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To my parents, who have encouraged me and supported me all these years.
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ΠΕΡΙΛΗΨΗ

1. ΕΛΛΕΙΠΤΙΚΗ ΔΗΜΙΟΥΡΓΙΑ ΠΛΕΓΜΑΤΟΣ ΣΕ ΠΕΔΙΑ ΠΟΥ ΠΕΡΙΕΧΟΥΝ ΠΟΛΛΑΠΛΑ ΕΓΚΛΕΙΣΜΑΤΑ ΚΑΙ ΥΠΟΚΕΙΝΤΑΙ ΣΕ ΜΕΓΑΛΕΣ ΠΑΡΑΜΟΡΦΩΣΕΙΣ

Ο ακριβής αριθμητικός υπολογισμός πολλών σημαντικών επιστημονικών και τεχνολογικών διεργασιών με ελεύθερες επιφάνειες ή κινουμένα σύνορα αποτελεί μεγάλη πρόκληση στον τομέα της έρευνας εδώ και πολλές δεκαετίες. Δύο τέτοιες διεργασίες είναι και αυτές που μελετώνται στην παρούσα εργασία: (α) φυσαλίδες μέσα σε ιξωδοελαστικά νήματα που υπόκεινται σε εφελκυσμό και (β) αλληλεπιδρούσες φυσαλίδες σε ακουστικό πεδίο ροής λαμβάνοντας υπ’ όψη και τις εξώδεις δυνάμεις. Φυσαλίδες ή κοιλότητες αναπτύσσονται σε λεπτά φίλμ κατασκευασμένα από μακρομόρια υψηλού μοριακού βάρους που χρησιμοποιούνται ως συγκολλητικά σε ένα πλήθος εφαρμογών με τη γενική ονομασία pressure sensitive adhesives (PSA’s). Οι φυσαλίδες αυτές μπορούν να εξελιχθούν σε νήματα με σημαντικές επιπτώσεις στις μηχανικές ιδιότητες του υλικού καθώς μπορούν να οδηγήσουν αρχικά στην αύξηση της μηχανικής αντοχής του υλικού και τελικά στην καταστροφή του. Από την άλλη, οι φυσαλίδες που πάλλονται και αλληλεπιδρούν σε ένα ακουστικό πεδίο ροής κατέχουν σημαντική θέση στη σύγχρονη επιστήμη και τεχνολογία, καθώς παίζουν σημαντικό ρόλο σε ένα πλήθος μηχανικών εφαρμογών, όπως η παραγωγή ατμού και η λειτουργία των στροβιλομηχανών, ο διαχωρισμός αερίου ή υγρού διασπαρμένου σε άλλο μη αναμίξιμο υγρό κ.τ.λ.

Οι υπολογιστικές μέθοδοι για την αριθμητική προσομοίωση τέτοιων προβλημάτων απαιτούν ισχυρές τεχνικές διακριτοποίησης που βασίζονται στη χρήση κατάλληλων πλεγμάτων. Τα πλέγματα είναι σύνολα από διακριτά σημεία κατά μήκος γραμμών που καλύπτουν το φυσικό πεδίο και πρέπει να ικανοποιούν κάποιες συγκεκριμένες ιδιότητες όπως ομαλότητα και ορθογωνιότητα κατά μήκος συγκεκριμένων συνόρων. Ανάλογα με τη μέθοδο που χρησιμοποιείται για τη δημιουργία των πλέγματος, οι αριθμητικές τεχνικές μπορούν να ταξινομηθούν και βασισμένοι σε Lagrangian, Eulerian και μικτές Lagrangian-Eulerian (ALE). Οι τεχνικές αυτές, αν και έχουν πολλά πλεονεκτήματα, οδηγούν σε μεγάλες παραμορφώσεις του πλέγματος και απαιτούν συχνή αναδημιουργία του, μειώνοντας έτσι την ακρίβεια της λύσης. Οι Dimakopoulos and Tsamopoulos (2003a), βασισμένοι σε προηγούμενες εργασίες
μεθόδους ιξωδοελαστικό περίπτωση (Karapetsas and Tsamopoulos 2008), όπου περιορίσματα μόνης κατάστασης (Tsamopoulos et al. 2008; Karapetsas and Tsamopoulos 2008), χρονομεταβαλλόμενων (Dimakopoulos and Tsamopoulos 2003a, 2003b, 2003c, 2004, 2007; Foteinopoulou et al. 2204, 2006; Karapetsas and Tsamopoulos 2006) και ανάλυσης ευστάθειας (Carvalho and Scriven 1999). Δυστυχώς όμως, όλα τα παραπάνω σχήματα αποτυγχάνουν στην περίπτωση που το πεδίο περιέχει εγκλείσματα τα οποία υπόκεινται σε ισχυρές παραμορφώσεις, όπως συμβαίνει στην περίπτωση αλληλεπιδροσών φυσαλίδων σε παλλόμενα πεδία ροής ή φυσαλίδων μέσα σε εξωδελαστικό νήμα που υπόκειται εφελκυσμό. Πιο συγκεκριμένα, με τις προαναφερθείσες μεθόδους επιδιώκεται η εξομάλυνση των γραμμών του πλέγματος σε συγκεκριμένα σημεία έτσι ώστε να μπορούν να αντιμετωπίσουν οι μεγάλες παραμορφώσεις. Στην περίπτωση των φυσαλίδων όμως, η εξομάλυνση αυτή εμφανίζεται σαν απόδημη σε σημεία που να μην είναι ιδιαίτερα ακόμη διακριτοποίηση προκειμένου να μην διενεργήσουν σε αριθμητικά σφάλματα. Τέτοια σημεία είναι οι πόλοι της φυσαλίδας. Το πρόβλημα αυτό αντιμετωπίζεται επιτυχώς, επεκτείνοντας την δουλειά των Dimakopoulos and Tsamopoulos (2003a), με δύο τρόπους στην παρούσα εργασία:

(a) στην περίπτωση των φυσαλίδων σε εξωδελαστικό νήμα, εφαρμόζοντας κατάλληλες συνθήκες κατανομής των κόμβων σε συγκεκριμένες εσωτερικές γραμμές του πλέγματος (ψευδό-σύνορα) που ξεκινάνε από τους πόλους της φυσαλίδας,

(β) στην περίπτωση των παλλόμενων φυσαλίδων, που υπόκεινται σε πιο ισχυρές παραμορφώσεις, με τον χωρισμό του φυσικού πεδίου σε υπό-πεδία καθένα από τα οποία περιγράφεται από το δικό του σύστημα συντεταγμένων και την επανένωσή τους για την επίλυση των εξισώσεων της ροής.

Έτσι, σε σχέση με τις προηγούμενες μεθόδους, κατάλληλες συνδυασμένες συνθήκες και περιορισμοί, όπως ορθογωνιότητα και κατάλληλη κατανομή των κόμβων πάνω σε συγκεκριμένες γραμμές του πλέγματος, μπορούν να εφαρμοστούν πιο εύκολα, ενώ δεν χρειάζεται πλέον η χρήση ελκτικών όρων σε γονίδες του πλέγματος ή ιδιαίτερα σημεία, μα ιδέα που είχε προταθεί από τους Dimakopoulos and Tsamopoulos (2003a). Επιπλέον, προκειμένου να ανεξαρτεί η πυκνότητα του πλέγματος γύρω από τις ελεύθερες επιφάνειες, όπου υπάρχουν οι μεγάλες παραμορφώσεις, καθώς και για να μειωθεί το υπολογιστικό κόστος, εφαρμόζεται μια τεχνική τοπικής πύκνωσης του πλέγματος. Η τεχνική αυτή
προτάθηκε αρχικά από τους Szabo and Babuska (1991) και εφαρμόστηκε αργότερα από τους Tsiveriotis and Brown (1993) σε προβλήματα με ελεύθερες επιφάνειες. Βασίζεται στην τομή των ορθογώνιων στοιχείων που δημιουργούνται αρχικά με τη μέθοδο κατασκευής του πλέγματος σε τέτσες μικρότερα ορθογώνια, εισάγοντας επιπλέον κόμβους στο κέντρο κάθε πλευράς του ορθογώνιου. Τελικά κάθε ορθογώνιο στοιχείο χωρίζεται σε δύο τρίγονα ενώ προκειμένου να ενωθούν διοικητικά αριθμοί στοιχείων χρησιμοποιείται μια ενδιάμεση ζώνη τριγονικών στοιχείων. Η μέθοδος αυτή, όχι μόνο μειώνει το υπολογιστικό κόστος, αλλά επιπλέον όπως αποδεικνύεται, αυξάνει και την ακρίβεια των υπολογισμών.

Για την επίλυση των εξισώσεων της ροής χρησιμοποιείται η μέθοδος των μικτών πεπερασμένων στοιχείων τροποποιημένη στην περίπτωση του ιξωδοελαστικού ρευστού προκειμένου να αντιμετωπιστεί ο υπερβολικός χαρακτήρας της εξίσωσης του καταστατικού μοντέλου. Το διάνυσμα της ταχύτητας και της θέσης προσεγγίζονται με τετραγωνικές συναρτήσεις βάσης ενώ η πίεση καθώς και ο τανυστής των τάσεων και του ρυθμού παραμόρφωσης στην περίπτωση του ιξωδοελαστικού ρευστού με γραμμικές συναρτήσεις βάσης. Προκειμένου να περιγραφεί η ιξωδοελαστική συμπεριφορά του πολυμερούς χρησιμοποιείται το καταστατικό μοντέλο που προτάθηκε από τους Phan-Thien and Tanner (1977).

Η εγκυρότητα της μεθόδου επαληθεύτηκε στο πρόβλημα του πολυμερούς νήματος με έλεγχο των αποτελεσμάτων με τη σύγκλιση με το πλέγμα. Οι προσομοιώσεις επαναλήφθηκαν με πλέγμα σχετικά αραιά αλλά και πολύ πικνό χωρίς τοπική πύκνωση και με πλέγμα με πύκνωση. Βρέθηκε ότι τα αποτελέσματα με πολύ πικνό χωρίς τοπική πύκνωση και με πλέγμα με πύκνωση συμπίπτουν ενώ το υπολογιστικό κόστος μειώθηκε κατά 30% και ο υπολογιστικός χρόνος κατά 80% στην περίπτωση χρησιμοποιήθηκε πλέγμα με τοπική πύκνωση. Στην περίπτωση του αραιού πλέγματος χωρίς πύκνωση τα αποτελέσματα απέκλιναν αρκετά σε σχέση με το πικνότερο πλέγμα, ιδιαίτερα στους πόλους της φυσαλίδας που είναι ένα ιδιαίτερα σημείο, δείγμα ότι απαιτείται πολύ καλή διακριτοποίηση στα σημεία εκείνα.

Στην περίπτωση των αλληλεπιδροντών φυσαλίδων, ο καλύτερος τρόπος ελέγχου της μεθόδου είναι ο υπολογισμός των ιδιοσυχνοτήτων των φυσαλίδων και ο έλεγχος τόσο της σύγκλισης τους με το πλέγμα όσο και της σύγκρισης τους με τις θεωρητικά προβλεπόμενες ιδιοσυχνότητες, όπως αυτές προκύπτουν για μια φυσαλίδα μέσα σε άπειρο ρέυστο. Ο υπολογισμός των ιδιοσυχνοτήτων γίνεται με γραμμική ανάλυση ευστάθειας γύρω από τη θέση ισορροπίας και θεωρώντας πολύ μικρή διαταραχή. Η επίλυση του προβλήματος ευστάθειας γίνεται με τη μέθοδο Arnoldi (Lehoucq et al. 1998). Αποδείχθηκε ότι προκειμένου οι ιδιοσυχνότητες που υπολογίζονται με τον αλγόριθμο μας να συγκλίνουν στις αναλυτικά
προβλεπόμενες, απαιτείται πολύ καλή διακριτοποίηση του πλέγματος και πολύ ομοιόμορφο πλέγμα γύρω από τις διεπιφάνειες των δύο υψιλού. Αυτό δε μπορούσε να επιτευχθεί με την αρχική μέθοδο των Dimakopoulos and Tsamopoulos (2003a) καθώς προέκυπταν πολύ παραμορφωμένα στοιχεία γύρω από τους πόλους των υψιλών που αυξανόταν το σφάλμα των υπολογισμών. Επιπλέον, η χρήση τοπικής πύκνωσης γύρω από τις διεπιφάνειες μείωσε σημαντικά τόσο το υπολογιστικό κόστος όσο και τον υπολογιστικό χρόνο επιτρέποντας μας τη χρήση πλέγματος με μεγάλο αριθμό στοιχείων γύρω από τις δύο υψιλών, πράγμα που δε ήταν αδύνατο να γίνει πριν καθώς, λόγω της πύκνωσης του πλέγματος σε όλο το υπολογιστικό πεδίο αυξάνονταν πολύ το υπολογιστικό κόστος και κατά συνέπεια και ο χρόνος.

Τέλος είναι σημαντικό να αναφέρουμε, ότι και στα δύο προβλήματα που μελετήθηκαν στην παρούσα εργασία, οι προσομοιώσεις προχώρησαν σε αρκετά μεγάλο χρόνο, τα σύνορα του φυσικού πεδίου μετατοπίστηκαν σημαντικά σε σχέση με την αρχική τους θέση και οι υψιλών υπέστησαν σημαντικές παραμορφώσεις χωρίς να χρειαστεί ανακατασκευή του πλέγματος. Αυτό είναι πολύ σημαντικό καθώς έτσι μειώνεται στο ελάχιστο το αριθμητικό σφάλμα που εισέρχεται με τη μέθοδο της παραμορφώσης που εφαρμόζεται στην περίπτωση της ανακατασκευής του πλέγματος. Ιδίωτερα σημαντικό είναι τη εφαρμογή της μεθόδου που αναπτύχθηκε, σε προβλήματα τρισδιάστατης γεωμετρίας, όπως είναι η κίνηση και η παραμορφώση υψιλών που βρίσκονται εκτός του άξονα συμμετρίας ή η αλληλεπίδραση περισσότερων των δύο υψιλών σε ακουστικό πεδίο.

2. ΕΠΙΔΡΑΣΗ ΤΟΥ ΙΣΩΔΟΥΣ ΣΕ ΔΥΟ ΑΛΛΗΛΕΠΙΔΡΩΣΕΙΣ ΚΑΙ ΠΑΡΑΜΟΡΦΟΥΜΕΝΕΣ ΦΥΣΙΛΙΔΕΣ ΛΟΓΩ ΒΗΜΑΤΙΚΗΣ ΜΕΤΑΒΟΛΗΣ ΤΗΣ ΠΙΕΣΗΣ

Όπως αναφέρθηκε ήδη, η δυναμική των υψιλών κατέχει μια σημαντική θέση στη σύγχρονη επιστήμη και τεχνολογία. Είναι γνωστή η καταστροφική επίδρασή τους σε αντλίες, κινητήρες και προπέλες λόγω φαινομένων σπηλαίωσης (Rayleigh 1917). Ο αρχικός σχηματισμός υψιλών κατά το βρασμό είναι το κλειδί για την παραγωγή ατμού και τη λειτουργία των στροβιλομηχανών, ενώ έχει προταθεί η χρήση ακουστικών κυμάτων για την αρχική συσσωμάτωση και τον εν συνεχεία διαχωρισμό αερίου ή υγρού διασπαρμένου σε άλλο μια αναμίξιμο υγρό όταν το σύστημα βρίσκεται σε συνθήκες μειωμένης βαρύτητας ή πρέπει να αποφευχθεί η χρήση χημικών (Batchelor 1967). Επιπλέον η κατάρρευση τους
μπορεί να προκαλέσει εξαιρετικά μεγάλη αύξηση της θερμοκρασίας και εντοπισμένες χημικές αντιδράσεις (sonochemistry; sonoluminescence, Ohl et al. 1999), χρησιμοποιούνται σαν μέσα μεταφοράς φαρμάκων σε συγκεκριμένα σημεία του σώματος (Li et al. 2003) ενώ τα τελευταία χρόνια έχει αναδειχθεί η χρήση τους στην βιοϊατρική και την υπερηχητική ηχοκαρδιογραφία (Goldberg et al. 2001; Tsigilis and Pelekasis 2008).

Είναι γνωστό από πειράματα στην ηχητική σπηλαίωση (acoustic cavitation), ότι όταν δύο φυσιαλίδες πάλλονται σ’ένα ρευστό, είτε έλκονται αν ταλαντώνται με την ίδια φάση, είτε απομακρύνονται αν ταλαντώνται εκτός φάσης. Επομένως, όταν δύο φυσιαλίδες είναι του ίδιου μεγέθους και, επομένως έχουν την ίδια ιδιοσυχνότητα, αναπτύσσουν ελκτικές δυνάμεις ανεξάρτητα του είδους της μεταβολής της πίεσης στο περιβάλλον ρευστό, με αποτέλεσμα να έλκονται ή και να συνενώνονται (Kornfeld and Suvorov 1944). Επιπλέον, όταν στο περιβάλλον ρευστό επιβάλλεται βηματική μεταβολή της πίεσης, τη συχνότητα του είναι μηδενική και οι δύο φυσιαλίδες θα πάλλονται με συχνότητα κάτω από τη συχνότητα συντονισμού τους, και θα έλκονται συνεχώς ανεξάρτητα από το σχετικό τους μέγεθος. Η συνισταμένη των υδροδυναμικών δυνάμεων που αναπτύσσονται ονομάζεται δευτερογενής δύναμη ‘Bjerknes’ και είναι γνωστό από τις αρχές του περασμένου αιώνα ότι, σε πρώτη προσέγγιση, είναι ανάλογη του ήγκου της κάθε φυσιαλίδας και του αντίστροφου του τετραγώνου της απόστασής τους, δηλ. υπακούει σε νόμο παρόμοιο με εκείνο της παγκόσμιας έλξης. Επίσης από πειράματα είναι γνωστό ότι δύο ή περισσότερες φυσιαλίδες βρισκόμενες σε ακουστικό πεδίο μπορεί να διατηρούν τις αποστάσεις τους, σχηματίζοντας πολύπλοκες δομές και μη υπακούοντας στον προηγούμενο νόμο (Mettin et al. 1997). Για λεπτομερέστερη παρουσίαση της πληθώρας των φαινομένων που έχουν παρατηρηθεί και μερικούς αναλυθεί σε παρόμοια πεδία ροής με την συμμετοχή φυσιαλίδων βλέπε και το βιβλίο του Leighton (1994).

Στο παρελθόν έχουν προσομοιωθεί οι άλληλεπιδράσεις δύο φυσιαλίδων με χρήση της μεθόδου των συνοριακών στοιχείων και υποθέτοντας αντίστοιχη κύκλωση και αστροβλήμα της ροής (Pelekasis and Tsamopoulos 1993a, b), ότι οι φυσιαλίδες παραμένουν σφαιρικές, βρίσκονται σε σχετικά μεγάλη απόσταση μεταξύ τους και οι ιξώδεις δυνάμεις περιορίζονται σε ένα συνοριακό στρώμα γύρω από την κάθε φυσιαλίδα (Pelekasis et al. 2004). Λόγω των σημαντικών αυτών περιορισμών, οι προσομοιώσεις αυτές δε μπορούσαν να παρακολουθήσουν την κίνηση των φυσιαλίδων καθώς αυτές πλησιάζαν πολύ η μία την άλλη, αλλά και συχνότερα του αναμενόμενου προέδρου λιγότερο του παραμορφώσεων της επιφάνειάς τους ή αντίθετα δεν επέτρεπαν και τέτοιες παραμορφώσεις. Για την εξάλειψη αυτών των μειονεκτημάτων στην παρούσα εργασία έχει ληφθεί πλήρης υπόψη το ιξώδες του περιβάλλοντος ρευστού και, επομένως, ο αριθμός
Ohnesorge \( Oh = \left( \frac{\mu^* \sigma^2}{\rho^* R_{\text{s}}^2} \right)^{1/2} \) είναι πεπερασμένος, όπου \( \mu^* \), \( \rho^* \) το ιξώδες και η πυκνότητα του ρευστού αντίστοιχα, \( \sigma^* \) η επιφανειακή τάση και \( R_{\text{s}}^* \) η ακτίνα της αριστερής φυσαλίδας. Προς τούτο έχουμε αναπτύξει μια νέα αριθμητική μέθοδο και έχουμε κάνει προσομοιώσεις για μεγέθη φυσαλίδων 5–1000 \( \mu m \) όπως απαιτούν τα σχετικά πειράματα.

