}$, for a Neo Hookean membrane.

The effect of the initial strain on the capsule shape is much more dramatic as seen in Figure 3(b) where the pre-strain, α is varied from 0 to 0.15 for capsule under similar flow conditions with $Br = 10^{-4}$. At low levels of pre-strain, the capsule is highly deformed and the rear end buckles to form a concave shape. For an initial strain of $\alpha = 0.10$, the buckle has almost disappeared and the rear of the capsule is nearly flat. As the initial strain is increased further the membrane is in tension everywhere and the buckle disappears. This transition from concave to convex has been used to estimate the material properties of capsule in channel flow (Lefebvre & Barthes-Biesel, 2007; Lefebvre, et al., 2008). The effect of varying the amount of initial pre-strain on the meridional and azimuthal tensions is seen in Figure 4. The increase in α raises the tension uniformly along the surface of the capsule. The tension is everywhere positive in the meridional direction irrespective of the initial strain while only becoming uniformly positive in the azimuthal direction for $\alpha > 0.10$. The channel parallel wrinkles are caused by negative azimuthal tensions. We therefore, set $\alpha = 0.10$ for the rest of the simulations to ensure the membrane stays in tension and is not artificially stabilized by the axisymmetric nature of the problem.

The deformation of a capsule flowing in a channel is strongly dependent on the relative size of the capsule. Small capsules do not feel the confining effect of the wall and flow in a region of low shear and therefore have relatively small deformations and remain nearly spherical. As the capsule becomes larger the fluid flow around the capsule is confined to a thin annulus between the capsule and channel wall. A lubrication type flow exists here which can generate large stresses on the membrane and large extra pressure loss in the system (Secomb & Hsu, 1996). The effect of capsule size on the shape and deformation of the capsule is shown in Figure 5 for a Neo-Hookean membrane with $Ea = 0.10$. The meridional and azimuthal strains are plotted as a function of the normalized arc length in Figure 6. For small capsules the deformation is small and the capsule remains spherical. Larger capsules show increased deformation and the strain increases rapidly as $\kappa \rightarrow 0.9$. The meridional strain is largest near the front of the capsule as it stretches out into an elongated shape. Towards the rear of the capsule strain remains small as the flow is pushing the rear of the capsule into itself. The azimuthal strain takes on an almost sinusoidal form with areas of high extension at the front and areas of compression in the middle as the capsule is forced into a narrower shape. The region of large strain near the front of the capsule indicates the most likely area where the membrane would fail if overstrained.

Figure 5. Family of capsule shapes for different sizes $\kappa = 0.4$ (innermost), 0.5, 0.6, 0.7, 0.8, and 0.9 (outermost), for Neo-Hookean membranes with $Ea = 0.10$, $Re = 100$, $\alpha = 0.10$, and $Br = 10^{-4}$.

In addition to the local membrane properties we also plot the capsule velocity and the extra pressure loss as a function of capsule size in Figure 7. These macroscopic quantities show a very strong relationship to the capsule size. The velocity is a decreasing function of capsule size as is expected from previous studies on droplet flow in channels. Very small capsules will flow at the local fluid velocity which is twice the mean velocity on the centerline. Large capsules move slowly as the thin annulus between the capsule and the channel wall restricts the flow around the capsule. The extra pressure loss depends on how much the capsule obstructs the otherwise Poiseuille flow. Small capsules create a relatively small disturbance to the bulk flow while large capsules nearly block the channel causing large pressure loss. Large capsules can significantly increase the pressure loss of the system as in the current scaling the non-dimensional pressure loss per unit length is 8.