Προκειμένου να μελετηθεί η αλληλεπίδραση μεταξύ των δύο φυσαλίδων, θεωρούμε ότι αυτές περιέχουν αέρα, είναι αρχικά σφαιρικές του ίδιου ή διαφορετικού όγκου και βρίσκονται σε ισορροπία με το περιβάλλον ρευστό που είναι νερό. Σε μεγάλη αλλά πεπερασμένη απόσταση από τις δύο φυσαλίδες εφαρμόζουμε βηματική μεταβολή της πίεσης σε χρόνο \( t \geq 0 \). Οι πλήρεις εξισώσεις Navier-Stokes επιλύονται με τη μέθοδο των μικτών πεπερασμένων στοιχείων κατά Galerkin. Για τη χρονική ολοκλήρωση του συστήματος των εξισώσεων επιλέχθηκε η η-αναλυτή Euler, με αυτοματοποιημένη ρύθμιση του χρονικού βήματος μέσω αναλυτής πρόβλεψης. Οι εξαιρετικά μεγάλες παραμορφώσεις των διεπιφανειών αντιμετωπίζονται επιτυχώς με την κατασκευή ενός δομημένου πλέγματος τμηματικά (block-structured), όπως περιγράφεται στο κεφάλαιο 1 της παρούσας εργασίας. Το σύστημα των εξισώσεων ορμής και συνέχειας επιλύεται σε κάθε χρονική στιγμή, μέχρι σύγκλιση με τροποποιημένη Newton-Raphson και στη συνέχεια, αφού έχουν υπολογιστεί οι ταχύτητες και η πίεση, υπολογίζονται οι νέες θέσεις των κόμβων.

Με την παρούσα μελέτη αποδείξαμε ότι η αρχή του νόμου του Bjerknes ισχύει και στην περίπτωση των ιξώδων ρευστών αλλά με κάποιες καινούριες απόψεις: (α) η σταθερά της αναλογικότητας του νόμου εξαρτάται αναλυτικά από τις ιξώδες δυνάμεις, (β) η παραμόρφωση των φυσαλίδων αποτελεί τον κανόνα και όχι την εξάρτηση για φυσαλίδες μεγαλύτερες των 100 \( \mu m \) και προσανάτος θα οδηγήσει στην κατάρρευση τους παρόλο που οι τριχοειδείς δυνάμεις και το ιξώδες τείνουν να εξομαλύνουν τους κυματισμούς που εμφανίζονται στην διεπιφάνειά τους και (γ) η δύναμη της μεταξύ τους αλληλεπίδρασης αυξάνεται, και επομένως, ο χρόνος που απαιτείται για τις δύο φυσαλίδες να πλησιάσουν μειώνεται με τη μείωση του αριθμού Ohnesorge, την αύξηση της πίεσης του περιβάλλοντος ρευστού και της διατομής που επιβάλλεται στην πίεση, οδηγώντας έτσι, σε μείωση της περιόδου ταλάντωσης του όγκου. Ποιο συγκεκριμένα, όσο αυξάνεται το μέγεθος των φυσαλίδων, η επιτάχυνση τους αυξάνεται και οι τριχοειδείς δυνάμεις μειώνονται. Έτσι οι μικρότερες φυσαλίδες παίρνουν ένα πεπλατσιμένο σχήμα, ενώ όσο το μέγεθος τους αυξάνει, αρχίζουν να αναπτύσσονται παραμορφώσεις στην πλευρά την αντίθετη της κινήσης των φυσαλίδων, οι οποίες γίνονται πιο έντονες όσο αυξάνεται το μέγεθος των φυσαλίδων και
οδηγούνται ακόμα και σε παραμορφώσεις ολόκληρης της επιφάνειας τους όταν οι φυσαλίδες γίνονται της τάξης του 1mm και κάτω από συγκεκριμένες συνθήκες, όπως είναι η μεγάλη μεταξύ τους απόσταση και η μικρή διαταραχή της πίεσης του περιβάλλοντος ρευστού. Οι παραμορφώσεις που αναπτύσσονται στις επιφάνειες των φυσαλίδων, οφείλονται είτε σε αστάθειες τύπου Rayleigh-Taylor λόγω της κίνησης τους, είτε σε αρμονικό (harmonic) ή υπό-αρμονικό (sub-harmonic) συντονισμό με τις ταλαντώσεις του όγκου της φυσαλίδας με άλλες αρμονικές διαταραχές της επιφάνειας. Γενικότερα, οι ελκτικές δυνάμεις εξαρτώνται ισχυρά από τον αριθμό Ohnessorge και από την πίεση του περιβάλλοντος ρευστού καθώς αυτά καθορίζουν επιπλέον την έκταση της παραμόρφωσης και την οπισθέλκουσα δύναμη λόγω του ιξώδους.

3. ΕΠΙΔΡΑΣΗ ΤΟΥ ΙΞΩΔΟΥΣ ΣΕ ΔΥΟ ΑΛΛΗΛΕΠΙΔΡΩΣΕΙΣ ΚΑΙ ΠΑΡΑΜΟΡΦΟΥΜΕΝΕΣ ΦΥΣΑΛΙΔΕΣ ΛΟΓΩ ΤΑΛΑΝΤΩΜΕΝΟΥ ΠΕΔΙΟΥ ΠΙΕΣΗΣ

Σε συνέχεια του προηγούμενου κεφαλαίου, μελετάται η επίδραση του ιξώδους στην κίνηση και παραμορφώση φυσαλίδων στην περίπτωση που στο περιβάλλον ρευστό ασκείται ένα πεδίο πίεσης το οποίο ταλαντώνεται με το χρόνο. Στην περίπτωση αυτή έχει βρεθεί ότι οι δύο φυσαλίδες αποχωρούν όταν η επιβαλλόμενη συχνότητα βρίσκεται μεταξύ των φυσικών συχνοτήτων (natural frequency) των δύο φυσαλίδων, ενώ έλκονται σε κάθε άλλη περίπτωση. Οι Pelekasis and Tsamopoulos (1993b) προσομοίωσαν φυσαλίδες μεγέθους 1mm, ίσες ή άνισες, σε νερό για διάφορες επιβαλλόμενες συχνότητες και για σχετικά μικρές μεταβολές της πίεσης και βρήκαν συμφωνία με τη θεωρία του Bjerknes τόσο στις ίσες όσο και στις άνισες φυσαλίδες. Επίσης παρατήρησαν είτε μια τάση των φυσαλίδων να διασπασθούν εξαιτίας των ιχνών ταλαντώσεων του όγκου τους, είτε τη βίαιη κατάρρευσή τους ενώ διατηρούν το σφαιρικό τους σχήμα εξαιτίας χρονομεταβαλλόμενης σπηλαίωσης (transient cavitation). Πιο πρόσφατα οι Mettin et al. (1997) παρατήρησαν ότι η αλληλεπιδρώσα δύναμη μεταξύ των δύο φυσαλίδων μπορεί να γίνει από ελκτική, απωστική ή το αντίστροφο, όταν η μεταξύ τους απόσταση μειώνεται, και ενώ ήταν αρχικά σε απόσταση πολύ μεγαλύτερη της ακτίνας τους. Οι δύο παραπάνω ερευνητές καθώς και άλλοι που μελέτησαν παρόμοια φαινόμενα δεν έλαβαν υπόψη τους τις ιξώδεις δυνάμεις του ρευστού. Πιο πρόσφατα, οι Pelekasis et al. (2004), θεώρησαν ότι οι ιξώδεις δυνάμεις περιορίζονται σε ένα συνοριακό στρώμα γύρω από την επιφάνεια της κάθε φυσαλίδας, και παρατήρησαν ότι για φυσαλίδες
μεγέθους μέχρι 100 μμ, τη ταχύτητα μεταφοράς των φυσαλίδων μπορεί να αλλάξει πρόσημο καθώς αυξάνεται η μεταβολή της πίεσης του περιβάλλοντος ρευστού και υπό συνθήκες κοντά στο κατώτερο του Blake (Blake threshold). Επιπλέον, οι Pelekasis et al. (2004) θεώρησαν ότι οι δύο φυσαλίδες παραμένουν σφαιρικές λόγω του ότι βρίσκονται σε πολύ μεγάλη μεταξύ τους απόσταση.

Στην παρούσα εργασία λαμβάνονται υπόψη οι ιδιότητες δυνάμεις του ρευστού και επιπλέον επιτρέπεται η παραμορφωση των φυσαλίδων. Όπως και στην περίπτωση της μηδενικής μεταβολής της πίεσης, οι δύο φυσαλίδες είναι αρχικά σφαιρικές του ιδίου ή διαφορετικού όγκου και βρίσκονται σε ισορροπία με το περιβάλλον ρευστό ενώ σε χρόνο t ≥ 0 επιβάλλεται συνιμιτοειδής μεταβολή της πίεσης στο περιβάλλον ρευστό και σε μεγάλη απόσταση από τις φυσαλίδες. Η επίλυση των εξισώσεων και η κατασκευή του πλέγματος γίνεται όπως αναφέρθηκε στο προηγούμενο κεφάλαιο. Τα μεγέθη των φυσαλίδων που μελετήθηκαν κυμαίνονται από 30 μμ μέχρι 1 mm για την αριστερή φυσαλίδα ενώ το μέγεθος της δεξιάς φυσαλίδας είναι 50-100% το μέγεθος της αριστερής. Βρέθηκε ότι όταν οι δύο φυσαλίδες είναι του ίδιου όγκου πάντα έλκονται. Στην περίπτωση που οι φυσαλίδες είναι μεγέθους 1 mm και πάλλονται με επιβαλλόμενη συχνότητα κοντά στη 2η ή 3η ιδιωσυνάρτηση (mode) των φυσαλίδων, σε σχετικά μεγάλη απόσταση μεταξύ τους και σχετικά μεγάλη διαταραχή της πίεσης του περιβάλλοντος ρευστού, επικρατεί ο συντονισμός μεταξύ της μηδενικής ιδιωσυνάρτησης (zeroth mode) και ανώτερων ιδιωσυναρτήσεων που σχετίζονται με το σχήμα της φυσαλίδας αναγκάζοντας τις φυσαλίδες να παραμορφωθούν στην πλευρά της αντίθετης της κατεύθυνσης της κίνησης τους (spherical cap shapes). Στην περίπτωση μικρότερων φυσαλίδων και σε μικρή σχετικά απόσταση μεταξύ τους, επικρατεί ο συντονισμός μεταξύ της μηδενικής ιδιωσυνάρτησης και της επιβαλλόμενης συχνότητας προκαλώντας τη μεγάλη αύξηση του όγκου της φυσαλίδας.

Στην περίπτωση που η αριστερή φυσαλίδα είναι μεγέθους 1 mm και η δεξιά μικρότερον όγκου, τότε η μεταξύ τους απόσταση και επομένως η επιτάχυνση, καθώς και το μέγεθος της επιβαλλόμενης μεταβολής της πίεσης καθορίζουν ποια φυσαλίδα θα παραμορφωθεί και ποιο φαίνοντα όταν επικρατήσει. Συνήθως όταν η μεταξύ τους απόσταση είναι μεγάλη και οι φυσαλίδες πάλλονται με επιβαλλόμενη συχνότητα κοντά στη 2η ή 3η ιδιωσυνάρτηση της μιας από τις δύο φυσαλίδες, επικρατεί ο συντονισμός μεταξύ της μηδενικής ιδιωσυνάρτησης και κάποιων από τις ανώτερες ιδιωσυναρτήσεις της μιας ή της άλλης φυσαλίδας. Σε περίπτωση που οι δύο φυσαλίδες είναι σε μικρότερη αρχική απόσταση τότε συνήθως η επιτάχυνση επικρατεί και κάθε πιθανότητα για οποιοδήποτε συντονισμό.
εκμηδενίζεται. Όταν η κινούσα συχνότητα βρίσκεται μεταξύ των φυσικών συχνοτήτων των δύο φυσαλίδων, τότε οι ελεκτικές δυνάμεις επικρατούν στην περίπτωση που η διαταραχή που επιβάλλεται στην πίεση του περιβάλλοντος ρευστού είναι μικρή, ενώ δεν είναι ξεκάθαρο ποιες δυνάμεις θα επικρατήσουν όταν το μέγεθος αυτής αυξηθεί, καθώς οι φυσαλίδες παραμορφώνονται γρήγορα και οι προσομοιώσεις σταματάνε πρόωρα.

Όταν το μέγεθος της αριστερής φυσαλίδας μειωθεί, η δεξιά εξακολουθεί να είναι μικρότερο μεγέθους, και η επιβαλλόμενη συχνότητα εξακολουθεί να είναι μεταξύ των φυσικών συχνοτήτων των δύο φυσαλίδων τότε ελεκτικές δυνάμεις επικρατούν σε μικρές διαταραχές της πίεσης του περιβάλλοντος ρευστού ενώ όσο η διαταραχή αυτή αυξάνει οι παραμορφώσεις των φυσαλίδων επικρατούν σε μικρότερο χρόνο και οι προσομοιώσεις παύουν να συγκλίνουν πριν γίνει ξεκάθαρο ποια από τις δύο δυνάμεις θα επικρατήσει.

Τέλος, στην περίπτωση που η κινούσα δύναμη είναι εκτός του διαστήματος των φυσικών συχνοτήτων των δύο φυσαλίδων πάντα ελεκτικές δυνάμεις επικρατούν.

4. ΑΝΟΔΟΣ ΚΑΙ ΠΑΡΑΜΟΡΦΩΣΗ ΦΥΣΑΛΙΔΑΣ ΥΠΟ ΣΥΝΘΗΚΕΣ ΜΟΝΙΜΗΣ ΡΟΗΣ ΣΕ ΝΕΥΤΩΝΙΚΑ ΚΑΙ ΙΣΩΔΟΠΛΑΣΤΙΚΑ ΡΕΥΣΤΑ

Τα ιξωδόπλαστικά ρευστά είναι υλικά τα οποία συμπεριφέρονται ως στερεά για μικρές τιμές της τάσης, ενώ πέρα από μια κρίση τιμή (τάση διαρροής), συμπεριφέρονται ως γενικευμένα Νευτωνικά ρευστά. Το μέγεθος και το σχήμα της φυσαλίδας σε τέτοια ρευστά επηρεάζει σημαντικά πολλές φυσικές και χημικές διεργασίες αλλά και τις ιδιότητες των τελικών προϊόντων. Φυσαλίδες σχηματίζονται π.χ. κατά τη διάρκεια εξόρυξης πετρελαίου ή κατά την παραγωγή διαφόρων προϊόντων όπως τρόφιμα (σοκολάτα, μαγονέζα κλπ.) ή κοσμητικά (κρέμες, σαμπουάν, κτλ.). Στο παρέλθον η κίνηση μιας φυσαλίδας σε Νευτωνικό ρευστό έχει μελετηθεί εκτενέστατα από πολλούς ερευνητές τόσο αριθμητικά (Ryskin and Leal 1984) όσο και πειραματικά (Bhaga and Weber 1981; Duineveld 1995). Ωστόσο η ροή σε ιξωδόπλαστικά ρευστά έχει μελετηθεί ελάχιστα (Dubash and Frigaard 2004). Ιδίατερο ενδιαφέρον παρουσιάζει το γεγονός ότι α) η φυσαλίδα μπορεί να παγιδευτεί στο ρευστό στην περίπτωση που η άνωση δεν υπερβαίνει την τάση διαρροής και β) η παραμόρφωση της διεπαφής διαφέρει ποιοτικά σε σύγκριση με την περίπτωση Νευτωνικού ρευστού.

Στην παρούσα εργασία εξετάζεται η άνωδος μιας φυσαλίδας λόγω άνωσης σε ένα Νευτωνικό ή σε ένα ιξωδόπλαστικό ρευστό υποθέτοντας αξιονική συμμετρία και μόνιμη κατάσταση. Η πίεση και η ταχύτητα ανόδου της φυσαλίδας προσδιορίζονται από την
απαιτησή ότι ο όγκος της παραμένει σταθερός και το κέντρο μάζας της παραμένει στο κέντρο του συστήματος συντεταγμένων, αντίστοιχα. Για την περιγραφή της ιξωδοπλαστικής συμπεριφοράς του υλικού χρησιμοποιείται το συνεχές καταστατικό μοντέλο, το οποίο προτάθηκε από τον Papanastasiou (1987). Προκειμένου να επιλυθεί αριθμητικά το σύστημα των εξισώσεων της ροής χρησιμοποιείται η μέθοδος των μικτών πεπερασμένων στοιχείων κατά Galerkin. Το φυσικό πεδίο μετατρέπεται σε ένα σταθερό με το χρόνο υπολογιστικό πεδίο που επιλέχθηκε να είναι ο όγκος που καταλαμβάνει το ρευστό στην περίπτωση σφαιρικής φυσαλίδας. Για τη διακριτοποίηση του χώρου χρησιμοποιούνται τριγωνικά στοιχεία καθώς αυτά προσαρμόζονται πιο εύκολα στις μεγάλες παραμορφώσεις. Σε κάθε στοιχείο το διάνυσμα της ταχύτητας και της θέσης προσεγγίζονται με τετραγωνικές συναρτήσεις μικρότερης βάσης ενώ η πίεση με γραμμικές συναρτήσεις βάσης. Το σύστημα των εξισώσεων ορμής και συνέχειας επιλύεται ταυτόχρονα με ένα σύστημα οιονεί ελλειπτικών μερικών διαφορικών εξισώσεων, όπως αυτό προτάθηκε από τους Dimakopoulos and Tsamopoulos (2003a), και το οποίο επιτρέπει την παρακολούθηση των μεγάλων παραμορφώσεων της ελεύθερης επιφάνειας της φυσαλίδας, μέχρι να επιτευχθεί σύγκλιση με τη μέθοδο Newton-Raphson. Στη συνέχεια, αφού γνωρίζουμε το πεδίο των ταχυτήτων, μπορούμε να υπολογίσουμε τον ταντότητα των τάσεων και τη δεύτερη αναλλολογήτη αυτού.

Η ακρίβεια των λύσεων εξακριβώνεται με τοπική ενίσχυση του πλέγματος ενώ η πιστοποίηση του κώδικα έγινε με σύγκριση με προηγούμενα πειραματικά και θεωρητικά αποτελέσματα για Νευτωνικά ρευστά και βρέθηκε ότι οι προβλέψεις είναι σε πολύ καλή συμφωνία με αυτά. Σε περιπτώσεις που ήταν εφικτό επεκτέιναμε προγενέστερες εργασίες σε υγιλότερες τιμές των αριθμών Reynolds και Weber. Σε ένα ιξωδοπλαστικό ρευστό, προσδιορίζουμε το σχήμα της φυσαλίδας, την ταχύτητα της και το σχήμα της επιφάνειας διαρροής για ένα ευρύ φάσμα ιδιοτήτων υλικού, που εκφράζονται σε όρους των αδιάστατων αριθμών Bingham \( Bn = \tau^* / \rho^* g^* R_b^* \), Bond \( Bo = \rho^* g^* R_b^2 / \gamma^* \) και Αρχιμήδη \( Ar = \rho^2 g^* R_b^* / \mu_o^2 \), όπου \( \rho^* \) είναι η πυκνότητα, \( \mu_o^* \) το ιξώδες, \( \gamma^* \) η επιφανειακή τάση, \( \tau^* \) το επιφάνειακό του υλικού, \( g^* \) η τάση, \( R_b^* \) η επιφάνεια της βαρύτητας και \( R_b^* \) η ακτίνα μιας σφαιρικής φυσαλίδας ίδιου όγκου. Για όλες τις τιμές των παραμέτρων που εξετάσαμε, το υλικό δεν παραμορφώνεται πέρα από μια πεπερασμένη περιοχή γύρω από τη φυσαλίδα, και κάτω από συγκεκριμένες συνθήκες (όπως μικρούς αριθμούς \( Bn \) και μεγάλους αριθμούς \( Bo \) ) δεν παραμορφώνεται ούτε στην πλευρά που είναι αντίθετη στην κίνηση της φυσαλίδας. Η πεπερασμένη αυτή περιοχή μειώνεται καθώς ο αριθμός Bingham αυξάνει. Αντίθετα με ότι
συμβαίνει σε ροή ρευστού Bingham γύρω από σφαίρα όπου για μεγάλους $Bn$, εμφανίζεται στερεά περιοχή στους πόλους της σφαίρας (Beris et al. 1984), στην περίπτωση της φυσαλίδας περιοχές με στερεό εμφανίζονται στον ισημερινό της φυσαλίδας. Καθώς ο αριθμός $Bn$ αυξάνεται, η ταχύτητα ανόδου της φυσαλίδας μειώνεται, οι επιφάνειες διαρροής στο επίπεδο του ισημερινού και μακριά από την φυσαλίδα αυξάνονται, μέχρι που συνενώνονται και αυτή παγιδεύεται. Επίσης είναι αξιοσημείωτο να αναφέρθει, ότι σε μικρούς αριθμούς Bingham ($Bn = 0.01$) τα σχήματα των φυσαλίδων μοιάζουν πάρα πολύ με αυτά του Νευτωνικού ρευστού με τη διαφορά ότι ελαφρώς μη-συμμετρικά σχήματα εμφανίζονται ακόμα και όταν $Ar = 0$, αλλά ο αριθμός $Bo$ αρκετά μεγάλος (μικρή επιφανειακή τάση-εύκολα παραμορφώμενη φυσαλίδα), μια συμπεριφορά που έχει παρατηρηθεί και από τους Gueslin et al. (2006) σε μη-Νευτωνικά ρευστά. Καθώς ο αριθμός Bingham αυξάνει και πλησιάζει την κρίσιμη τιμή του, η φυσαλίδα τείνει να πάρει ένα σφαιρικό σχήμα για $Bo < 5$, ενώ για $Bo \geq 5$ η φυσαλίδα τείνει να πάρει ένα σχεδόν συμμετρικό επίμηκες σχήμα.
CHAPTER 1

On The Elliptic Mesh Generation in Domains Containing Multiple Inclusions and Undergoing Large Deformations

1.1 Introduction

The accurate numerical simulation of many scientifically and technologically important processes with free or moving boundaries has been a challenging research area for many decades. Computational methods for numerical simulation of such problems require powerful discretization techniques based on the use of appropriate grids. These are discrete sets of points along lines well covering the physical domain, which must satisfy some specific properties like smoothness and orthogonality along certain boundaries so that the accuracy and the stability of the calculation is guaranteed (Khamayseh et al. 1999). In particular, orthogonality only near the moving boundary is often necessary to achieve accurate results, for example, in simulations of flows where boundary layers arise.

Depending on the method generating the computational grid, the available numerical approaches can be classified as Lagrangian, Eulerian and mixed Lagrangian-Eulerian. In the Lagrangian formulation, the coordinate system is moving with the fluid following its local velocity. This method has several useful properties since the interfaces can be specifically delineated and precisely followed, the free-surface boundary conditions are easily applied and curved grid boundaries of any arbitrary shape can be treated. However, it has some significant disadvantages since the grid becomes very often severely distorted and consequently demands multiple reconstructions. Indicatively, Saksono and Peric (2006) have used a Lagrangian method for simulating the oscillations of droplets and the stretching of a liquid bridge, where a remeshing procedure proved to be an essential feature for improving the overly distorted finite elements. On the other hand in the Eulerian formulation, the grid points remain fixed relative to the observer, while the fluid moves through the cells. This method has the advantage of being able to handle extreme interface distortions, but the interface is not as sharp and requires a special procedure to locate it with some accuracy. Hirt and Nichols (1981) implemented the Volume of Fluid (VOF) method in an Eulerian hydrodynamics code in order to study a variety of highly complicated free surface flows. A significant improvement for Eulerian methods is the front tracking method (Unverdi and Tryggvason
1992; Zacharioudaki et al. 2007) because it determines the interface explicitly using a separate grid for it in addition to that used for the fluid volume.

An intermediate approach is the arbitrary Lagrangian-Eulerian (ALE) method, in which each node of the mesh moves independently of the local fluid velocity. Its main advantage is that it reduces the number of remeshing procedures, and consequently it reduces the projection errors that are introduced after such a remeshing cycle, especially in the continuity equation. However, remeshing techniques still may be needed even in the ALE method. This can be minimized by employing a curvilinear coordinate system that conforms to the moving boundary. The irregular physical domain is mapped onto a simple and time-independent computational one in which the moving boundary coincides with one of the coordinate surfaces (or part of it) and in which it is trivial to generate the mesh. There are two ways to do this by using either algebraic expressions or partial differential equations. The algebraic grid generation methods are based on simple interpolation functions (Smith 1982). However, with this procedure problems arise related to smoothness, node overlapping and grid-line folding (Thompson and Soni 1999). Hence heuristic rules must be introduced for controlling the mesh development. Moreover, this technique is restricted to simple initial shapes and small deformations.

The elliptic mesh generation schemes are based on the solution of a partial differential equation (PDE) for each computational coordinate; see an extensive review by Thompson, Warsi and Mastin (1982). The simplest of the mesh generation algorithms is conformal mapping, where the Cauchy-Riemann equations are satisfied. Conformal meshes are smooth and orthogonal and when the boundary shape is the only constraint on the mesh generated, they are usually the most efficient ones (Thompson et al. 1982). However, conformal mapping does not allow control of mesh spacing. Orthogonal meshes (Ryskin and Leal. 1983; Christodoulou et al. 1992) become then the simplest choice, since they are less restricted than conformal meshes. Christodoulou and Scriven (1992) in particular have extended the earlier work in Ryskin and Leal (1983) incorporating new features in the system of the differential equations, by minimizing a functional which quantifies the deviation of the mesh from an orthogonal one that satisfies generalized Cauchy-Riemann equations and by including forcing terms. This work was further improved by Tziveriotis and Brown (1992) who proposed a ‘mixed mapping method’. It seemed to allow independent control of mesh spacing in each direction which is important when deformations of the free surface preferentially arise in one direction. To improve the accuracy of the solution vector on the interface, they also proposed
a non-conforming two-to-one element splitting scheme (Tsiveriotis and Brown, 1993), for the transition from a coarser mesh in the bulk to a finer one close to the interface.

All these ideas have formed the basis for the elliptic grid generation scheme introduced by Dimakopoulos and Tsamopoulos (2003a). It is a very robust and flexible method which takes into consideration all the intrinsic features of the developing surface and the deforming control volume. It has been tested in a wide range of numerical simulations (Dimakopoulos and Tsamopoulos 2003a, 2003b, 2003c, 2004, 2007; Foteinopoulou et al. 2004, 2006; Karapetsas and Tsamopoulos 2006, 2008; Tsamopoulos et al. 2008) and proved very satisfactory even at very large deformations. The main advantages of this elliptic grid generation scheme are:

- It can be used to solve a variety of problems such as: transient problems (Dimakopoulos and Tsamopoulos 2003a, 2003b, 2003c, 2004, 2007; Foteinopoulou et al. 2004, 2006; Karapetsas and Tsamopoulos 2006), steady state problems (Tsamopoulos et al. 2008; Karapetsas and Tsamopoulos 2008), and determine their stability (Carvalho and Scriven 1999) requiring minimum changes in the numerical algorithm and so a minimum input from the user.
- Large deformations can be simulated with minimum or even without remeshing cycles. Thus, it reduces errors due to frequent variable interpolations between meshes.
- Structured meshes can be adopted for minimizing the error dispersion/amplification (Kallinderis and Kontzialis 2006) and improve numerical stability and accuracy.

A similar method is the pseudosolid mesh generation technique (Sackinger et al. 1996), which treats the material as a compressible, elastic solid and solves Cauchy’s equilibrium equation to determine the location of the nodal positions. However, with this method remeshing is often necessary since it has not been adopted to allow large distortions of the mesh (Sackinger et al. 1996; Madosu and Cairncross 2003). Actually this issue is closely related with the boundary conditions that should be used. These must be physically consistent with the governing equations, which is not always possible. Such natural conditions for the pseudosolid method do not include important constraints such as prespecified node distribution or line orthogonality along specific parts either of the boundary or in the interior of the control volume leading to severe distortion of the mesh near a static contact point (see fig. 14 in Madosu and Cairncross 2003).

All these ALE-type methods for generating a structured grid fail when the domain contains inclusions and especially if their shapes undergo large deformations or the simulations are carried out for long times. This is expectable because they inevitably smooth
out the mesh near any singular point, such as a corner (slope discontinuity of any variable on any boundary) or a point of large curvature or the poles of the bubbles included in the physical domain in our specific applications. This smoothing appears as a repulsion of the mesh lines away from such singular points. On the contrary, this is exactly where a higher discretization is needed for accurate computations. This makes imperative the special and careful treatment of the inclusions.

Body-fitted curvilinear coordinates for domains containing 2D bodies with fixed boundaries have been proposed earlier. The simpler such method maintains the connectivity of the domain and represents the inclusion(s) by empty slab(s) or slit(s) (Thompson et al. 1985). Then, both coordinate lines in computational space experience a discontinuity at certain points on its boundary. As explained above, this leads to failure of computations, and more so in moving boundary problems. The second method (Thompson et al. 1985; Thompson et al. 1974; Villamizar et al. 2007) transforms the domain into a simply connected one by introducing as many branch-cuts as needed at arbitrary positions to connect once the inclusions with each other and another branch-cut to connect one of the internal bodies with the external boundary of the domain. Typically, one of the coordinates is assigned the same constant value on all the internal interfaces and all the branch-cuts between the bodies and another value at the external boundary, whereas the other coordinate takes two different constant values on the cut between one of the bodies and the outer interface. This is an O-type opening of the domain. A different positioning of the cuts leads to a C-type opening, etc. In each one of the numerous computational domains that may be created (Thompson et al. 1985), this procedure makes even the interfaces of the inclusions in physical space external boundaries transforming the multiply connected domain to a simply connected one. Each cut appears as two segments on the transformed boundary, each segment corresponding to the two branches of the cut in physical space. However, there at least two disadvantages in applying this method: (i) the two branches of each cut comprise re-entrant boundaries and one of them has a different orientation in computational space requiring special treatment to impose continuity of the dependent variables and their derivatives there and (ii) the resulting mesh may not have the desired distribution of nodes and may require a lot of effort to adjust them as needed. Moreover, in deforming inclusions this adjustment may require modification in time, thus increasing the computational effort and time. The last available method (Thompson et al. 1985; Thompson 1987; Baker 2005) breaks up the physical domain into several smaller blocks or subdomains and then generates separate meshes in each individual block. Hence, it has been called multiblock or block-structured or domain decomposition.
method. It can be used in either simply or multiply connected domains. In the second case it may be coupled with the previous method of introducing branch-cuts. Each subdomain is chosen to be geometrically much simpler than the entire configuration and, thus, to be more easily discretizable by a quasi-elliptic method, for example. On the boundaries of each subdomain mesh points are introduced just as in actual domain boundaries. Across the boundaries of the subdomains the meshes maybe unmatched or patched without enforcing continuity of mesh lines or with enforcing continuity of the mesh lines or even of their slopes. In the above order, these three possibilities offer more advantages to the numerical solutions, but also become more difficult in generating the mesh. For example, when mesh line continuity is enforced, the location of the interface nodes requires an additional data indexing procedure to link the subdomains across the interfaces. In spite of generating meshes of higher quality, the difficulty in automating the multiblock method with mesh continuity has inhibited its application to moving boundary problems.

The main contribution of this paper is the presentation of a new methodology for generating accurate meshes in domains with deforming inclusions with or without domain decomposition. The presentation is confined to problems with axial symmetry in the interest of reducing the storage requirements and the computing time. Clearly these problems have their 3D counterparts and, because of their technological importance, we are currently extending the present numerical method to deal with them. We test our scheme and we present results for two problems of scientific and technological interest: (i) bubble growth in viscoelastic filaments undergoing stretching and (ii) bubble interactions in an acoustic field fully accounting for viscous effects. In addition, we apply our numerical technique along with an appropriate mesh refinement methodology in order to limit the large number of grid points only in regions where they are needed the most.

The physics and motivation to study the chosen two problems are given in the following two subsections. The governing equations are given in section 1.2 and the general solution methods in section 1.3. Section 1.4 is dedicated to the specific procedures and methods for mesh generation in domains with deforming inclusions. There we will show that the first example can be solved accurately using a single domain with different mappings of segments of the physical boundaries to segments of the computational boundaries and with imposing the node distribution along lines that emanate from the poles of the bubbles. These lines play the role of pseudo-boundaries. In essence, this method corresponds to introducing branch-cuts along the axis of symmetry and using the second of the three methods we discussed above for solving problems with inclusions. This idea, when applied to the second
example, fails completely as we show with the two most promising mappings among a variety of mappings we have tried. Indeed, the resulting grids are too skewed and irregular and cannot follow closely the deforming boundaries of the inclusions. Now splitting the domain to subdomains, each one having its own curvilinear coordinate system, becomes imperative. The entire region is treated as a single one when writing and solving the governing equations. The curved interfaces bounding the subregions form internal interfaces across which information must be transferred. Thus, this problem can be solved accurately for long times by efficiently advancing some of the ideas from the third of the methods mentioned above. In section 1.5 we give numerical results using the optimum methods for each problem.

1.1.1 Bubble growth in Newtonian and viscoelastic filaments undergoing stretching

Bubbles or cavities develop in thin films of materials made by block copolymers (such as those based on styrene-isoprene triblocks or acrylates) that are extensively used nowadays as self-adhesives or pressure sensitive adhesives (PSAs). PSAs, in particular, have the ability to average stresses over large volumes of material, thus avoiding the sharp stress concentrations responsible for the failure of structural glassy adhesives. Controlling their adhesive properties is important, since it governs their suitability in non-structural bonding applications. Additionally, understanding the role of the small cavities that propagate along the material and cause its fracture at high deformation levels and how they are affected by the viscoelastic properties of the filament is critical in our ability to design new polymeric materials with optimal adhesive properties. In the literature, theoretical or numerical studies of bubble dynamics have been restricted either to spherically symmetric bubbles growing in an infinite non-Newtonian liquid (Kim 1994; Brujan 1999) or to the transient deformation of a single bubble or droplet in a uniaxial extensional flow of Newtonian or viscoelastic liquids for which the flow field far away from the bubble or droplet is known (Papanastasiou et al. 1984; Bousfield et al. 1988). More recently, Foteinopoulou, Mavratzas and Tsamopoulos (2004) have studied the deformation of a single bubble in a Newtonian or viscoelastic filament undergoing stretching. Later they extended their work to multiple bubbles that grow and deform simultaneously in a Newtonian liquid (Foteinopoulou et al. 2006), but the material deformations remained smaller than in testing experiments because of the need for higher mesh refinement close to the moving interfaces.
1.1.2 Bubble interactions in an acoustic field fully accounting for viscous effects

Bubble dynamics in acoustic fields has been studied extensively. In particular, the interaction of pulsating bodies in a fluid was first studied by V. F. K. Bjerknes (1906, 1909). Pulsating bubbles interact with nearby solid surfaces and also, interact with each other with a force that can be attractive or repulsive depending on whether they oscillate in or out of phase, respectively. In the linear limit and for inviscid fluids, it can be shown that its magnitude is proportional to the bubble volumes and inversely proportional to the square of their distance. This type of force is known as the secondary (or mutual) Bjerknes force and is responsible for several interesting dynamic phenomena. The mutual Bjerknes force plays an important role in many acoustic phenomena or engineering applications such as the formation of bubble grapes (Parlitz et al. 1999), the purification of liquid melts, the separation of a gas from its solution in a liquid, etc. Over the past decades a significant amount of research has been devoted to the study of single bubble dynamics (see Plesset and Prosperetti (1977) for a review on earlier work on the subject), as well as in the problem of bubble-bubble interaction (Doinikov and Zavtrak 1995). The theoretical approach to the secondary Bjerknes force assuming inviscid fluids by Pelekasis and Tsamopoulos (1993a, 1993b) has produced interesting results in a wide range of forcing frequencies, pressure amplitudes and bubble sizes. The surface of the bubbles has been allowed to deform from spherical retaining its axial symmetry. However, in those studies neglecting fluid viscosity led to very large bubble deformations that frequently ended up in bubble breakup. This makes necessary the examination of the effect of fluid viscosity on the bubble dynamics not only to determine if it reduces these large deformations but also to examine how it modifies the secondary Bjerknes force.

1.2 Governing equations

In both problems, we consider two initially spherical gas bubbles which are at rest in a stationary fluid. We assume axial symmetry around the line connecting their centers of mass and that the surrounding fluid is incompressible with density $\rho^*$, whereas the density and viscosity of the gas in the bubbles are much smaller than those of the liquid. Hence in general, the pressure inside the bubbles varies with time only and according to a polytropic law. In what follows an asterisk indicates a dimensional quantity.

The flow in the liquid is governed by the momentum and mass conservation equations, which in their dimensional form are:
\[
\rho^* \frac{D\mathbf{u}^*}{Dt^*} - \nabla^* \cdot (-P^* \mathbf{I} + \mathbf{\tau}^*) = 0
\]  
\[
\nabla^* \cdot \mathbf{u}^* = 0
\]  

(1.1) \hspace{1cm} (1.2)

where \( \frac{D}{Dt^*} \) stands for the convective derivative, \( \nabla^* \) for the gradient operator, \( \mathbf{u}^* \) and \( P^* \) are the velocity vector and pressure in the liquid, respectively, and \( \mathbf{\tau}^* \) is the extra stress tensor, which is generally split into a purely viscous part, \( 2\mu^*_s \dot{\gamma}^* \) and a polymeric contribution \( \mathbf{\tau}_p^* \):

\[
\mathbf{\tau}^* = 2\mu^*_s \dot{\gamma}^* + \mathbf{\tau}_p^*
\]  

(1.3)

where \( \mu^*_s \) is the Newtonian (solvent) viscosity and \( \dot{\gamma}^* \) is the rate of strain tensor defined as

\[
\dot{\gamma}^* = \frac{1}{2} (\nabla^* \mathbf{u}^* + \nabla^* \mathbf{u}^*\tau). 
\]

For a Newtonian fluid, \( \mathbf{\tau}_p^* = 0 \), whereas for a polymeric material the viscoelastic part of the extra stress tensor is related to the rate of strain tensor through a constitutive equation that describes the rheology of the polymer. As such we use the differential model that has been proposed by Phan-Thien and Tanner (PTT) (1977) assuming affine motion of the polymer chains:

\[
Y(\tau_p^*) \mathbf{\tau}_p^* + \lambda^* \mathbf{\tau}_p^* - 2\mu_p^* \dot{\gamma}^* = 0
\]  

(1.4)

where \( \lambda^* \) is the material relaxation time which is related to its elastic behavior, \( \mu_p^* \) the polymer viscosity and the symbol \( \hat{\cdot} \) over the viscoelastic stress denotes the upper convected Maxwell derivative defined as

\[
\hat{\mathbf{\tau}}_p^* = \frac{D\tau_p^*}{Dt^*} - (\nabla^* \mathbf{u}^*)^\top \cdot \tau_p^* - \tau_p^* \cdot \nabla^* \mathbf{u}^*
\]  

(1.5)

where the superscript \( T \) stands for the transpose of a tensor and the exponential form (Phan-Thien and Tanner 1978) of the PTT model is used:

\[
Y(\tau_p^*) = \exp \left[ \frac{\epsilon_{\text{PTT}}}{\mu_p^*} \lambda^* \mathbf{\tau}_p^* \right]
\]  

(1.6)

The parameter \( \epsilon_{\text{PTT}} \) in the PTT model imposes an upper limit to the elongational viscosity, which is inversely proportional to this parameter. Moreover \( \epsilon_{\text{PTT}} \) is related to the shear and extensional thinning of the polymeric material.

We note that for a Newtonian liquid, the extra stress tensor, \( \mathbf{\tau}^* \), is not an additional unknown, but it is calculated directly from the velocity field. However, for a viscoelastic model, such as the PTT model chosen here, the stress components are unknown quantities
which should be calculated through the constitutive equation. The hyperbolic nature of the latter necessitates for its accurate solution in various viscoelastic flows at high material elasticities, the Elastic-Viscous Split Stress (EVSS-G) method (Brown et al. 1993). This method splits the polymeric part of the extra stress tensor into a purely elastic, \( \Sigma^* \), and a viscous part:

\[
\tau_p^* = \Sigma^* + 2\mu_p^*\dot{\gamma}^*
\]  

(1.7)

Moreover, an independent and continuous interpolation, \( G^* \), of the components of the velocity gradient tensor, \( \nabla^*u^* \), is introduced wherever the latter arises in the constitutive equation:

\[
G^* = \nabla^*u^* .
\]  

(1.8)

For more details see (Dimakopoulos and Tsamopoulos 2004; Foteinopoulou et al. 2004; Brown et al. 1993). In summary, for a Newtonian fluid, eqs. (1.1)-(1.3) need to be solved with \( \tau_p^* = 0 \), whereas for a viscoelastic fluid the entire set of eqs. (1.1)-(1.8) must be solved simultaneously.