We now consider the effect of changing the Reynolds number on the flow and deformation of capsules. Based on previous work on the inertial effects on droplet flow, it is expected that increasing the Reynolds number will increase the deformation of the capsules (Carroll & Gupta, 2014). A comparison of capsules flowing at different Reynolds numbers can be seen in Figure 8 where the pressure field and streamlines for the flow are also shown. The inertial effects only begin to become apparent in the capsule shape for $Re \geq 50$. As the inertial effects become important the capsule becomes longer and narrower. The pressure is seen to locally increase in the gap between the capsule and the channel wall forcing it into a narrower shape. The front of capsule become more pointed and the rear of the capsule becomes flattened. The meridional and azimuthal strains as a function of the normalized arc length for varying Reynolds numbers are shown in Figure 9. The lengthening of the capsule leads to an increase in the meridional strain particularly in the front of the capsule. For $Re = 200$, there is a rapid increase in the meridional and azimuthal strains at the very front of the capsule. This local increase could cause the membrane to rupture near the front of the capsule at larger values of Re . Consequently, the limiting value of the elastic capillary number at which the Neo-Hookean capsule is no longer stable will depend on the Reynolds number. As the flow tends to become unstable and the time

required to reach steady state increases at high Reynolds numbers, the simulations were limited to $Re \leq 225$.

Figure 6. (a) Meridional and (b) azimuthal strain as a function of the normalized arc length for capsules of varying sizes for a Neo-Hookean membrane with $Ea = 0.10$, $Re = 100$, $\alpha = 0.10$, and $Br = 10^{-4}$.

Figure 7. Capsule velocity and extra pressure loss as a function of capsule size for a Neo-Hookean membrane with $Ea = 0.10$, $Re = 100$, $\alpha = 0.10$, and $Br = 10^{-4}$.

$Re = 0.1$

$Re = 100$

$Re = 200$

Figure 8. Streamlines (lower half) and pressure contours (upper half) at $Re = 0.1$, 100, and 200 for a Neo-Hookean capsules for $\kappa = 0.9$, $Ea = 0.10$, $\alpha = 0.10$, and $Br = 10^{-4}$.

Figure 9. Effect of Reynolds number on the (a) meridional and (b) azimuthal strain as a function of the normalized arc length for Neo-Hookean capsules with $\kappa = 0.9, Ea = 0.10, \alpha = 0.10, Br = 10^4$.

Next, we consider the effect of different membrane constitutive equations on the capsule deformation and mobility. A comparison of capsule shapes for Neo-Hookean and Skalak law

membranes with different membrane parameters, $C = 0.1$ and $C = 1$, is shown in Figure 10(a-c) for $Re = 0.1, 100$, and 200 . The Neo-Hookean membrane is much more deformed than either of the Skalak membranes. The Skalak membrane with $C = 0.1$ shows greater deformation than $C = 1$ membrane and also has a concave rear end as opposed to the convex shape of the $C = 1$ membrane. The increase in deformation with Reynolds number is quantified by the excess area $(A-A_0)/A_0$, where A_0 is the area of the undeformed capsule as shown in Figure 10(d). The excess area increases as Re becomes large although there is a slight decrease in A/A_0 for smaller values of Re for the more deformable Neo-Hookean and Skalak capsules with $C = 0.1$. The deformation of the Neo-Hookean capsule is seen to increase faster than the Skalak law capsules as the Skalak law is a strain hardening law while the Neo-Hookean law is strain softening. The meridional and azimuthal strains of the Neo-Hookean and Skalak law membranes are shown in Figure 11 for $Re = 100$. A large strain is again seen at the front of the Neo-Hookean capsule which is not seen for either of the Skalak law capsules. The $C = 0.1$ capsule shows a similar, but larger in magnitude, strain compared to the $C = 1$ capsule.

The effect of increasing the Reynolds number on the capsule velocity and extra pressure loss for these capsules is shown in Figure 12. The more deformable Neo-Hookean capsules show a larger velocity and lower pressure loss than the Skalak law capsules. The velocity is seen to monotonically increase with Re for all the capsules. The extra pressure loss decreases with Re for the more deformable Neo-Hookean and Skalak law capsule with $C = 0.1$ while the Skalak law capsule with $C = 1$ displays a slight maximum in pressure loss around $Re = 100$. The increase in capsule mobility comes from the deformation of the capsules into a narrower shape as Re increases. The deformation increases the gap between the capsule and the channel wall reducing the extra pressure loss. The non-monotonic trend seen for the $C = 1$ capsule is due to capsule becoming slightly wider at an intermediate Re before elongating into a narrow shape at higher Re .