Along the free surface of the bubbles, the velocity field should satisfy a local force balance between the capillary forces, viscous and elastic stresses in the liquid and pressure inside each bubble \( i \) :

\[
n \cdot (-P_i^I + \tau^*) = -P_{gi}^*n + 2H^*\sigma^*n
\]  

(1.9)

where \( P_{gi}^* \) is the pressure inside bubble \( i \), \( \sigma^* \) is the surface tension, assumed to be the same in all liquid/air interfaces, \( n \) is the outward (for the fluid domain) unit normal to each free surface and \( 2H^* \) is its mean curvature which is defined as:

\[
2H^* = -\nabla^* \cdot n, \quad \nabla^* = (I - nn) \cdot \nabla^*
\]  

(1.10)

The pressure inside each bubble varies following the instantaneous changes in the bubble volume according to:

\[
P_{gi}^* = P_{gio}^* \left( \frac{V_{io}^*}{V_i^*} \right)^\gamma , \quad i = 1, 2
\]  

(1.11)

where \( P_{gio}^* \) and \( V_{io}^* \) are the initial pressure and the volume of bubble \( i \), \( V_i^* \) its instantaneous volume and \( \gamma \) is taken to be equal to 1.4. The volume of each bubble is calculated after each time step through:

\[
V_i^* = \iiint dV_i^*, \quad i = 1, 2
\]  

(1.12)
where $dV^*_1 = r^* dr^* dz^* d\theta$ when the bubble interface is described in cylindrical coordinates, and $dV^*_2 = r^*_s \sin \theta dr^*_s d\theta d\phi$ when spherical coordinates are used. In general, the subscript $s$ indicates spherical coordinates. Additionally, the shapes of the free surfaces are determined by invoking the kinematic condition:

$$\frac{dF^*}{dt^*} = u^*$$

(1.13)

where $F^*$ denotes the position vector of the interface, which is given by the following expressions $F^*_r = r^* e_r + z^* e_z$ and $F^*_s = r^*_s e_r$, when cylindrical or spherical coordinates are used, respectively. Along the axis of symmetry the usual symmetry conditions are imposed: (a) the normal to the axis component of velocity vector is set to zero and (b) the tangential to the axis component is symmetric.

1.2.1 Cavities inside a filament undergoing stretching

The liquid filament is assumed to have initially a cylindrical outer surface with a uniform radius $R^*_o$ and to be confined between two solid and coaxial disks each of radius $R^*_co$ also, located at initial distance $H^*_o$. The filament is permanently bonded on both disks and is being stretched by pulling the upper disk with a constant velocity $U^*_o$, while the lower disk remains stationary. Due to the assumption of axial symmetry, both bubbles inside the filament are assumed to lie along its axis of symmetry. Their radii are initially $R^*_1$ and $R^*_2$, respectively, and their centers are located at distances $h^*_1$ and $h^*_2$ above the lower disk. The initial distance of the centers of the bubbles is denoted as $L^*_{oo} = h^*_2 - h^*_1$. A schematic of the system considered is shown in Fig. 1.1. As the upper disk is being pulled, the height $H^*(t^*) = H^*_o + U^*_o t^*$ of the filament increases, both bubbles deform and translate along the filament axis, and all liquid/gas interfaces get distorted.
Figure 1.1 Schematic of two spherical cavities inside an initially cylindrical filament.

In order to readily describe the filament interface, it is convenient to formulate this problem in cylindrical coordinates, although this choice complicates the description of the bubble surfaces. The center of the coordinate system is located at the center $O$ of the lower disk. The axial symmetry reduces this problem to a two-dimensional one, defined in the region enclosed by the outer surface of the liquid and the axis of symmetry of the cylinder or the bubble surfaces in the radial direction and by the two disks in the axial direction. We scale all lengths with the radius of the first bubble $R_{b1,0}^*$, velocities with the pulling velocity $U_o^*$, time with $R_{b1,0}^*/U_o^*$ and stresses and pressure with a viscous scale $\mu^* U_o^*/R_{b1,0}^*$ where the total dynamic viscosity is $\mu^* = \mu_s^* + \mu_p^*$. Hereafter, a variable without an asterisk indicates the corresponding dimensionless variable. Similarly, the equations governing this problem, when they are rendered dimensionless, retain their form, except for the momentum balance, the constitutive law and the interfacial force balance which become:

$$Re \frac{Du}{Dt} + \nabla P - \nabla \cdot \Sigma - 2 \nabla \cdot \dot{\gamma} = 0 \quad (1.14)$$

$$Y(\tau_p)\Sigma + De \dot{\Sigma} + 2De(1-\beta) \dot{D} - 2(1-\beta)(1-Y(\tau_p))D = 0, \quad Y(\tau_p) = \exp \left[ \varepsilon_{PTT} \frac{De}{1-\beta} tr\tau_p \right] \quad (1.15)$$
\[ \mathbf{n} \cdot (-P \mathbf{l} + \mathbf{t}) = -P_{gi} \mathbf{n} + \frac{2H}{Ca} \mathbf{n}, \quad i = 1, 2, 3 \]  

(1.16)

where \( D = \frac{1}{2}(G + G^T) \) and the four dimensionless numbers that arise are the Reynolds number, \( Re = \frac{\rho U^*_0 R^*_0}{\mu^*_0} \), the Deborah number, \( De = \frac{\lambda U^*_0}{R^*_0} \), which is a measure of fluid elasticity, the solvent viscosity ratio \( \beta = \frac{\mu^*_s}{\mu^*_0} \) and the capillary number \( Ca = \frac{\mu^*_0 U^*_0}{\sigma^*_0} \), expressing the ratio of viscous to capillary forces. In this problem eq. (1.16) is applied not only along the bubble-liquid interfaces (then, \( i = 1, 2 \) and \( P_{gi} \) stands for the time-varying, gas pressure inside bubble \( i \)), but also along the liquid-air interface, (then \( i = 3 \) and \( P_{gi} = 0 \) sets the surrounding air pressure to zero). The pressure inside each bubble and the corresponding volume of the bubbles is calculated via eqs. (1.11) and (1.12), respectively. Along the axis of symmetry the usual symmetry conditions are used, written in cylindrical coordinates:

\[ u_r = 0 \]

(1.17)

\[ \frac{\partial u_z}{\partial r} = 0 \]  

(1.18)

### 1.2.2 Interacting bubbles in an acoustic field

Initially, the two bubbles are spherical, surrounded by a viscous liquid and at equilibrium. Hence the initial pressure inside them is set solely by capillarity. Subsequently, they are set in motion by a step change in the far field pressure. This abrupt change in pressure causes volume oscillations in the bubbles, which, in turn, generate a disturbance in the pressure around them. The later induces a force between them which is always attractive, for a step change in pressure, (see Bjerknes (1906, 1909)) and a deformation of their interfaces, depending on the distance between them and the fluid properties. Fig. 1.2 illustrates a schematic of this flow geometry. The two bubbles are initially spherical with radii \( R^*_{bA}, R^*_{bB} \) and distance \( D^* \) between their two centers of mass. A convenient way to describe the far-field spherical symmetry of the pressure and velocity fields is to introduce a spherical coordinate system centered at the middle of the distance between the bubble centers. This choice complicates the description of the bubble surfaces, as in the previous problem, while the axial symmetry reduces it to a two-dimensional one defined in the region enclosed by the outer spherical surface and the axis of symmetry or the bubble surfaces.
We scale all lengths with the radius $R_{b_{A}}^{*}$ of the left bubble. Due to the absence of a characteristic velocity, surface tension is used for making velocity, time and pressure dimensionless. So, we scale them with $(\sigma^{*}/R_{b_{A}}^{*}\rho^{*})^{1/2}$, $(R_{b_{A}}^{*3}\rho^{*}/\sigma^{*})^{1/2}$ and $(\sigma^{*}/R_{b_{A}}^{*})$, respectively. The flow is governed by the momentum and mass conservation equations, eq. (1.1) & (1.2), and only the momentum balance is modified when written in dimensionless form:

$$\frac{D\mathbf{u}}{Dt} + \nabla P - Oh \nabla \cdot \left( \nabla \mathbf{u} + \nabla \mathbf{u}^{T} \right) = 0 \quad (1.19)$$

The dimensionless number that arises in it is the Ohnesorge number, $Oh = \left( \mu_{i}^{*2}/\rho^{*}R_{b_{A}}^{*}\sigma^{*} \right)^{1/2}$, a measure of viscous over inertia and capillary forces. For time greater than zero, the pressure at infinity increases over its static value $P_{s}$ as:

$$P_{\infty} = P_{s}(1 + \varepsilon), \quad (1.20)$$

where $\varepsilon$ is a measure of the applied disturbance. Along the free surface of the bubbles, we impose eq. (1.9) which in dimensionless form here becomes

$$\mathbf{n} \cdot (-P\mathbf{I} + \mathbf{t}) = P_{\infty}^{*} + 2H\mathbf{n}, \quad i = A, B \quad (1.21)$$

where $i = A, B$ stands for the interface of either bubble. The pressure inside each bubble is calculated via eq. (1.11), while their volume is calculated in spherical coordinates via eq.
Along the axis of symmetry, if spherical coordinates are used for the flow problem the symmetry conditions become:

\[ u_\theta = 0 \]  \hspace{1cm} (1.22)

\[ \frac{\partial u_r}{\partial \theta} = 0 \]  \hspace{1cm} (1.23)

The infinite domain of the fluid is truncated to a finite spherical domain around the two bubbles with a radius much larger than the bubble radius so this boundary does not affect the flow around the two bubbles. This is facilitated using the open boundary condition suggested by Papanastasiou, Malamataris and Ellwood (1992).

### 1.3 Numerical Implementation

#### 1.3.1 Elliptic grid generation

In order to accurately and effectively simulate moving boundary flows in domains with deforming inclusions we have chosen the mixed finite element method to discretize the velocity, pressure and extra stress (for viscoelastic materials only) fields, combined with an advanced elliptic grid generator for the initial construction and subsequent motion of the mesh nodes in the liquid domain. The set of equations generating the location of the grid points in the entire domain or in each subdomain is capable to relocate them in response to the evolution of the free surface. Their distribution over the domain is readjusted dynamically to keep a relatively uniform or smoothly varying concentration of nodes in the entire physical domain, without relying on prior knowledge of the interface location and deformation or intervention during the calculations or placing non-physical restrictions on its shape.

In particular, a mapping of the physical (sub)domain is used onto a fixed with time computational domain. This is schematically represented as \((X,Y,t) \rightarrow (\xi,\eta,t)\), where \(J\) is the Jacobian of the transformation. According to this mapping, every point particle being at time \(t\) at a position with coordinates \((X,Y)\) in physical space is mapped to a point particle in a new plane with global coordinates \((\xi,\eta)\). The \((X,Y)\) coordinates stand for either cylindrical \((r,z)\) or spherical coordinates \((r,\theta)\). Subsequently, a mesh is generated in computational space with the desired properties. Then the positions of the nodes in physical space are computed by solving a set of partial differential equations. The three essential properties of a mapping are: smoothness, orthogonality and concentration of the (coordinate) curves along which the mesh points lie in physical space (Thompson et al. 1974; Saltzman
and Brackbill 1982). The coordinate lines that are parallel to the deforming interface must follow closely its large distortions and even concentrate near it in order to better resolve the boundary conditions there, without the strong requirement that they remain orthogonal to the rest of the boundaries (Tsiveriotis and Brown 1992). On the other hand, the coordinate lines normal to the interface must intersect them nearly orthogonally. Keeping these in mind, Dimakopoulos and Tsamopoulos (2003a), concluded that the following system of quasi-elliptic partial differential equations combines these features:

$$\nabla \cdot \left( \frac{F(\eta)}{F(\xi)} \nabla \eta \nabla + (1 - \varepsilon_1) \nabla \eta \right) = 0$$  \hspace{1cm} (1.24)

$$\nabla \cdot \nabla \xi = 0$$  \hspace{1cm} (1.25)

Eq. (1.24) generates the curves on which $\eta$ is a constant. The introduction of the term with the square root here, allows them to be nearly normal to the highly deforming interface. Eq. (1.25) generates the curves on which $\xi$ is a constant. These are nearly parallel to the interface and must follow it while it deforms. Its large deformations may lead to highly obtuse or highly acute angles with its neighboring boundaries. This necessitates relaxation of orthogonality between these other boundaries and the $\xi$-coordinate lines making the square root term inappropriate in eq. (1.25) as clearly demonstrated in [13]. In the expressions above $F(q), q = \xi, \eta$ is given by:

- $F(q) = r^2 + \eta^2$ (when cylindrical coordinates are used)  \hspace{1cm} (1.26a)
- $F(q) = r^2 + \eta^2 \theta^2$ (when spherical coordinates are used)  \hspace{1cm} (1.26b)

in which when the variable $q$ appears as a subscript it indicates a partial derivative with respect to it. Also, $\varepsilon_1$ is an empirically chosen parameter, ranging between 0 and 1, that controls the smoothness of the mapping relative to the degree of orthogonality of the mesh lines. This parameter is adjusted by trial and error and in the following simulations is set equal to 0.1.

The way the mesh generating equations, eqs (1.24) - (1.25), are written implies that $(\xi, \eta)$ are unknown functions, while $(X,Y)$ are the independent variables. This is preferred over its inverse, which is actually the case, because it makes the transformation one-to-one provided that its curvature is non-positive and the boundary of the computational domain is convex. These can be achieved by construction (Dvinsky 1991). Moreover, the flow equations are originally written in the physical domain with independent variables $(X,Y)$, so we need
to transform the entire set so that \((\xi, \eta)\) are the independent variables. This procedure, although straightforward, adds to the complexity of the formulation by introducing new spatial and temporal derivatives in the governing equations according to the chain rule of differentiation:

\[
\frac{\partial}{\partial t} = \frac{\partial \xi}{\partial X} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial X} \frac{\partial}{\partial \eta}, \quad \frac{\partial}{\partial \xi} = \frac{\partial \xi}{\partial X} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial X} \frac{\partial}{\partial \eta}, \quad \frac{\partial}{\partial \eta} = \frac{\partial \xi}{\partial Y} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial Y} \frac{\partial}{\partial \eta}.
\] (1.27a, b, c)

Clearly time is independent of either the original or the mapped coordinate system, \(t = \hat{t}\), so that in these expressions \(\partial t / \partial X = \partial t / \partial \xi = 0\), etc., and the coefficient of the time derivative \(\partial / \partial \hat{t}\) is unity. The partial differentiations, e.g. \(\partial \xi / \partial t\), are implied under constant location in the physical space making these derivatives nonzero. Similarly, the partial time derivatives of the coordinates in physical space under constant location in computational space, \((X, Y)\), that correspond to the given node locations in computational space. Therefore, in eqs (1.24)-(1.27), the derivatives of the coordinates in physical space with respect to those in physical space must be expressed in an inverse manner. This is readily accomplished using the metrics and the Jacobian of the transformation and, for example, we obtain

\[
\xi_X = \frac{Y_\eta}{|J|}, \quad \xi_Y = -\frac{X_\eta}{|J|}, \quad \xi_\eta = \frac{X_\eta Y_\eta - Y_\eta X_\eta}{|J|}, \quad \text{where} \quad |J| = \left| X_\xi Y_\eta - X_\eta Y_\xi \right|.
\] (1.28)

Equally important for the quality of the constructed mesh are the boundary conditions and the constraints on eqs. (1.24) & (1.25). So, on the fixed parts of the boundary we replace the mesh generating equations with the equation that defines the boundary curve, while the remaining degree of freedom is used for controlling the node distribution there:

\[
\frac{d^2 \tilde{F}(q)}{dq^2} = 0, \quad q = \xi, \eta
\] (1.29a)

where

- \(\tilde{F}(q) = \int_0^q \sqrt{w_1 r_q^2 + w_2 z_q^2} \, dq\) (when cylindrical coordinates are used) \(1.29b\)
- \(\tilde{F}(q) = \int_0^q \sqrt{w_1 r_q^2 + w_2 r_q^2 \theta_q^2} \, dq\) (when spherical coordinates are used) \(1.29c\)

and \(w_1 + w_2 = 2\). In the above equation, \(\tilde{F}(q)\) is a weighted arc-length along the free surface and \(w_1, w_2\) are two weights, which have to be adjusted by trial and error to optimize performance. Setting \(w_1 = w_2 = 1\), distributes the nodes equally on the free surface, which is useful only when the deformation of the free surface is not very large in one of the directions. This constraint is imposed via a penalty formulation. More details and examples on the effect
of \( w_1, w_2 \) are given in Dimakopoulos and Tsamopoulos (2003a). It is noteworthy that for the quality of the constructed mesh, spacing of the nodes can be more important than orthogonality of the coordinate lines. Finally, on the free surfaces, the kinematic condition, eqs (1.13), is imposed on them, while the remaining degree of freedom is controlled again by eqs (1.29).

When accumulation of the coordinate lines towards certain boundaries is necessary, specific stretching functions are introduced in the computational domain (Chung 2002). For example, when an increased concentration of mesh lines is required close to the bottom of the computational domain at the boundary located at \( \xi = L \) the following expressions are used:

\[
Y = \eta, \quad X = K \frac{(\zeta + 1) - (\zeta - 1) \left( \frac{\zeta + 1}{\zeta - 1} \right)^{\frac{(\zeta - L)}{K}} + 1}{\left( \frac{\zeta + 1}{\zeta - 1} \right)^{\frac{(\zeta - L)}{K}}}
\]  

(1.30a, b)

where \( K \) is the length of the domain along the \( X \)-direction and \( \zeta \) is a parameter that controls the density of the coordinate lines and is chosen empirically, \( 1 < \zeta < \infty \). More specifically the closer to unity \( \zeta \) is, the denser the coordinate lines are near \( \xi = L \).

The discretization of the computational domain is based on triangular elements after the splitting of each rectangular element generated by the above procedure into two triangular ones in a way that will preserve the local symmetries. Triangular elements are preferred because they conform better to large deformations of the physical domain and can sustain larger distortions than the rectangular ones without making the Jacobian of the local transformation to the parent element singular. Further details about the construction of the mesh and the boundary conditions will be discussed for each case separately.

### 1.3.2 Local mesh refinement

To increase the local accuracy in regions of particular interest or in regions with sharp variations of the solution vector such as those along the bubble surface or other highly deforming interfaces, the element refinement (h-) method has been applied. The h-method has been suggested by Szabo and Babuska (1991) who subdivided the elements on which the measure of error was larger than a prescribed tolerance. Tsiveriotis and Brown (1993), also applied it in a free boundary problem by introducing a transition layer of non-conforming quadrilateral elements, and found that the local refinement technique is essential in cases where elliptic grid generators are used because it relaxes the requirements on the mapping
equations and adds more flexibility to the handling of the three important characteristics of the grid mentioned above.

Figure 1.3  Stages of the mesh refinement: (a) initial mesh with rectangular elements, (b) certain rectangular elements are split in four smaller ones, (c) Insertion of transition triangular elements and (d) each rectangular element is split in two triangular ones.

In Fig. 1.3, the four stages of mesh refinement methodology in two directions around a corner are illustrated. A coarse mesh, initially tessellated in rectangular elements, is refined by adding nodes located in the centroid of each element and in the middle of each element’s side. To accommodate the two regions with different number of elements, an intermediate zone of triangular elements is created. In the final stage all the rectangular elements are split into two triangular ones as already described. As we will demonstrate with specific examples this local refinement not only reduces the computational cost, but also increases the accuracy of our calculations considerably. For retaining the bandwidth of the Jacobian matrix as small as possible, the numbering of the nodes and consequently of the unknowns is based on a hierarchical method where nodes with smaller $\xi$ or $\eta$ (depending on which direction we count first) values are accounted first.

1.3.3 Mixed finite element method

The velocity vector as well as the position vector of the nodes are approximated with 6-node Lagrangian basis functions, $\phi^i$, and the pressure, the stress tensor and the rate of strain
The finite element/Galerkin method is employed, which after applying the divergence theorem results into the following weak forms of the momentum balance:

\[
\int_\Omega \left[ \mathbf{R}_e \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) \phi^i + \nabla \phi^i : (-\mathbf{P}_I + \Sigma + 2\dot{\gamma}) \right] \, d\Omega - \int_\Gamma \left[ \mathbf{n} \cdot (-\mathbf{P}_I + \Sigma + 2\dot{\gamma}) \right] \phi^i \, d\Gamma = 0,
\]

for the filament undergoing stretching and

\[
\int_\Omega \left[ \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) \phi^i + \nabla \phi^i : (-\mathbf{P}_I + Ohr) \right] \, d\Omega - \int_\Gamma \left[ \mathbf{n} \cdot (-\mathbf{P}_I + Ohr) \right] \phi^i \, d\Gamma = 0
\]

for the bubbles in the acoustic pressure field, while the mass balance becomes

\[
\int_\Omega \psi^i \nabla \cdot \mathbf{u} \, d\Omega = 0
\]

where \( d\Omega \) and \( d\Gamma \) are the differential volume and surface area respectively. The surface integral that appears in the momentum equation is split into as many parts as the boundaries of the physical domain and the relevant boundary condition is applied therein. In order to avoid dealing with the second order derivatives that arise in the boundary integral of the interface, through the definition of the mean curvature, \( H \), we use the following equivalent form:

\[
2H \mathbf{n} = \frac{dt}{ds} - \frac{\mathbf{n}}{R_2}
\]

where the first term describes the change of the tangential vector \( \mathbf{t} \) along the free surface, \( R_2 \) is the second principal radius of curvature, and \( \mathbf{n} \) is the unit normal vector on the free surface. The weak form of the mesh generating equations in general form is derived similarly by applying the divergence theorem:

\[
\int_\Omega \left( \varepsilon_1 \frac{F(\eta)}{F(\xi)} + (1-\varepsilon_1) \right) \nabla \eta \cdot \nabla \phi^i \, d\Omega + L \int_\Gamma \frac{\partial \phi^i}{\partial \eta} \sqrt{F(\eta)} \, d\eta = 0
\]

\[
\int_\Omega \nabla \xi \cdot \nabla \phi^i \, d\Omega = 0
\]

where \( F(\eta) \) and \( F(\xi) \) are given by eq. (1.26), the penalty parameter is \( L = O(10^3 - 10^5) \) and the line integral is along the free surface.

The weak form of eq. (1.8) for the velocity gradient tensor is given by:

\[
\int_\Omega (\mathbf{G} - \nabla \mathbf{u}) \psi^i \, d\Omega = 0
\]
Finally, the constitutive equation is a hyperbolic equation for the elastic part of the stress tensor and is solved by the Stream-line Upwind Petrov-Galerkin (SUPG) method (Brooks and Hughes 1982):

\[
\int_{\Omega} \left[ Y(\tau_p) \Sigma + D \Sigma + 2D(1 - \beta) D - 2(1 - \beta)(1 - Y(\tau_p)) D \right] \Psi' d\Omega = 0
\]

where the weighting function $\Psi'$ is formed from the finite element basis function for the elastic stress tensor according to Zienkiewicz and Taylor (2000):

\[
\Psi' = \psi' + \frac{\Delta t_{n+1}}{2} u \cdot \nabla \psi'
\]

where $\Delta t_{n+1}$ is the current time step. The derivation of eq. (1.37) is based on the characteristic Galerkin method (Codina 1998) and guarantees that the upwind term in the modified basis function vanishes as $\Delta t \to 0$.

### 1.3.4 Time integration and solution procedure

In order to integrate accurately the governing equations in time, the implicit Euler method, which is an A-stable approximation, with time stepping adaptation, is used. This method has been suggested as a very efficient and robust alternative to the more expensive finite element methods. More specifically, if by $f(\kappa)$ we denote the set of equations to be integrated, its approximate form, using backward finite differences is

\[
\kappa_{n+1} - \kappa_n = f(\kappa_{n+1})
\]

where the subscript $n$ stands for the previous time instant and $\kappa$ is the entire unknown vector which includes velocities, pressure, projected rate of strain and stresses. The difference $t_{n+1} - t_n$ defines the current time step $\Delta t_{n+1}$. The strategy for changing the time step is based on the estimation of the local truncation error, which is the difference between the accurate approximation $\kappa_n$, and an explicitly predicted one $\kappa_n^p$:

\[
\kappa_n^p = \kappa_{n-1} + \Delta t_{n-1} \dot{\kappa}_{n-1}
\]

\[
\Delta t_{n+1} = \Delta t_n \left( \frac{\epsilon}{\|d_n\|} \right)^{1/2} \equiv \Delta t_{e}
\]

where $\epsilon$ is a user defined tolerance, $\| \cdot \|$ stands for the Euclidean norm and $d_n = \kappa_n - \kappa_n^p$ is the difference between the predicted and the accurate solution at $t_n$ (Gresho et al. 1980).
The resulting set of algebraic equations is solved by the modified Newton-Raphson iteration scheme. This method proceeds by not updating after each cycle the Jacobian matrix and its factorized form, unless a criterion of decreased convergence rate is violated. Moreover, in the case of transient calculations a Picard iteration scheme is used for solving the set of non-linear equations at each time step and simultaneously decreasing the memory requirements. The total set of equations is split in two sub-sets: the first one consists of the mass and momentum balances and the other one consists of the mesh equations. These are solved independently from each other, using only the necessary information from the other sub-problem. When the fluid exhibits viscoelastic behavior, then the extra-stress unknowns are also solved separately according to the following algorithm (Fortin and Fortin 1989):

For each time step solve iteratively until convergence Problems 1-4:

- **Problem 1**: The mass and momentum balances for \( \mathbf{u}^{i+1}_{n+1} \) and \( P^{i+1}_{n+1} \) keeping \((X,Y)^i_{n+1}, G^{i}_{n+1}\) and \( \Sigma^{i}_{n+1} \) fixed.

- **Problem 2**: The mesh equations for \((X,Y)^i_{n+1}\) keeping \( \mathbf{u}^{i+1}_{n+1}, P^{i+1}_{n+1}, G^{i}_{n+1}\) and \( \Sigma^{i}_{n+1} \) fixed.

- **Problem 3**: The continuous approximation of the rate of strain tensor \( G^{i}_{n+1} \) keeping \( \mathbf{u}^{i+1}_{n+1}\) and \( P^{i+1}_{n+1}, (X,Y)^i_{n+1}, \) and \( \Sigma^{i}_{n+1} \) fixed.

- **Problem 4**: The viscoelastic constitutive equation for \( \Sigma^{i}_{n+1} \) keeping \( \mathbf{u}^{i+1}_{n+1}\) and \( P^{i+1}_{n+1}, (X,Y)^i_{n+1}\) and \( G^{i}_{n+1} \) fixed.

This is an efficient method for decoupling the nonlinear equations because it results in considerably smaller Jacobian matrices, which are easier to handle. The convergence of the entire scheme is ensured by the automatic time adaptation, because the predicted solution does not differ too much from the exact one and the Newton/Kantorovich sufficient condition is satisfied (Cockburn 2001). In order to improve the effectiveness of the scheme and to avoid undesirable increases of the time step, an upper bound is placed on the latter by the number of Picard iterations. So the new time step, \( \Delta t_{n+1} \), is determined by

\[
\Delta t_{n+1} = \min(\Delta t_c, \Delta t_p) \tag{1.42}
\]

where \( \Delta t_c \) is given from Eq. (1.41) and \( \Delta t_p \) is given by

\[
\Delta t_p = \Delta t_p \left( \frac{\text{desired number of Picard cycles}}{\text{actual number of Picard cycles}} \right)^{1/4}.
\]

Usually, the desired number of Picard iterations is equal to the actual ones at the first integration step increased by 3-4.
In addition, the Jacobian matrix of each sub-problem that results after the application of the Newton Raphson solution technique, is stored in Compressed Sparse Row (CSR) format and the linearized system is solved by using PARDISO, a robust direct sparse matrix solver (Schenk and Gärtner 2004, 2006). A Fortran 90 code was written for this purpose and was run on a workstation with dual Xeon CPU at 2.8 GHz.

1.4 Generation of initial meshes

1.4.1 Cavities inside a filament undergoing stretching

Although the domain to be discretized contains inclusions because of the presence of the bubbles in the filament, the assumption of axial symmetry makes it simply connected. Actually, the segments of the axis of symmetry connecting each disk to one of the bubbles and the bubbles with each other play the role of branch-cuts in the corresponding 3D geometry. Then as discussed in the introduction, each segment of the axis of symmetry can retain the same position, while each bubble surface is mapped onto two different segments of the axis of symmetry in the computational domain. In particular, each bubble surface is mapped onto segments with \( \xi = 0 \) and \( Z^l_i \leq \eta \leq Z^u_i \), where \( Z^l_i \) and \( Z^u_i \) are the coordinates of the south \((l)\) and north \((u)\) pole of the lower \((i = 1)\) or the upper \((i = 2)\) bubble. The resulting computational domain is shown in Fig. 1.4 to be confined between the initial filament surface, which is a perfect cylinder, \( \xi = R_{co} \) and its axis of symmetry, \( \xi = 0 \). Clearly, this shape of the computational domain is different from even the initial shape of the filament containing bubbles of a specific shape and size and, hence, it is necessary to construct the corresponding initial mesh in the physical domain. To do so, we developed a continuation procedure in which the mesh equations, eq. (1.24) & (1.25), are solved together with the appropriate boundary conditions. As boundary conditions, we impose the locations of all the boundaries of the liquid except for the surfaces of the bubbles and the node distribution equations therein, which are generated by eq. (1.29). On the boundaries corresponding to the bubble surfaces we impose the following equations that define the two ellipsoids with the same poles as each bubble:

\[
\frac{r^2}{b^2} + \frac{(z-z_{i,0})^2}{R_{bi,0}^2} = 1, \tag{1.43}
\]
where $z_{i,0}$ is the initial axial position of the center of bubble $i$. Initially, the boundary is a straight line coinciding with the axis of symmetry, but subsequently it takes the shape of an ellipsoid when the parameter $b$ in eq. (1.43) increases from zero and finally becomes a hemisphere when $b$ is equal to the initial radius of the $i$ bubble, $R_{b,i,0}$. These changes in the domain shape and the discretizing mesh must be introduced gradually, so, we increase the value of the parameter $b$ gradually from $0.01R_{b,i,0}$ to $R_{b,i,0}$ by zeroth order continuation. When the transient problem is solved, eq. (1.43) is replaced with the kinematic condition, eq. (1.13), written in cylindrical coordinates. A similar kinematic condition determines the time-dependent location of the outer filament surface.

![Figure 1.4 Computational $(\xi, \eta)$ domain of the bubbles in a filament problem. The bubble surfaces are mapped onto the thicker line segments.](image)

The mesh that is generated in this manner is shown in fig. 1.5a. For clearer viewing, the mesh we show here is quite coarse, but a much finer mesh was used in order to produce the results in this paper. We observe that the mesh is not acceptable near the poles of the bubbles, where the repulsion of the mesh lines is clearly seen, as discussed in the introduction. An easy remedy of this is to impose the generalized distributions, eq. (1.29) along the $\eta$-lines, that begin from the poles of each bubble and reach the air-liquid interface (Fig. 1.4). Since a higher concentration of nodes is needed in the regions closer to the bubbles, along these lines we use $w_1 = 0.1$ and $w_2 = 1.9$ in eq. (1.29). The mesh generated after the application of eq. (1.29), is shown in Fig. 1.5b. It consists of more uniform elements all around the two bubbles. With the introduction of these “internal” lines withpreset node distributions, in essence, we introduce internal boundaries in the computational domain which
somewhat resembles domain decomposition. Thus, we eliminate the need for adding attractive terms on corners or on the bubble poles in these elliptic equations, something we have used elsewhere successfully (Dimakopoulos and Tsamopoulos 2003b). When we introduced such attractive terms on the bubble poles here, the resulting mesh was not as uniform as the one shown in fig. 1.5b. Additionally, the mesh refinement technique described in section 1.3.1 is used here due to the large mesh deformations expected in the region near the bubbles and the filament-air free surface and the need to resolve them very accurately, especially because of the hyperbolic nature of the constitutive law. Typical meshes with and without local mesh refinement will be shown in the results section.

Figure 1.5 Initial mesh for the bubble-filament problem (a) using the equidistribution condition only at the boundaries of the mesh problem and (b) using additional generalized distributions along the $\eta$-lines that begin from the poles of each bubble and reach the air-liquid interface, with $w_1 = 0.1$ and $w_2 = 1.9$.

1.4.2 Interacting bubbles in an acoustic field

Given the success and simplicity of the previous method in dealing with the bubbles included in the filament, it was first attempted for this problem to construct the mesh following a similar method. More specifically, given that here very far from both bubbles the pressure and velocity fields have spherical symmetry, a spherical coordinate system is more appropriate. Also, it seems reasonable to position its center at the middle of the distance between the centers of the two bubbles. The physical domain $(r, \theta)$ (see fig. 1.2) is mapped
on the computational domain \((\xi, \eta)\) (see fig. 1.6), as follows: The first and third segments, \(0 \leq \xi \leq \xi_{A1}\) and \(\xi_{A2} \leq \xi \leq R_\infty\), of the line \(\eta = 0\) (left boundary) correspond to the line segments \(OA_1\) and \(A_2A_3\) in the physical domain, while its second segment \(\xi_{A1} \leq \xi \leq \xi_{A2}\) corresponds to the surface of the left bubble. Similarly, the first and third segments, \(0 \leq \xi \leq \xi_{B1}\) and \(\xi_{B2} \leq \xi \leq R_\infty\), of the line at \(\eta = \pi\) (right boundary) correspond to the line segments \(OB_1\) and \(B_2B_3\), while its second segment \(\xi_{B1} \leq \xi \leq \xi_{B2}\) corresponds to the surface of the right bubble, which is generally of different size.

**Figure 1.6** Computational \((\xi, \eta)\) domain for the bubble-bubble interaction problem, when the center of the spherical coordinate system is positioned at the middle of the distance between the centers of the two bubbles. The bubble surfaces are mapped onto the thicker line segments.

The line segments \(0 \leq \eta \leq \pi\) at \(\xi = 0\) and at \(\xi = R_\infty\) correspond to the center of the coordinate system and to the far field boundary in physical space, respectively. In other words, the four segments on the axis of symmetry corresponding to branch-cuts are mapped in pairs on opposite boundaries of the computational domain, while each bubble surface is also mapped on the same opposite boundaries. The center of the coordinate system and the outer circular boundary are mapped on the bottom and top boundaries, respectively, in the computational space. To avoid the repulsion of the mesh lines by the bubble poles, the node locations on the lines of constant \(\xi\) emanating from both poles of each bubble are controlled.

As in the previous case, this choice of computational domain necessitates the construction of an initial physical domain (containing bubbles of the desired shape and size). This is achieved via the same continuation procedure in which the mesh equations, eq. (1.24) & (1.25), written
in spherical coordinates, are solved together with the boundary conditions which set the locations of all the boundaries of the liquid except for the surfaces of the bubbles and the node distribution equations therein, which are generated by eq. (1.29). On the bubble surfaces, a condition similar to eq. (1.43) is imposed and meshes of gradually increasing values of the parameter $b$ are generated, until both bubbles attain a spherical shape. The resulting initial mesh is shown in fig. 1.7, after splitting each rectangle into 2 triangles in a way that preserves the local symmetries. This mesh seems to be quite satisfactory. Unfortunately, as the bubbles get distorted with time the computations fail to converge. This is attributed to the asymmetry in discretizing the two poles of each bubble. This is observed first by the increasing error in pressure at the poles of the bubbles, especially when the bubbles are relatively small and eventually leads to unacceptable errors.

![Figure 1.7](image)

**Figure 1.7** Part of the initial mesh for the bubble-bubble interaction problem when the mapping of fig. 1.6 is used.

In a second attempt to generate the mesh for accurate calculations, it was decided to remedy this problem by placing the center of the coordinate system at the center of one of the two bubbles, e.g. the right bubble, see fig. 1.8a. Then, the surface of this bubble would be described simply and exactly by these spherical coordinates and, hence, it would be symmetrically discretized. In order to improve the discretization of the left bubble also, we impose the node locations on the $\xi$-lines starting from the poles of the left bubble at $\eta = 0$ all the way to $\eta = \pi$ on which the generalized node distributions, eq.(1.29), are imposed. Finally, the small asymmetry in the far field boundary condition which is introduced by the presence
of the second bubble should not affect the solution since this boundary is not only located very far away from both bubbles but also the open boundary condition is applied there. Hence and although “the branch-cuts” remain the same, the physical domain $(r, \theta)$ (fig. 1.8a) is mapped onto a different computational one $(\xi, \eta)$ (fig. 1.8b). In particular, the surface of the right bubble is mapped onto the entire bottom boundary $0 \leq \eta \leq \pi$ at $\xi = R_b$, and the left bubble onto the line segment $\xi_1 \leq R_b \leq \xi_2$ at $\eta = 0$, the left boundary. This is also a very promising arrangement out of a host of others. The locations $\xi_1$ and $\xi_2$ correspond to the right and left poles, respectively, of the left bubble from where the $\xi$-lines emanate. In order to construct the two bubbles initially the equation of a circle with radius equal to the radius of the bubble is used directly for the right bubble, while for the left bubble the continuation procedure and eq. (1.43) in spherical coordinates is used as described before.

Figure 1.8 Illustration of: (a) the coordinate system in physical space and (b) the computational domain of the bubble-bubble interaction problem, when the center of the coordinate system is placed at the center of the right bubble. The bubble surfaces are mapped onto the thicker line segments.
The fixed parts of the domain are imposed as boundary conditions, while the node distribution equations, eq. (1.29), are imposed at the line of symmetry ($\theta = 0, \theta = \pi$) and at $r = R_e$. Fig. 1.9 depicts a close up of the initial mesh around the two spherical bubbles with rectangular elements for reasons of clarity. This initial mesh seems satisfactory. However, drawing the pressure profile around the surface of two equal bubbles at $t = 10^{-4}$ and for $Oh^{-1} = 20$ and $P_s = 28$, fig. 1.10 we observe two things: (i) The pressure in both bubble surfaces deviates from its expected value of $\sim 28$, something we had noted with the previous mesh to lead to failure of computations and (ii) This deviation is about 2 orders of magnitude larger in the left bubble the center of mass of which does not coincide with the center of the coordinate system.

![Figure 1.9](image.png)

**Figure 1.9** Part of the initial mesh near the bubbles for the bubble-bubble interaction problem when the mapping of fig. 1.8 is used. For clarity we show rectangular elements only.

![Figure 1.10](image.png)

**Figure 1.10** Pressure variation along the moving surface of (a) the right bubble and (b) the left bubble for the mesh of fig. 1.9, at $t = 10^{-5}$, for $R_{gb} = 1$, $Oh^{-1} = 20$, $P_s = 28$, $\varepsilon = 1$, $D = 5$ and $R_\infty = 30$. 

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Moreover, when the transient problem is solved and the bubbles undergo large deformations, the mesh around the left bubble is highly distorted and several elements are quite skewed. This leads to inaccuracies in the solution and to the breaking down of the computations after a while. On the other hand, the mesh around the right bubble remains much less distorted and follows the bubble deformations nicely. An example of the mesh around quite distorted bubbles of equal radius with $Oh^{-1} = 6.5$ and $P_s = 1000$ is shown in fig. 1.11.

![Figure 1.11 Deformation of the mesh near the bubbles at $t = 0.3$ when the mapping of fig. 8 is used for $R_{a,b} = 1$, $Oh^{-1} = 6.5$, $P_s = 1000$, $\varepsilon = 1$, $D = 5$ and $R_\infty = 30$. For clarity we show rectangular elements only.](image)

All the above lead us to the conclusion that in order to obtain optimal results for this geometry, the mesh around the two bubbles must be particularly fine, the elements must remain close to orthogonal and equilateral triangles and, more importantly, both bubble surfaces must be individually discretized, so that the error on their poles is decreased as much as possible. This naturally leads to the requirement that the physical domain (see fig. 1.12) is decomposed into three parts: (a) one part around each bubble described by a separate spherical coordinate system with a center that coincides with the initial centroid of each bubble (parts A & B) and (b) a third part that will cover the rest of the domain with a center that coincides with the middle of the segment connecting the initial bubble centroids (part C), see fig. 1.12a. All parts are constructed separately using the elliptic grid generation equations.
(eq. (1.14) & (1.15)) defined on local spherical coordinate systems. At the final stage, the three sub-domains are reunited to form the original one.

**Figure 1.12** (a) Schematic of the decomposition of the physical domain into 3 parts, and the mapping to a computational \((\xi, \eta)\) domain of (b) Part A, (c) Part B and (d) Part C. The bubble surfaces are mapped onto the thicker line segments.