Figure 10. Comparison of capsule shapes for (a) $Re = 0.1$, (b) $Re = 100$, (c) $Re = 200$ and (d) excess area as a function of Reynolds number for Neo-Hookean and Skalak law membranes with $\kappa = 0.9$, $Ea = 0.10$, $\alpha = 0.10$, and $Br = 10^{-4}$.

Figure 11. (a) Meridional and (b) azimuthal strain along the normalized arc length for Neo-Hookean and Skalak membranes for $Re = 100$, $\kappa = 0.9$, $\alpha = 0.10$, and $Br = 10^{-4}$.

Figure 12. Effect of Reynolds number of the capsule velocity, (a) and extra pressure loss, (b) for Neo-Hookean and Skalak law, $C = 0.1$ and 1 , membranes with $\kappa = 0.9$, $Ea = 0.10$, $\alpha = 0.10$, and $Br = 10^{-4}$.

Figure 13. Family of capsule shapes for different elastic capillary numbers, $Ea = 0.03$ (innermost), 0.05, 0.07, 0.09, and 0.11 (outermost) for (a) Neo-Hookean (b) Skalak, $C = 0.1$, and (c) Skalak, $C = 1$ membranes with $\kappa = 0.9$, $Re = 100$, $\alpha = 0.10$, $Br = 10^{-4}$.

The effect of varying Ea on the capsule shape is shown Figure 13 for both Neo-Hookean and Skalak type membranes with the Skalak law parameter set to $C = 0.1$ and 1. At low Ea , the capsules have a similar shape with a convex rear end. As Ea increases, the capsules elongate and the rear end flattens. For the Neo-Hookean and Skalak membrane with $C = 0.1$ the rear end becomes concave at larger Ea while the Skalak membrane with $C = 1$ remains convex. The Neo-Hookean capsule deforms the greatest followed by the Skalak with $C = 0.1$ and then the Skalak with $C = 1.0$ capsules.

The buckling transition from a convex to concave rear end can be more clearly seen in Figure 14(a) where the meridional curvature at the rear end of the capsule is shown. At a small Ea the Neo-Hookean and Skalak capsule with $C = 1$ have similar values for curvature while the Skalak capsule with $C = 0.1$ shows a smaller curvature indicating a flattening of the surface. The transition from convex to concave occurs as the curvature transitions from positive to negative. The Skalak capsule with $C = 0.1$ becomes concave at a smaller Ea than the Neo-Hookean membrane even though the overall deformation as measured by the excess area is smaller indicating a difference in the way the capsule deforms. The Skalak law with $C = 1$ remains convex for the range of Ea studied although the trend would suggest a transition at higher Ea . The maximum strain within the membrane is shown in Figure 14(b) as a function of Ea . As expected from the plots of excess area, the strain is highest within the Neo-Hookean membrane and lowest in the Skalak law membrane with $C = 1$. The strain within the Skalak law capsules seems to be varying linearly with Ea while the Neo-Hookean membrane shows a rapid increase in strain at larger Ea due to its strain softening behavior. Based on Figure 14(b) it would seem that the strain in the Neo-Hookean capsule is growing rapidly and steady shapes will not exist for Ea larger than 0.120. As reported previously (Li, et al., 1988), if Ea is too large, the Neo-Hookean capsule will continuously deform until it ruptures while the Skalak type capsule will remain stable. As the Skalak capsule is strain hardening it is not expected to show this failure mechanism.

Figure 14. (a) Rear meridional curvature and (b) Maximum meridional strain as a function of elastic capillary numbers for Neo-Hookean and Skalak membranes with $\kappa = 0.9$, $Re = 100$, $\alpha = 0.10$, $Br = 10^{-4}$.

The limiting Ea , the last stable value of Ea before the capsule fails, is highly dependent on the size of capsule. Neo-Hookean capsules were simulated at different sizes with increasing Ea until the deformation of the capsule was seen to increase without bound and no stable shape was found. The limiting elastic capillary number as a function of drop size is plotted in Figure 15(a) for Neo-Hookean capsules with $Re = 100$. The limiting elastic capillary number is a decreasing function of κ as the deformation greatly increases with the confinement of the capsule. Once the deformation is large enough, the strain-softening nature of Neo-Hookean membrane causes the capsule to continuously deform in an attempt to match the viscous stress at its surface. This limiting Ea only represents a theoretical limit for the capsule stability based on the Neo-Hookean law being valid for any level of strain. The membrane could rupture or deviate from the Neo-Hookean behavior before this theoretical limit is reached. Similarly, while the Skalak law membranes do not show a limiting Ea in this sense, there will obviously exist a limiting Ea where the membrane fails. The limiting Ea will also depend on the Reynolds number. This can be seen clearly in Figure 15(b) where the maximum meridional strain for a Neo-Hookean capsule is plotted as a function of Ea at different Reynolds numbers. As the deformation becomes larger, the Reynolds number has a larger effect on the membrane strain. This increase in maximum strain with Re will shift the limiting elastic capillary numbers to lower values. At a Reynolds number of 200, the highest stable capsule has $Ea = 0.10$ compared with 0.12 for the low $Re = 0.1$ simulations.

Finally, Figure 16 shows the capsule velocity and extra pressure loss as a function of Ea for large $\kappa = 0.9$ capsules at $Re = 100$ for Neo-Hookean and Skalak law membranes. The increase in deformability with increases in elastic capillary number leads to an increase in the capsule velocity. The extra pressure loss is very large at small Ea and rapidly decreases as Ea becomes larger. The extra pressure loss is still large even at the limiting Ea as compared to a fluid droplet of the same size due to the rigid boundary of the capsule. The Skalak law capsule with $C = 1$ is less deformable than the other capsules and as a result shows a slower velocity and larger extra pressure loss. This result is similar to that seen for increases in the Reynolds number.

Figure 15. (a) Limiting elastic capillary number as a function of capsule size at $Re = 100$ and (b) maximum meridional strain as a function of elastic capillary number for varying Reynolds number at $\kappa = 0.9$ for Neo-Hookean membranes with $\alpha = 0.10$, $Br = 10^{-4}$.

Figure 16. Effect of elastic capillary number on the (a) capsule velocity and (b) extra pressure loss for Neo-Hookean and Skalak law membranes with $\kappa = 0.9$, $Re = 100$, $\alpha = 0.10$, and $Br = 10^{-4}$.

6. #Conclusions

Numerical simulations were performed for capsules flowing in cylindrical channels for Reynolds numbers ranging from 0.1 to 225. Membrane bound capsules were studied for two different membrane constitutive equations, the Neo-Hookean and Skalak laws. The Neo-Hookean membranes displayed a strain softening behavior which led to greater deformations while the Skalak law membranes were strain hardening depending on the value of the parameter C . For larger values of C , capsules were rigid and showed very little deformation. The Neo-Hookean capsules displayed a behavior of continuous deformation when the elastic capillary number was above a limiting value. The limiting Ea was found to be a function of the capsule size. The Skalak capsules with their strain hardening membrane did not display a limiting Ea for the range of parameters studied. Increases in the level of membrane strain at higher Reynolds numbers shifted the limiting elastic capillary number to smaller values. It was found that the shape tended to be the most important factor in determining the drop velocity or extra pressure drop. The change in shape at higher Reynolds number caused the capsule to travel faster. A similar effect was also seen in droplet flow at higher Reynolds number. However, the changes in drop velocity and extra pressure loss were monotonic with increasing Re unlike droplet flow in cylindrical channels at finite Reynolds number (Carroll & Gupta, 2014). An axisymmetric numerical model requires a finite bending resistance and pre-strain to prevent the channel parallel buckling. However, this restricts the deformation that the capsules will experience at higher Reynolds numbers. A full three dimensional model for the inertial flow of capsules would be required to overcome several restrictions in an axisymmetric model such as limited deformation, capsule-capsule interaction, and tumbling and tank treading motions. Three dimensional simulations would also be useful for studying flows in non-axisymmetric geometries like square and rectangular channels seen in microfluidic systems as well as complicated geometries like vasculature.

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7. #References

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