For constructing the meshes around the two bubbles (parts A & B), each physical sub-domain with local coordinates \((r, \theta)\) is mapped separately to a computational domain with \((\xi, \eta)\) coordinates. For both subdomains, the two segments from the line of symmetry are mapped to the left and the right boundary \(R_{bi} \leq \xi \leq L_i, \ i = A, B\) with \(\eta = 0\) or \(\eta = \pi\) corresponding to \(\theta = 0\) or \(\theta = \pi\), see fig 1.12b and 1.12c. Each bubble surface is mapped to the bottom boundary \(0 \leq \eta \leq \pi\) with \(\xi = R_{bi}\) \((i = A, B)\) so that the centre of mass of each bubble coincides with the origin of the local coordinate system. The extent of the subdomain around each bubble, which is also related to the initial distance between the two bubbles, is mapped to the top \(\xi = L_i\), where \(L_i\) is the radius of the outer spherical boundary of the part \(i\) and we take \(L_A = L_B\) always. Moreover, the location of the boundaries \(A_iC_2E_1\) and \(E_1D_1B_4\) in physical space is determined by two sets of equations: (a) up to a position that corresponds to
the local angle $0 \leq \theta \leq 3\pi/4$ for part A and to the local angle $\pi/4 \leq \theta \leq \pi$ for part B we impose the equation of a circle with a radius equal to the length $L_i$ of each part, (b) for the rest of each boundary, $OE_i$, we impose the equation of a straight line, see fig. 1.12a. The remaining degrees of freedom at all boundaries are used to distribute the nodes at equal distances, hence $w_1 = w_2 = 1$, along these boundaries through eq. (1.29) in a spherical coordinate system. Having constructed the mesh for parts A & B the location of the boundaries $A_iC_2E_i$ and $E_iD_2B_4$ and the nodes on them are used as input data for the boundary $A_4C_2E_4D_2B_4$ of part C. More specifically, first we define the third physical domain, C, to be a spherical shell with center at the middle of the distance between the centroids of the two bubbles, inner radius $L_c$ ($L_c = OA_4 = OB_4$) and outer radius equal to the radius where the far field boundary condition is applied, $R_\infty$. Then this physical domain is mapped to a computational domain with ($\xi, \eta$) coordinates that is bounded by the left and right boundaries $L_c \leq \xi \leq R_\infty$ at $\eta = 0$ or $\eta = \pi$ corresponding to line segments on the axis of symmetry, $A_4A_3$ and $B_4B_3$, respectively, while its inner and outer spherical surface correspond to $0 \leq \eta \leq \pi$ at $\xi = L_c$ or at $\xi = R_\infty$, see fig. 1.12d. Subsequently, the initial physical domain is constructed by the previously described continuation procedure. In particular, here the inner spherical surface is pulled towards the $A_4C_2E_4D_2B_4$ boundary in physical space. Simultaneously, the locations of the nodes, along the $\eta = \pi/2$ -line that corresponds to the line $E_1E_2$ are relocated according to:

$$
\frac{r_{si} - R_\infty}{\xi_{si} - R_\infty} = \frac{r_{s1} - R_\infty}{L_c - R_\infty}, \quad i = 1, 2, \ldots, N
$$

(1.44)

where $N$ is the total number of nodes along this $\eta$ -line, $r_{si}, \xi_{si}$ are the coordinates of node $i$ on it in physical and computational space, respectively and $r_{s1}$ is the radial coordinate of the first node on it that changes at each continuation step. For the degrees of freedom setting the locations of the nodes on all boundaries, eq. (1.29) with $w_1 = w_2 = 1$ is used. Moreover, for each computational domain eq. (1.30) is used as needed for concentrating the coordinate lines along the corresponding inner boundary $\xi = R_{hA}, R_{hB}$, or $L_c$, with an appropriate value of $\zeta$: usually $1.05 \leq \zeta \leq 1.2$. After the construction of the three individual domains, we construct the entire mesh by merging all 3 domains. This is also used as an initial state for the transient problem.
The discretization of the entire physical domain is presented in Fig. 1.13a, while a magnified view close to the bubbles is presented in Fig. 1.13b. Clearly, the mesh nodes are evenly distributed around both bubbles. Despite this fine discretization, it was soon realized that an even finer mesh is required close to the bubble surfaces, in order to compute the eigenvalues of bubble shape deformation to at least 3 significant digits. This highly sensitive computation is accomplished accurately without unnecessarily increasing the mesh where this is not needed, i.e. away from the bubbles, by following the mesh refinement technique described in section 1.3.1. In Fig. 1.13c a magnified view of the mesh in the vicinity of the two bubbles is given. Three refinement levels are used for higher local resolution of the flow. Details of the mesh around the pole of the right bubble are presented in Fig. 1.13d and verify the capability of the proposed method to generate nearly optimal grids.
Figure 1.13 Typical initial mesh for the bubble-bubble interaction problem (a) the entire domain, (b) a region around the bubbles with uniform mesh for the entire domain, (c) a region around the bubbles with a 3-level refinement around each bubble and (d) a region around the pole of the right bubble with 3-level refinement. In figures (a) and (b) only rectangular elements are shown for clarity.
In fig. 1.14a,b we present two unequal bubbles after they have undergone several volume oscillations and have translated towards each other, while in fig 1.15 we present only the right of two equal interacting bubbles. In both cases the liquid is taken to be water and the dimensionless parameters change in response to changes in the size of the bubbles. The combined volume and shape oscillation with bubble translation has resulted in large deformation especially of the right bubble in fig 1.14 and of both bubbles in the second case (fig. 1.15). In fact in the case of fig. 15, where the inverse Ohnesorge number is large, the bubbles become highly deformed and we are able to capture accurately a very fast moving jet that emanates from the bubble side which is away from the other bubble. Eventually this will pierce the bubble and will cause its collapse, a well known phenomenon. The dynamically adjusting mesh follows very nicely the jet and the swelling that appears in its head along with every other detail on the bubble surface. It is quite challenging to capture this interface with multiple folds of varying amplitude, even if it appeared in a single bubble. This example clearly shows the advantages of splitting the domain into subdomains which closely follow the local interfaces and the quasi-elliptic method for generating the mesh. Characteristic of the specific meshes will be described in the next section.
Figure 1.14 Deformation of the mesh when the mapping of fig. 1.12 is used. (a) a region around both bubbles, (b) a magnification around the right bubble at $t = 0.39$ for $R_{bb} = 0.5$, $Oh^{-1} = 85$, $P_s = 137$, $\varepsilon = 1$, $D = 3$ and $R_\infty = 30$.

Figure 1.15 Deformation of the mesh when the mapping of fig. 1.12 is used. The mesh is magnified around the right bubble and the left and right pole of the bubble at $t = 0.651$ for $R_{bb} = 1$, $Oh^{-1} = 270$, $P_s = 1375.51$, $\varepsilon = 0.3$, $D = 9.9$ and $R_\infty = 30$. 
There are several advantages of the above methodology for generating a mesh. More specifically, (i) the grid is structured with mesh lines remaining nearly orthogonal to the highly deforming boundaries which is essential to very accurately resolving the boundary conditions on these boundaries even at high values of fluid inertia or fluid elasticity; (ii) the grid is structured not only around the above regions where the solution exhibits rapid variation, but also in the entire domain, when it is well known that structured grids have better properties related with error distribution and propagation compared to unstructured ones (Jester and Kallinderis 2003; Kallinderis and Nakajima 1994); and (iii) during the transient simulations resulting in large domain deformations grid restructuring is not needed at all and variable interpolations are not required or kept to a minimum. All these benefits are essential in the case of a moving boundary problem because of the hyperbolic character of the kinematic condition, not to mention the hyperbolic character of the viscoelastic constitutive law. For this reason, a moving boundary problem is susceptible to artificial short wave instabilities, unless an optimal discretization technique is adopted. Therefore, using in this case a local orthogonal spherical coordinate system around each bubble, we can decrease the local errors and perform simulations for long times. The implementation is simple, and its specific steps for creating the initial mesh are described above. Subsequently, in order to perform the transient calculations we just replace the essential conditions on the moving boundaries \( r_s = R_{bh} \) and \( r_s = R_{bd} \), with the kinematic ones (eq. (1.13)) and follow the solution algorithm described in section 1.3.2.

It must be mentioned that our numerical experimentation showed that for the solution of the flow problem a global coordinate system can be safely used without introducing any numerical instability. This is also very convenient from a programming point of view, since no extra geometric transformations are necessary.

1.5 Numerical examples

1.5.1 Cavities inside a filament undergoing stretching

For simplicity, we assume that the two spherical bubbles are of equal radius \( R_{b1} = R_{b2} = 1 \), with their centers located symmetrically with respect to the middle plane of the filament at distances \( h_1 = 2 \) and \( h_2 = 7 \) from the lower disk, respectively. The ratio of the initial filament height to the bubble radius is \( H_o = 9 \), while the initial aspect ratio of the filament is \( \Lambda = H_o / R_{c0} = 2.25 \). The liquid that surrounds the two bubbles is viscoelastic with
\( De = 1, \ \varepsilon_{PTT} = 0.03 \) and \( \beta = 0.01 \). Since PSAs are materials with very high dynamic viscosities (close to \( 10^7 \text{Pas} \)), the resulting Reynolds number is practically zero.

The meshes used to discretize the liquid domain are constructed as discussed in section 1.4.1 and are denoted by U or M, indicating either a uniform or a locally refined mesh, respectively. For example mesh U1 consists of 960 triangular elements with 21 nodes around each bubble surface. More details about all the meshes that are used for this problem are given in Table 1.1. In Fig. 1.16 we show three snapshots of the filament and the bubbles inside it at times \( t = 0, t = 5 \) and \( t = 11.5 \).

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Number of radial elements before refinement</th>
<th>Number of axial elements before refinement</th>
<th>Number of triangles after refinement (if used)</th>
<th>Number of nodes on free surface after refinement</th>
<th>( \Delta r ) around the free surface after refinement</th>
<th>( \Delta z ) around the free surface after refinement</th>
</tr>
</thead>
<tbody>
<tr>
<td>U1</td>
<td>10</td>
<td>48</td>
<td>960</td>
<td>21</td>
<td>0.2</td>
<td>0.314</td>
</tr>
<tr>
<td>U2</td>
<td>80</td>
<td>84</td>
<td>61440</td>
<td>161</td>
<td>0.025</td>
<td>0.04</td>
</tr>
<tr>
<td>M1</td>
<td>10</td>
<td>48</td>
<td>5664</td>
<td>161</td>
<td>0.025</td>
<td>0.04</td>
</tr>
<tr>
<td>M2</td>
<td>14</td>
<td>64</td>
<td>10752</td>
<td>225</td>
<td>0.018</td>
<td>0.028</td>
</tr>
</tbody>
</table>

Table 1.1 Characteristics of the meshes used in the filament stretching problem. Triple local refinement has been performed for the M family of meshes around the bubble surface at the locations: \( \xi = R_c / 20, R_c / 10, R_c / 5 \) and single local refinement has been performed along the filament free surface in the range: \( 0.9R_c \leq \xi \leq R_c \).

The bubbles remain symmetric with respect to the mid-plane of the filament at all times. The mesh U1 is depicted here. Although this mesh is satisfactory for the relatively small initial deformations of the filament, at longer times and larger deformations non physical angles appear at the surfaces of the bubbles and particularly at their poles closer to each disk. Clearly, more nodes are needed in order to describe accurately the highly deforming bubble surfaces. However, despite the coarse discretization, no remeshing techniques are required and even larger deformations of the domain boundaries can be followed. In order to increase the accuracy of the computations, one option is to increase the number of triangular elements throughout the domain to, for example, 61440 and the number of nodes along each bubble surface to 161. This is mesh U2. Now the surfaces of the bubbles are captured very
satisfactorily even after they are highly deformed, but the computational time increases to prohibitive levels.

![Deformations of the mesh U1 with a uniform tessellation of $10 \times 48$ 1D dimensional elements in the radial and axial direction, respectively, at times (a) $t = 0.0$, (b) $t = 5.0$ and (c) $t = 11.5$. The dimensionless parameters are $De = 1$, $Re = 0$, $Ca = 10$, $\varepsilon_{PTT} = 0.03$, $\beta = 0.01$, $\Lambda = 2.25$, $H_0 = 9$, $R_{h_1} = R_{h_2} = 1$, $h_1 = 2$ and $h_2 = 7$.]

More specifically using 960 triangular elements the simulation requires almost 5 hours in order to reach the same final time of $t = 11.5$, while using 61440 elements the simulation takes almost 10 days. In order to reduce the memory requirements and simultaneously the computational time, while keeping the same accuracy in the calculations, we applied the local refinement technique described in section 1.3.1. Here the local refinement was performed in one direction only, the radial one, resulting in unnecessarily finer mesh all along the axis of symmetry. Also three grading levels were introduced around the axis of symmetry and each
bubble surface and a single grading level along the liquid-surrounding air interface. The number of the nodes along each bubble surface is retained at 161. However, the total number of the triangular elements decreases significantly from that in mesh U2 to 5664 (mesh M1). The resulting decrease in the CPU time is impressive, since the simulation in this case takes almost 12 hours to reach the same final time. If the local refinement was performed in both the radial and the axial directions around the bubbles surfaces only, the reduction in both memory requirements and computation time would have been even larger. In Fig. 1.17 we show snapshots of mesh M1 at times $t = 0$, $t = 5$ and $t = 11.5$, while in Fig. 1.18 we show a magnified view around the top and the bottom of the upper bubble at two different times, $t = 5$ and $t = 11.5$, for the same mesh, M1. From these figures we can clearly observe that the mesh remains very uniform around the bubble and that its skewness is reasonably restricted. In an even closer view around the bottom of the upper bubble (fig. 1.18c3), one can observe the inception of a cusp at the bubble pole. This is similar to the well documented inverted teardrop shape that a bubble assumes when it rises in a viscoelastic liquid (Bird et al. 1987).

Figure 1.17 Deformation of the mesh M1 for the flow and geometric parameters and times of figure 1.15 with triple local refinement around the bubble surfaces, $\xi \leq R_{c,\sigma} / 20$, $R_{c,\sigma} / 10$, $R_{c,\sigma} / 5$, and single along the liquid one, $0.9R_{c,\sigma} \leq \xi \leq R_{c,\sigma}$.
Figure 1.18 Details of the mesh of fig. 1.17(b) (b1, b2) and fig. 1.17(c) (c1, c2, c3), around the top and the bottom of the upper bubble in the left and the right part of the figure respectively.
Fig. 1.19 shows the evolution of the pressure, $P$, and components of the stress tensor, $\tau_p$, with time at the points on the bubble surface that are most critical for determining the accuracy of the calculations, i.e. the poles and the equatorial plane of the bubble, for four different meshes: U1, U2, M1, and M2. The model parameters are those already mentioned before. The results are given for one of the two bubbles, the upper one, because of the symmetry of the problem. Fig. 19a shows the pressure, $P$, and the stress tensors, $\tau_{\theta\theta,p}$, $\tau_{rz,p}$, and $\tau_{zz,p}$ for the north pole of this bubble. We can see that convergence of the results depends critically on the discretization on the free surface. Indeed meshes U2 and M1, where the discretization of the free surface is exactly the same, give identical and converged results, while using the finer mesh M2 does not offer higher accuracy at least in the scale shown in these figures, although computing with this mesh is more expensive. This means that using either a coarser mesh than M1 away from the bubbles, or a finer mesh than M1 on the bubbles surfaces does not affect the solution. In contrast, when the coarsest uniform mesh U1 is used, the solution shows a continuously increasing deviation from the solutions obtained with the other three meshes. Similar is the conclusion by examining the evolution of the solution for the pressure $P$ and the stress components $\tau_{zz,p}$, $\tau_{rz,p}$, and $\tau_{rr,p}$, at the south pole of the bubble (Fig. 1.19b). While the results for the denser meshes (M1, M2 and U2) are in very good agreement, except close to the end of the calculations, the solution for the coarser mesh U1 differs from early on. The elements on the free surface of this mesh, given in fig. 1.16, are not enough to accurately describe its large deformations at longer times. In other words, at short times where no significant deformation of the bubble occurs, the solution with mesh U1 is in agreement with the solutions with the finer meshes. As time increases and the deformations become significant, the solution with this mesh deviates and when the bubble forms a cusp at the south pole only the finest mesh on its surface remains accurate. In contrast with the upper and the lower pole of the bubble, the solution at the equatorial plane (Fig. 1.19c) seems not to be affected by the mesh as much. Indeed, the deformations at the equatorial plane are smoother and even the coarsest mesh is sufficient to describe accurately the free surface there.
(a)

(b)
Figure 1.19 Evolution with time of (a) $P$, $\tau_{\theta\theta, p}$, $\tau_{rz, p}$, $\tau_{zz, p}$ for the upper pole of the upper bubble, (b) $P$, $\tau_{zz, p}$, $\tau_{rz, p}$, $\tau_{rr, p}$ of the lower pole of the upper bubble and (c) $u_z$, $u_r$, $\tau_{rr, p}$, $\tau_{rz, p}$ of a point near the equatorial plane of the upper bubble for the indicated meshes. The dimensionless parameters are those in fig. 1.16.

Fig 1.20 presents contour plots of the velocities, the pressure and the stress components at $t = 5.0$, obtained with mesh M1. We observe that all the contour lines are smooth and no ‘wiggles’ appear anywhere. We can also observe that all profiles are symmetric with respect to the instantaneous mid-plane of the filament, except of course for the velocity $U_z$. This velocity component takes its highest values at the upper disk, which is the one that causes the entire motion and deformation, while it takes zero values at the lower disk which remains motionless.
1.5.2 Interacting bubbles in an infinite domain

Having generated the entire mesh by uniting the three parts of the domain, it is easier to use cylindrical coordinates to write the governing equations in each node. In this way, the following two tests have been performed.

1.5.2.1 Calculation of the eigenvalues of the system

Perhaps the most demanding and strict tests to determine the accuracy of the simulations for this problem is to examine the convergence with mesh refinement of the eigenvalues of the corresponding free boundary problem. This is readily achieved by assuming that initially no flow exists and the bubbles are spherical due to capillarity and, then, subjecting all the flow variables including the bubble shapes to an infinitesimal disturbance. In addition to convergence with mesh refinement, we can compare our predictions with the analytically obtained eigenvalues for an isolated bubble surrounded by a viscous liquid, which have been reported by Miller and Scriven (1968). To this end, we only

Figure 1.20 Contours of (a) $u_r$, (b) $u_z$, (c) $P$, (d) $\tau_{rr,p}$, (e) $\tau_{rz,p}$, (f) $\tau_{zz,p}$, (g) $\tau_{\theta\theta,p}$ at $t = 5.0$ for the dimensionless parameters of fig. 1.16.
need to position the two bubbles as far apart as allowed by our current hardware/software configuration.

More specifically, the normal modes of the system are computed by assuming that all variables are split into their base values and a small disturbance.

\[
\begin{bmatrix}
    u(r,z,\theta,t) \\
    P(r,z,\theta,t) \\
    P_{gb}(r,z,\theta,t) \\
    x(r,z,\theta,t)
\end{bmatrix}
= \begin{bmatrix}
    u_b(r,z) \\
    P_b(r,z) \\
    P_{gb}(r,z) \\
    x_b(r,z)
\end{bmatrix}
+ \delta \begin{bmatrix}
    u_p(r,z) \\
    P_p(r,z) \\
    P_{gb}(r,z) \\
    x_p(r,z)
\end{bmatrix} e^{\omega t}
\]  

(1.45)

where the new subscripts \( b \) and \( p \) indicate the equilibrium (base) state and the perturbed one, respectively, \( \delta \ll 1 \) is the amplitude of the infinitesimal disturbance and \( x \) denotes the position vector of the mesh nodes. As noted in Carvalho and Scriven (1999), by invoking the domain perturbation approach only the positions of nodes on the free surfaces need to be perturbed as part of the overall disturbance. This is achieved by setting the domain perturbation to:

\[
x_p = H^{(0)}(x_b) h' n
\]  

(1.46)

where \( n \) is the unit normal to the unperturbed boundary, \( h' \) is a scalar function related to the amplitude of the perturbation for the mesh nodes and \( H^{(0)} \) is the Heaviside function:

\[
H^{(0)}(x_b) = \begin{cases} 
1, & x_b \in \Gamma \\
0, & x_b \in \Omega
\end{cases}
\]  

(1.47)

Thus \( H^{(0)}(x_b) \) vanishes inside the unperturbed liquid domain, whereas it is equal to one on its boundaries, allowing only the nodes at the moving boundary to be displaced as determined by \( h' \).

Substituting expressions (1.45) into the governing equations, including the kinematic equation (1.13) and the equation of state that describes the pressure inside the bubble (1.11), and neglecting terms of order higher than linear in the perturbation parameter, \( \delta \), we obtain a generalized eigenvalue problem of the form:

\[
\mathbf{J} \mathbf{Y} = \omega \mathbf{M} \mathbf{Y}
\]  

(1.48)

where \( \mathbf{J} \) is the Jacobian matrix, \( \mathbf{M} \) is the mass matrix, \( \omega \) are the eigenvalues and \( \mathbf{Y} \) the corresponding eigenvectors. In order to solve the eigenvalue problem, we used the Arnoldi method as it is implemented in the Arpack library (Lehoucq et al. 1998). This method is capable of iteratively computing a relatively small fraction of the entire spectrum of eigenvalues and in particular those that have the largest magnitude. Since we are interested in
enhancing convergence to a specific portion of the spectrum and in order to limit the fraction of the eigenvalues to be computed each time, we used the shift-and-invert transformation:

\[(J - \lambda M)^{-1}MY = \nu Y, \quad \text{where} \quad \nu = \frac{1}{c - \lambda}.\]  

(1.49)

This transformation is efficient because not only it turns the generalized eigenvalue problem into a simple one but also it computes the eigenvalues that are closer to the user-provided complex number \(\lambda\), since the eigenvalues \(\nu\) of eq. (1.49) that are largest in magnitude correspond to the eigenvalues \(c\) of the original problem that are nearest to the shift constant \(\lambda\) in absolute value. The accuracy of the converged eigenpairs is checked independently by evaluating a-posteriori the residual \(|JY_n - cMY_n|\).

The computed eigenvalues are compared with those that arise from the analytical solution of Miller and Scriven (1968) for individual bubbles which gives the eigenvalues \(c\) by the implicit expression:

\[
c^2 = \frac{1 + 2}{\omega^2} \left[ \frac{(2l + 1)\omega^2 R_{\nu}^2 - 2(l - 1)(l + 1)(2l + 1 - \omega^2 R_{\nu}^2 Q_{l+1/2}^{H})}{2l + 1 - \omega^2 R_{\nu}^2 Q_{l+1/2}^{H} + \omega^2 R_{\nu}^2 / 2} \right] - 1, \quad i = A, B, \quad l = 2, 3, \ldots \]  

(1.50)

where \(\omega^2 = \left(c^* \rho^* / \mu^* \right)^{1/2}\) and \(c^* = \left(\sigma^* (l + 1)(l - 1)(l + 2) / R_{\nu}^3 \rho^* \right)^{1/2}\) is the frequency of oscillation, if the liquid is assumed to be inviscid and the gas in the bubble does not contribute to the dynamics of the problem, as we have already assumed. In these expressions, \(l\) corresponds to the index of the Legendre polynomial characterizing the shape of the bubble. The analytical solution does not apply for volume oscillations of the bubble \((l = 0)\) or bubble translation \((l = 1)\). The real part, \(c_R\), of \(c\) is the amplification or decay factor, the imaginary part, \(c_I\), is the angular frequency and \(Q_{l+1/2}^{H} = \frac{H_{l+1/2}^{(1)}(\omega^2 R_{\nu}^2)}{H_{l+1/2}^{(1)}(\omega^2 R_{\nu}^2)}\); \(H_{l+1/2}^{(1)}\), \(H_{l+1/2}^{(1)}\) are the half-integral-order Hankel functions of first kind. The oscillation frequency and decay factor are obtained numerically assuming the value of the Ohnesorge number and properties of water at 25°C and atmospheric pressure by solving eq. (1.50) using standard software.

The eigenvalue problem required 12-24 hours to complete, depending on the flow parameters, before the local refinement technique was introduced, while it required only \(1/2\)-1 hours following this procedure. In addition, the maximum number of nodes that could be used
before the local refinement with our current hardware, was up to 150 along each bubble surface due to the high computational cost, and the requirement of a gradual coarsening of the mesh away from the bubbles resulting in a total of 36720 triangles. On the contrary up to 2250 nodes along each free surface can be used after the local refinement increasing the accuracy of our computations, as discussed below. Table 1.2 presents the characteristics of the meshes that we used. Only in the M family of meshes three levels of local refinement have been introduced near the bubble surfaces as detailed in the table. Special attention has been paid so that the aspect ratio of the elements near the bubbles does not deviate from unity significantly. This can be seen in the minimum values of their sides in the r- and z-directions (in a cylindrical coordinate system). The reduction of both these values near the bubbles through local mesh refinement is noteworthy.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Part A or B (radial, azimuthal) elements before refinement</th>
<th>Part C (radial, azimuthal) elements before refinement</th>
<th>Number of triangles after refinement (if used)</th>
<th>Number of nodes on free surface after refinement</th>
<th>$\Delta r_{\text{min}}$ around the free surface after refinement</th>
<th>$\Delta z_{\text{min}}$ around the free surface after refinement</th>
</tr>
</thead>
<tbody>
<tr>
<td>U3</td>
<td>(120,72)</td>
<td>(10,108)</td>
<td>36720</td>
<td>145</td>
<td>0.044</td>
<td>0.004</td>
</tr>
<tr>
<td>M3</td>
<td>(37,40)</td>
<td>(10,60)</td>
<td>15360</td>
<td>641</td>
<td>0.01</td>
<td>0.002</td>
</tr>
<tr>
<td>M4</td>
<td>(37,80)</td>
<td>(10,120)</td>
<td>30720</td>
<td>1281</td>
<td>0.005</td>
<td>0.002</td>
</tr>
<tr>
<td>M5</td>
<td>(37,140)</td>
<td>(10,210)</td>
<td>53760</td>
<td>2241</td>
<td>0.003</td>
<td>0.002</td>
</tr>
<tr>
<td>U4</td>
<td>(14,72)</td>
<td>(100,108)</td>
<td>25632</td>
<td>145</td>
<td>0.044</td>
<td>0.063</td>
</tr>
<tr>
<td>M6</td>
<td>(16,24)</td>
<td>(50,36)</td>
<td>9792</td>
<td>385</td>
<td>0.016</td>
<td>0.004</td>
</tr>
<tr>
<td>M7</td>
<td>(16,40)</td>
<td>(50,60)</td>
<td>16320</td>
<td>641</td>
<td>0.010</td>
<td>0.004</td>
</tr>
</tbody>
</table>

Table 1.2 Characteristics of the meshes used for the bubbles in an acoustic field problem. Local refinement has been used for the M family of meshes only. In meshes M3-M5 a three-level local refinement has been used around each bubble surface at the following distances in the computational domain: $R_{hi} \leq \xi \leq 1.008R_{hi}$, $1.008R_{hi} \leq \xi \leq 1.026R_{hi}$, $1.026R_{hi} \leq \xi \leq 1.036R_{hi}$, while in meshes M6-M7 the three levels of refinement were introduced at: $R_{hi} \leq \xi \leq 1.014R_{hi}$, $1.014R_{hi} \leq \xi \leq 1.029R_{hi}$, $1.029R_{hi} \leq \xi \leq 1.039R_{hi}$.
\(Oh^{-1}(= Re) = 5\)

<table>
<thead>
<tr>
<th>l</th>
<th>Miller &amp; Scriven</th>
<th>M3</th>
<th>M4</th>
<th>M5</th>
<th>U3</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.5252 ± 1.9697i</td>
<td>1.5344 ± 1.9918i</td>
<td>1.5298 ± 1.9807i</td>
<td>1.5278 ± 1.9760i</td>
<td>1.5648 ± 2.0674i</td>
</tr>
<tr>
<td>3</td>
<td>2.7030 ± 3.7877i</td>
<td>2.7092 ± 3.8040i</td>
<td>2.7061 ± 3.7958i</td>
<td>2.7047 ± 3.7923i</td>
<td>2.7301 ± 3.8599i</td>
</tr>
<tr>
<td>4</td>
<td>4.0400 ± 5.6620i</td>
<td>4.0452 ± 5.6754i</td>
<td>4.0426 ± 5.6687i</td>
<td>4.0415 ± 5.6658i</td>
<td>4.0625 ± 5.7214i</td>
</tr>
<tr>
<td>5</td>
<td>5.5513 ± 7.6212i</td>
<td>5.5560 ± 7.6326i</td>
<td>5.5536 ± 7.6270i</td>
<td>5.5526 ± 7.6245i</td>
<td>5.5712 ± 7.6723i</td>
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</tbody>
</table>

\(Oh^{-1}(= Re) = 20\)

<table>
<thead>
<tr>
<th>l</th>
<th>Miller &amp; Scriven</th>
<th>M3</th>
<th>M4</th>
<th>M5</th>
<th>U3</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.7252 ± 3.2205i</td>
<td>0.7288 ± 3.3094i</td>
<td>0.7270 ± 3.2652i</td>
<td>0.7262 ± 3.2461i</td>
<td>0.7389 ± 3.5996i</td>
</tr>
<tr>
<td>3</td>
<td>1.2677 ± 5.8998i</td>
<td>1.2704 ± 5.9661i</td>
<td>1.2690 ± 5.9330i</td>
<td>1.2685 ± 5.9188i</td>
<td>1.2786 ± 6.1887i</td>
</tr>
<tr>
<td>4</td>
<td>1.9367 ± 8.8197i</td>
<td>1.9392 ± 8.8755i</td>
<td>1.9379 ± 8.8476i</td>
<td>1.9374 ± 8.8356i</td>
<td>1.9468 ± 9.0642i</td>
</tr>
<tr>
<td>5</td>
<td>2.7302 ± 11.9906i</td>
<td>2.7328 ± 12.0400i</td>
<td>2.7314 ± 12.0153i</td>
<td>2.7308 ± 12.0047i</td>
<td>2.7401 ± 12.2070i</td>
</tr>
</tbody>
</table>

\(Oh^{-1}(= Re) = 40\)

<table>
<thead>
<tr>
<th>l</th>
<th>Miller &amp; Scriven</th>
<th>M3</th>
<th>M4</th>
<th>M5</th>
<th>U3</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.4041 ± 3.3754i</td>
<td>0.4074 ± 3.6618i</td>
<td>0.4061 ± 3.5214i</td>
<td>0.4053 ± 3.4596i</td>
<td>0.4145 ± 4.5098i</td>
</tr>
<tr>
<td>3</td>
<td>0.7074 ± 6.1694i</td>
<td>0.7102 ± 6.3867i</td>
<td>0.7088 ± 6.2789i</td>
<td>0.7082 ± 6.2322i</td>
<td>0.7173 ± 7.0828i</td>
</tr>
<tr>
<td>4</td>
<td>1.0857 ± 9.2425i</td>
<td>1.0885 ± 9.4262i</td>
<td>1.0870 ± 9.3347i</td>
<td>1.0864 ± 9.2953i</td>
<td>1.0957 ± 10.0309i</td>
</tr>
<tr>
<td>5</td>
<td>1.5384 ± 12.6049i</td>
<td>1.5414 ± 12.7676i</td>
<td>1.5398 ± 12.6864i</td>
<td>1.5392 ± 12.6515i</td>
<td>1.5487 ± 13.3088i</td>
</tr>
</tbody>
</table>

Table 1.3 Comparison of eigenvalues derived either semi-analytically [62] or numerically with the indicated meshes, for an isolated bubble at various \(Oh^{-1}\) numbers (\(D = 17, R_\infty = 30\)).

Table 1.3 summarizes the computed eigenvalues for bubbles of equal size, \(R_{s2} = 1\), at a relatively large distance between their centers \(D = 17\), when the far field boundary is taken at \(R_\infty = 30\). We have verified that neither one of the two latter parameter values affect the computed eigenvalues by increasing the distance to \(D = 24\) and the boundary location to \(R_\infty = 45\). Results with one relatively uniform mesh, U3, and three meshes with local refinement, M3-M5, are given, for various values of \(Oh^{-1}\), which plays the role of a Reynolds
number for this problem. In the same table the semi-analytically calculated eigenvalues using eq. 50 for individual bubbles are also given. Clearly the very expensive calculations with the U3 mesh result in the least accurate values, whereas even the coarsest of the M family of meshes, M3, results in values closer to the semi-analytical ones for all values of $O\text{h}^{-1}$ numbers and all modes. Increasing the nodes on the free surface, the numerically computed eigenvalues tend monotonically to the semi-analytical ones. Even the higher eigenmodes, that involve larger contributions from higher Legendre polynomials and larger interfacial deformations, which should have been computed less accurately, are in very good agreement with the theoretical eigenvalues. On the other hand, the higher the $O\text{h}^{-1}$ number is, the lower the accuracy of the computed eigenvalues. This should have been anticipated since increasing $O\text{h}^{-1}$, increases the inertial over the viscous forces producing a sharper boundary layer around each bubble, which requires an even finer mesh to capture accurately the eigensolution. We also performed tests for the aspect ratio of the elements around the free surfaces. It is found that when all the elements around the free surface have the same or quite the same aspect ratio higher accuracy is achieved. This remark may explain the variation between eigenvalues resulting from the analytical expression and numerically computed ones. In our mesh the aspect ratio of the elements located between the two bubbles is smaller than unity whereas those located at their other poles are larger than unity.

Fig. 1.21 shows the relative error of each numerically computed eigenvalue with respect to each analytical counterpart in logarithmic scales. Clearly for all modes, there is a linear decrease of the error as the number of surface elements increase. On the contrary, the error does not depend in such a simple manner on the number of total nodes or elements, verifying that the number of surface elements is the most crucial factor for this computation. It is noteworthy that in all cases we have computed the inner product of the eigenvector for the modes $l = 2, 3, 4, 5$ with Legendre polynomials of various degrees and found that each eigenvector contained only the Legendre polynomial of degree 2, 3, 4, 5, correspondingly, testifying once more to the accuracy of the present calculations.
Figure 1.21 Relative error of each numerically computed eigenvalue with respect to its semi-analytical counterpart for meshes U3, M3, M4 and M5 and for $Oh^{-1} = 20$.

1.5.2.2 Transient simulations

Fig. 1.22, presents snapshots of the mesh around the bubbles at three different times: (a) $t = 0.28$, (b) $t = 0.4$ and (c) $t = 0.66$, and for two different meshes. At the left column of snapshots in Fig. 1.22 the mesh is finer near the bubble surfaces and becomes coarser slowly away from them (mesh U4 in Table 1.2). The total number of triangular elements is 25632, which corresponds to 220163 unknowns, while the number of nodes along each bubble surface is only 145. At the right column of snapshots in Fig. 1.22 the mesh in addition contains a three level refinement around the bubbles (mesh M6 in Table 1.2). The total number of triangular elements is smaller 9792 which correspond to less 85991 unknowns, whereas the number of nodes along each bubble interface is much higher 385. The two bubbles are equal, $R_{b_2} = 1$, their dimensionless initial distance is set to $D = 2.8$, which allows us to use a generally less refined mesh compared to that in the eigenvalue computations, and the outer boundary is $R_\infty = 30$. Moreover, the dimensionless static pressure, $P_s$, is equal to 100. As initial disturbance a step change in pressure at the far-field is applied, with $\varepsilon = 1$ increasing the far field pressure by a factor of 2. The two bubbles undergo volume oscillations and simultaneously approach each other with time, as expected, since they oscillate in phase and attractive forces develop (Bjerknes 1906, 1909; Pelekasis and Tsamopoulos 1993a). From
Fig. 1.22 we can see that when local refinement is used, the mesh remains dense around the two bubbles until the end of the simulations. On the other hand when no local refinement used and as time passes the elements are deformed near the poles of the bubbles, with quite large and small aspect ratios between the two bubbles and away from it, respectively. If the simulations were allowed to continue further, remeshing would have been required.

Figure 1.22 Snapshots of the mesh around the two bubbles when the uniform mesh, U4, is used (left column) and when 3-level refinement mesh, M6, is used (right column) at (a) \( t = 0.28 \), (b) \( t = 0.4 \) and (c) \( t = 0.66 \). Dimensionless parameters are \( R_{bb} = 1 \), \( Oh^{-1} = 10 \), \( P_s = 100 \), \( \varepsilon = 1 \), \( D = 2.8 \) and \( R_\infty = 30 \). For mesh U4 only rectangular elements are shown.
Figure 1.23 Time evolution of the coefficients of the Legendre modes (a) $P_0$ and (b) $P_2$ for the decomposition of the left bubble interface, for three different meshes, U4, M6 and M7. Dimensionless parameters are those of fig. 1.22.
One way to examine closer the accuracy of the present dynamic computations, it is to decompose the bubble surface into Legendre modes. These are computed with respect to a spherical coordinate system with its origin located at the instantaneous centre of mass of each bubble. The Legendre coefficients of each mode are computed as follows:

\[ C_l = \int F_{si}(\theta)P_l(\theta)\sin(\theta)d\theta, \quad i = A, B; \quad l = 0, 1, 2, 3... \]  

(1.51)

where \( F_{si} \) is position of the interface of the \( i \) bubble. Then, it may be seen that the dominant modes for this case are those that correspond to the Legendre polynomials of degree zero and two. Fig 1.23 shows the time evolution of the coefficient, \( C_0 \) (Fig. 1.23a), of the zeroth degree Legendre polynomial, \( P_0 \), that is associated with volume oscillations, and the coefficient, \( C_2 \) (Fig. 1.23b), of the second degree Legendre polynomial, \( P_2 \), for the same parameters that we mentioned earlier. Positive values of the coefficient \( C_2 \) correspond to prolate bubble shapes (elongated along the axis of symmetry) whereas negative values to oblate bubble shapes (flattened at the bubble poles). Hence the bubble initially oscillates retaining a prolate shape, whereas at later times it attains both prolate and oblate shapes and finally only oblate shapes, since then the bubbles have approached and flattened each other considerably. These coefficients are compared for 3 different meshes, U4, M6 and M7; where U4 stands for a slowly graded mesh (without local refinement), while in meshes M6 and M7, 3 levels of refinement are used around the bubble surfaces. As can be seen in Fig. 1.23, both coefficients calculated with the U4 mesh deviate with time from those calculated with the other two meshes indicating that a very fine mesh around the bubble surfaces is indeed required in order to solve accurately this problem for longer times.

In Table 1.4, we give the relative error in pressure, the most sensitive of the variables computed in Newtonian fluids, at three positions on the surface of the left bubble (near its 2 poles and its equatorial plane) for meshes U4 and M6 with respect to the values obtained with mesh M7, at 3 different times. As previously, the finer the mesh around the two bubbles is the more accurate the calculated pressure is. More precisely, the relative error in pressure for the mesh U3 at \( t = 0.28 \) is \( \sim 1.3\% \) and increases up to \( \sim 8.5\% \) at \( t = 0.66 \) when the bubble has deformed appreciably. On the contrary, the relative error for the mesh M6 starts with \( \sim 0.1\% \) at \( t = 0.28 \) and does not exceed \( \sim 0.8\% \) at the end of the simulations. In addition to the larger error, the smoothly varying mesh here has a larger number of elements distributed throughout the domain around the bubbles, which necessitates fewer elements adjacent to the free surfaces in order to keep the computational cost at a reasonable level. This is exactly what the
local mesh refinement achieves, more elements on the highly deforming, free surfaces, where they are needed the most for higher accuracy in the calculations, and fewer elements away from them to the point that the total number of elements is smaller. The required computation times on a single node of our quad xeon machine are almost 2 weeks using the U4 mesh as opposed to 2 and 6 days for the M6 and M7 meshes, respectively.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>$z$</th>
<th>error (%)</th>
</tr>
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<tbody>
<tr>
<td>U3</td>
<td>−2.0</td>
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</tr>
<tr>
<td>M6</td>
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</tr>
<tr>
<td>U3</td>
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<tr>
<td>M6</td>
<td>−1.2</td>
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</tr>
<tr>
<td>M6</td>
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<td>0.16</td>
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$t = 0.28$

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<tbody>
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<td>U3</td>
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<td>4.72</td>
</tr>
<tr>
<td>M6</td>
<td>−2.0</td>
<td>0.23</td>
</tr>
<tr>
<td>U3</td>
<td>−1.2</td>
<td>4.82</td>
</tr>
<tr>
<td>M6</td>
<td>−1.2</td>
<td>0.25</td>
</tr>
<tr>
<td>U3</td>
<td>−0.4</td>
<td>4.84</td>
</tr>
<tr>
<td>M6</td>
<td>−0.4</td>
<td>0.25</td>
</tr>
</tbody>
</table>

$t = 0.4$

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<th>error (%)</th>
</tr>
</thead>
<tbody>
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<td>U3</td>
<td>−2.0</td>
<td>4.72</td>
</tr>
<tr>
<td>M6</td>
<td>−2.0</td>
<td>0.23</td>
</tr>
<tr>
<td>U3</td>
<td>−1.2</td>
<td>4.82</td>
</tr>
<tr>
<td>M6</td>
<td>−1.2</td>
<td>0.25</td>
</tr>
<tr>
<td>U3</td>
<td>−0.4</td>
<td>4.84</td>
</tr>
<tr>
<td>M6</td>
<td>−0.4</td>
<td>0.25</td>
</tr>
</tbody>
</table>

$t = 0.66$

<table>
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</tr>
<tr>
<td>M6</td>
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<td>0.72</td>
</tr>
</tbody>
</table>

Table 1.4 Relative error of the pressure at three different positions (around the poles and the equatorial plane) on the free surface of the left bubble at three different times:

$$error = \left| \frac{P_{z \text{, mesh}} - P_{z \text{, M7}}}{P_{z \text{, M7}}} \right|$$

Fig. 1.24 presents contour plots of both velocity components and the pressure at $t = 0.66$. The results are given in spherical coordinates with center located at the middle of the distance between the initial centroids of the two bubbles. The mesh used is M7 and no
remeshing is needed until the end of the simulation. The radial velocity, Fig. 1.24a (upper half), takes the highest and positive values between the two bubbles, while it takes negative values at the rear side of the bubbles. This velocity distribution indicates that the bubbles are contracting and approaching each other at this time instant, squeezing fluid away from the gap between them. If Stokes flow prevailed, the radial velocity should drop like \( \sim r^{-1} \) away from the bubbles. In the upper half of Fig. 1.24a we can see that it decreases with the radial distance, but does not exactly follow this rule, since the inverse Ohnesorge number is not small. The azimuthal velocity field, Fig. 1.24a (lower half), is symmetric with respect to \( \theta = \pi/2 \), because the two bubbles are equal and undergo in-phase oscillations. In agreement with the picture about the radial velocity, the azimuthal velocity takes negative values around the left bubble and positive values around the right bubble around their equators, but changes sign at their poles facing away from each bubble. It also takes zero values at \( \theta = 0 \), \( \theta = \pi \) and \( \theta = \pi/2 \), as it should. Finally the pressure field, Fig. 1.24b, attains radial symmetry not too far from the bubbles, verifying again that our choice to locate the outer boundary at \( R_\infty = 30 \) is a conservative one for this configuration. As can be seen in Fig. 1.24 the main changes in the velocity and pressure fields occur around and close to the two bubbles, explaining once more the need for a very fine mesh in that region and not in the area away from them.
1.6 Conclusions

The elliptic grid generator scheme proposed by Dimakopoulos and Tsamopoulos (2003a) has been successfully extended to problems where domains with inclusions are involved, the interfaces undergo large deformations and hyperbolic equations must be solved. Depending on the geometry, it has been found that the entire fluid domain can be either mapped onto a single computational domain or it must be divided into subdomains in order to generate the most suitable mesh. The initial mesh is generated by continuation techniques. The fluid problem is always solved in the entire domain and does not require restructuring and interpolation of the variables in a new mesh in order that the simulations retain their high accuracy. For optimizing the quality of the mesh, constraints (e.g. generalized node distributions) along specific surfaces of the geometry were imposed, alleviating in this way the stiffening of the scheme when exponential attractive terms are used in the elliptic equations (Dimakopoulos and Tsamopoulos 2003a, 2007). Another improvement that was incorporated herein is a local refinement algorithm, for increasing the resolution of the mesh along the free surfaces while keeping the computation cost as a low as possible.
The proposed schemes was tested in two highly demanding problems with free surfaces and complex geometries: (a) bubble growth in viscoelastic filaments undergoing stretching where a single domain with multiple mappings suffice and (b) interacting bubbles in a viscous medium, where splitting into subdomains and multiple mappings are necessary. In our first application the mesh is generated by enforcing the node distribution along lines passing through the singular points of the domain. In essence, these lines play the role of internal pseudo-boundaries, but the domain is not actually decomposed for generating the mesh. This approach may not always work as demonstrated by a couple of examples in our second application making the second method indispensable. This is based on decomposition of the physical domain to subdomains defined in local, even different, but most appropriate for each subdomain coordinate systems, while the flow equations are written in the entire domain. This method is the most powerful and general and we believe that it can be applied in any 3D problem. In both cases, we managed to reduce the memory requirements up to 30% and the computational time up to 80% by applying the local refinement method around the deforming interfaces for achieving accuracy similar with or higher than that of the finest mesh without local refinement. Despite the large deformation of the fluid volume, the accuracy of the calculations remained high throughout the simulations, and no remeshing was performed. Although the boundaries of the physical domain have actually moved a lot, the mesh generated by our quasi-elliptic method in the time independent computational domain does not need to be readjusted. This is important in order to decrease numerically induced instabilities, numerical diffusion and perform numerical simulations even with viscoelastic fluids.

Currently, we are working on the extension of this methodology to 3D domains. In this case, for example, the motion and deformation of multiply bubbles away from the axis of symmetry can be computed and the applications studied here or others, such as the dynamics of emulsions in flow, growth of cavitating bubbles behind hydrofoils can be accurately simulated. Certainly then, this methodology would have a greater impact.
CHAPTER 2

Viscous Effects On Two Interacting And Deformable Bubbles Under A Step Change In Pressure

2.1 Introduction

Bubble dynamics plays a central role in several practical applications and physical phenomena and, hence, it has challenged researchers for many decades. Often the generation, stabilization or interaction of bubbles is enhanced by introducing a pressure wave or other disturbance in the host liquid. Bubbles depending on their size, are trapped in pressure nodes (larger bubbles) or antinodes (smaller bubbles) of a standing pressure wave, feeling an effective force known as the primary Bjerknes force; Bjerknes (1906). There, owing to rectified diffusion of dissolved gases and volume pulsations, bubbles grow until they eventually reach a state of dynamic equilibrium that is characterized by stable radial oscillations; Leighton (1994). This process is part of what is called acoustic cavitation, originally investigated by Lord Rayleigh (1917) in an effort to explain the damage observed on propellers of high speed boats and submarines and originally attributed to collapsing bubbles in their vicinity. Lord Rayleigh (1917) described the generation and collapse of bubbles as a result of changes in the local pressure field in the absence of other surfaces in their vicinity. Besides their interaction with nearby solid surfaces, bubbles also interact with each other as each bubble moves due to fluid acceleration caused by the volume oscillations of another bubble. This force can be attractive or repulsive depending on whether the bubbles oscillate in or out of phase, respectively and is known as the secondary Bjerknes force, since it was first investigated by C.A. Bjerknes and his son V. F. K. Bjerknes (1906, 1909). The primary and the secondary Bjerknes forces were explained by postulating that every body that is moving in an accelerating fluid is subjected to a ‘kinetic buoyancy’ proportional to the product of the acceleration of the fluid, $g$, multiplied by the mass, $\rho V$, of the fluid displaced by the body: $F \sim g \rho V$. Bjerknes hoped to use this phenomenon to explain the effects of electromagnetism and gravitation. The analogy with these forces was supported by the fact that the secondary Bjerknes force is proportional to the sizes of the bubbles and inversely proportional to the square of the distance between their centers of mass.
Based on the reasoning that the primary Bjerknes force drives the bubble to pressure nodes or antinodes, Crum (1974) used a stationary pressure wave in the vertical direction to counterbalance gravity and trap the bubbles. In addition, via a second pressure wave he induced volume oscillations to the bubbles. Then he measured their relative velocity of approach in the horizontal direction and found that the secondary Bjerknes force is much smaller than the primary one. However, it can increase by increasing the frequency of the pulsations and consequently ultrasonic pressure variations can be used in separation processes in order to remove gases from gas/liquid dispersions Batchelor (1967). Moreover the secondary Bjerknes force is responsible for several interesting dynamic phenomena which, among others, include bubble coalescence, formation of stable bubble pairs that move together in the host liquid and the formation of satellite bubbles Kornfeld and Suvorov (1944). More recently the field of cavitation gained significant momentum, due to the remarkable phenomenon of single bubble sono-luminescence, Ohl, et al. (1999), which is associated with light emission during collapse of either a cavitating or a laser-induced bubble. When a cloud of bubbles are present, the effect is known as multi-bubble luminescence Matula et al. (1995). During the last decade there is an emerging biomedical application of bubbles in the form of contrast agents, which are micron size bubbles that are encapsulated in a lipid polymer or albumin shell. Today these bubbles are clinically established markers of vascularity and are used for quantitative blood flow and volume measurements, especially in ultrasound echocardiography Goldberg, et al. (2001), Tsiglifis and Pelekasis (2008). Controlled oscillations and collapse of such bubbles has also been used recently for enhanced drug and gene delivery, Li et al. (2003).

Over the past several decades a significant amount of research has been devoted, both in the study of single bubble dynamics (see Plesset and Prosperetti (1977) for a review on earlier work on the subject) and the problem of bubble-bubble interaction. In the later field, efforts to evaluate the secondary Bjerknes force in the context of linear oscillations, has been reported by Zabolotskaya (1984) and later on by Doinikov and Zavtrak (1995) and Doinikov (1999) who considered nonlinear interactions. More recently, Pelekasis et al. (2004) made a systematic effort to evaluate the two available mechanisms that explain the formation of stable bubble clusters, when bubbles oscillate below resonance under an intense acoustic disturbance, extending the earlier work of Oguz and Prosperetti (1990) and Mettin et al. (1997). In this effort, the viscous boundary layers around each bubble were systematically accounted for, but the bubbles were assumed to remain spherical because of the large interbubble distance and their small radius. Earlier Pelekasis and Tsamopoulos (1993a, b)
reported a detailed study of the volume and shape oscillations of two bubbles assuming that the surrounding liquid is inviscid. This assumption is acceptable for a bubble radius larger than 1mm. They examined a certain range of frequencies, pressures and pressure amplitudes, bubble sizes and distances. This is the only study to date in which the surface of each bubble was allowed to deform in response to capillary, pressure and inertia forces, while retaining their axial symmetry. The results of these simulations show agreement with the linear theory with respect to the influence of the separation distance, volumes of the bubbles, forcing amplitude and frequency upon the average acceleration acquired by the bubbles in relative motion. An important nonlinear result is the fact that when the Bond number, \( Bo = (\rho \langle g \rangle R^2) / \sigma \), based on the average acceleration, \( \langle g \rangle \), the bubble radius, \( R^* \), and the properties of the liquid (density, \( \rho^* \), and surface tension, \( \sigma^* \)), lies above a critical value, spherical-cap shapes appear. Such shapes have been reported by Davies and Taylor (1950) for steady rising bubbles. On the contrary, when \( Bo \) lies below a critical value, globally deformed shapes appear, which have been reported by Kornfeld and Suvorov (1944). More results along these lines have been reported in Pelekasis (1991). However in that study due to the assumption of negligible viscous effects, the bubble motion and deformation could not be followed for very long as they approached each other due to very large shape distortions, possibly leading to premature bubble breakup. Another aspect that was not included was bubble coalescence, which is known to occur under cavitation conditions. The process of bubble coalescence was studied numerically, for example, by Chen et al. (1998) in the context of rising bubbles using a control volume technique for the discretization of the surrounding fluid. The dynamic phenomena involved, however, in the interaction of cavitating or laser induced bubbles are more severe and of different nature, in view of the large disturbances that are applied, thus requiring a more sophisticated numerical approach.

In the present work the nonlinear interactions of two deforming bubbles of radius ranging between 5\( \mu m \) and 1mm, will be examined. In contrast to the previous work of Pelekasis and Tsamopoulos (1993a, b) viscous effects will be accounted in full. The two bubbles will be subjected to a step change in pressure at infinity. Since the far-field pressure remains constant in time its frequency is zero and both bubbles are driven below their resonance frequency. Consequently, they will always attract each other irrespective of their relative size. The highly deforming interfaces are accurately computed by a block-structured mesh, which closely follows their surfaces. In every block, a set of partial elliptic differential equations is solved to compute the location of the mesh nodes, a procedure developed first by
Dimakopoulos and Tsamopoulos (2003a). This method has been applied to a number of free-
or moving - boundary problems, such as the displacement of a Newtonian fluid from a tube Dimakopoulos and Tsamopoulos (2003c), the transient squeezing of a viscoplastic material between parallel disks, Karapetsas and Tsamopoulos (2006), the steady rise and deformation of a bubble in a Newtonian or a viscoplastic material Tsamopoulos et al. (2008), and the deformation of several bubbles during filament stretching Foteinopoulou et al. (2006). Very recently this method has been extended to problems with domains that contain multiple inclusions and require decomposition and/or multiple mappings, Chatzidai et al. (2008), and it is found to be very accurate, flexible and robust.

In §2.2 we present the governing equations and boundary conditions of the problem. In §2.3, we very briefly mention the numerical method of solution. The results for equal and unequal bubbles under a step change in the far-field pressure are presented in §2.4. Finally, conclusions are drawn in §2.5.

2.2 Problem Formulation

The motion and the nonlinear interactions of two gas bubbles surrounded by a viscous liquid is considered. Axisymmetry around the axis connecting the centers of mass of the two bubbles is assumed. The density of the gas inside the bubbles is assumed to be much smaller than that of the liquid $\rho^*$, so that the gas is considered to be inertialess. Therefore, its pressure varies only with time according to a polytropic law. Figure 2.1 illustrates a schematic of the flow geometry examined herein.

Figure 2.1 Schematic of the flow geometry and the coordinate system of the problem.
The two bubbles are initially spherical with radii $R_{b1}^*$, $R_{b2}^*$ and distance $D^*$ between the two centers of mass. All lengths are scaled with the radius $R_{b1}^*$ of the left bubble. Due to the absence of a characteristic velocity the surface tension $\sigma^*$ is used for making velocity, time and pressure dimensionless. So, velocity is scaled with $\left(\frac{\sigma^*}{R_{b1}^*} \right)^{1/2}$, time with $\left(\frac{R_{b1}^3 \rho^*}{\sigma^*}\right)^{1/2}$ and pressure with $\frac{\sigma^*}{R_{b1}^*}$. The dimensionless number that arise is the Ohnesorge number, $Oh = \left(\frac{\mu^*}{\rho^* R_{b1}^* \sigma^*}\right)^{1/2}$, where $\mu^*$ is the dynamic viscosity. The importance of surface tension can be measured through the initial hydrostatic pressure in the liquid, $P^*$. 

The motion of the fluid is induced by a step change in pressure at infinity, which means that for time greater than zero, the pressure at infinity is given by: 

$$P_\infty = P(1 + \varepsilon), \quad (2.1)$$

where $\varepsilon$ is a measure of the disturbance.

The flow is governed by the momentum and mass conservation equations, which in their dimensionless form are:

$$\frac{Du}{Dt} - \nabla \cdot \sigma = 0 \quad (2.2)$$
$$\nabla \cdot u = 0 \quad (2.3)$$

where $\sigma$ is the total stress tensor,

$$\sigma = -P I + \tau = -P I + Oh \left[ \nabla u + (\nabla u)^T \right] \quad (2.4)$$

where $u$ is the velocity vector and $\nabla$ denotes the gradient operator.

Along the free surface of the bubbles, the velocity field should satisfy a local force balance between the capillary forces, viscous stresses in the liquid and pressure inside the bubble:

$$n \cdot \sigma = P_{gi} + 2Hn, \quad i = 1, 2 \quad (2.5)$$

where $P_{gi}$ is the pressure inside each bubble, $n$ is the outward unit normal to the free surface and $2H$ is its mean curvature which is defined as:

$$2H = -\nabla \cdot n, \quad \nabla_s = (I - nn) \cdot \nabla \quad (2.6)$$

Moreover, along the bubble interface the kinematic condition must be imposed:
where $\frac{DF}{Dt} = \dot{u}$

(2.7)

where $F$ is the position vector of the interface, given by:

$F = r, \varepsilon$

(2.8)

The pressure inside each bubble varies adiabatically with the instantaneous volume:

$P_{gi} = P_{gio} \left( \frac{V_{i0}}{V_i} \right)^{\gamma}, \quad i = 1, 2$

(2.9)

where $P_{gio}$ and $V_{i0}$ are the initial pressure and the volume of each bubble, $V_i$ the instantaneous volume of each bubble and $\gamma$ is the polytropic constant that here is assumed equal to 1.4. The volume of each bubble is calculated in spherical coordinates after each time step through:

$V_i = \int_0^\pi R_i^3 \sin \theta d\theta \quad i = 1, 2$

(2.10)

where $R_i$ is the radial position of each bubble interface.

Along the axis of symmetry the usual symmetry conditions are applied:

$u_r = 0$

(2.11)

$\frac{\partial u_r}{\partial r} = 0$

(2.12)

The infinite domain of the fluid is truncated to a finite spherical domain around the two bubbles with a radius much larger than the bubble radius so this boundary does not affect the flow around the two bubbles. This is achieved using the open boundary condition suggested by Papanastasiou et al. (1992).

### 2.3 Numerical Solution

These equations are solved numerically using the mixed finite element method to discretize the velocity and pressure fields, combined with an advanced elliptic grid generator for the initial construction and subsequent motion of the mesh points in the liquid domain. Details of this method as it is applied in the present problem are given in Chapter 1, where a number of convergence tests are also reported to determine the number of elements required in the entire domain and on the bubble surfaces in particular to resolve the boundary layers that may arise in this problem.
A particular problem that arises during the progress of this simulation is the corrugated bubble surfaces and the translation of the bubbles very close to each other. At the first case, the discretization of the mesh becomes coarser and coarser within the troughs, while at the second case, becomes very dense at the side facing between the two bubbles. In both cases, the skewness of the elements increases, causing deterioration in the accuracy of the calculations and, possibly, the destabilization of the numerical scheme. In order to overcome these difficulties, the mesh is reconstructed when it is considered necessary, i.e. before the elements skewed much. The reconstruction of the mesh is based on the rarefaction or the condensing of the elements around the two bubbles, depending on the case. The basic steps of the entire procedure are:

(a) Construction of a new mesh with the procedure that described in Chapter 1 for the construction of the initial mesh. More specifically, the physical domain is splitted into three sub-domains which are mapped separately to a computational domain (see figure 1.12 of Chapter 1). Each computational domain is constructed as described in Chapter 1. In order to set the lengths of each computational domain around the two bubbles, the two physical domains around the bubbles (parts A and B of figure 1.12) considered to be a spherical shell with inner radius \( R_i \) (\( i = A, B \)) and outer radius \( L_i \). As the bubbles are not spherical any more, as inner radius is selected the maximum distance of the bubble surface from its center of mass, while the outer radius is defined by the location of the bubbles in the physical domain. Once the computational domain for each bubble has been constructed, a continuation procedure is followed on each bubble surface in order to take their final shape in the physical domain. The third sub-domain is constructed exactly as described in Chapter 1. The three individual domains are merged and the new entire mesh is constructed. Moreover, it must be mentioned, that the number of nodes on each bubble surface remain the same in the old and the new mesh, while the number of the elements around each bubble is increased or decreased, depending on the case. In the case that the bubble surfaces are very deformed and a very dense mesh is demanded around them, eq. (1.30) is used as needed for concentrating the coordinate lines along them, with an appropriate value of \( \zeta \).

(b) Since the new mesh has constructed, assigned values to velocity and pressure vectors at the new grid points, using interpolation techniques between the old and the new mesh. The slowest step in the above procedure is the continuation procedure of the free surfaces, especially when they are very deformed and a small continuation step is needed. On the other
hand, the duration of the step (b) is much shorter (a few seconds), despite the global character of the procedure.

2.4 Results

2.4.1 Normal mode analysis

Before proceeding with the nonlinear dynamics and in order to interpret and classify the numerical predictions, it is imperative to perform a normal mode analysis of the two deformable bubbles interacting in a Newtonian liquid. This will determine the frequencies and the damping rates of the system under small disturbances. Such data have not been reported before because even these reduced equations do not seem to be amenable to analytical treatment. Nevertheless, these data can be extracted with our numerical code by assuming that initially no flow exists and the two bubbles are spherical due to capillarity and, then, subjecting all the flow variables including the bubble shapes to an infinitesimal disturbance. More specifically, the normal modes of the system are computed by assuming that all variables are split into their base (static equilibrium) values and a small disturbance,

\[
\begin{bmatrix}
    u(r, \theta, t) \\
    P(r, \theta, t) \\
    P_{gb}(r, \theta, t) \\
    x(r, \theta, t)
\end{bmatrix}
= \begin{bmatrix}
    u_b \\
    P_b \\
    P_{gb} \\
    x_b
\end{bmatrix}
+ \delta \begin{bmatrix}
    u_p(r, \theta) \\
    P_p(r, \theta) \\
    P_{gib}(r, \theta) \\
    x_p(r, \theta)
\end{bmatrix} e^{\epsilon t}. \tag{2.13}
\]

Here the new subscripts \( b \) and \( p \) indicate the equilibrium and the perturbed states, respectively, \( \delta \ll 1 \) is the amplitude of the infinitesimal disturbance and \( x \) denotes the position vector of the mesh nodes including the nodes at the interfaces of the bubbles. Substituting expressions (2.13) into the governing equations, including the kinematic equation (2.7) and the equation of state that describes the pressure inside the bubble (2.9), and neglecting terms of order higher than linear in the perturbation parameter, \( \delta \), we obtain a generalized eigenvalue problem of the form,

\[
J Y = c M Y, \tag{2.14}
\]

where \( J \) is the Jacobian matrix, \( M \) is the mass matrix, \( c \) are the eigenvalues and \( Y \) the corresponding eigenvectors. In order to solve the eigenvalue problem, we used the Arnoldi method as it is implemented in the Arpack library (Lehoucq et al. 1998). This method is capable of iteratively computing a relatively small fraction of the entire spectrum of eigenvalues and in particular those that have the largest magnitude. Since we are interested in enhancing convergence to a specific portion of the spectrum and in order to limit the fraction
of the eigenvalues to be computed each time, we used the shift-and-invert transformation. For more details see Chatzidai et al. 2008.

On the other hand, analytical results of the simpler normal mode analysis for an isolated bubble in a Newtonian liquid have been reported in the literature. Comparing our numerical predictions for the computed eigenfrequencies in the limit of large distance between the bubble centers in comparison with their radii to the analytical expressions for a single bubble provides a strict and demanding test for the accuracy of our numerical simulations and an indication for the extend to which the computational mesh must be refined. In particular, assuming that (i) the surrounding liquid is incompressible, (ii) thermal effects are negligible (iii) the interface has no elasticity or intrinsic viscosity and that the bubble undergoes only radial oscillations, yields the classical Rayleigh-Plesset equation (Plesset and Prosperetti 1977; Brennen 1995; Tsiglifis and Pelekasis 2007). Further assuming that the disturbance amplitude is small and using the scales for the variables employed herein reduces it to the linearized equation,

$$R_p^* + 4\, \text{Oh} \, R'_p + \left\{ 3\gamma (P_b + 2) - 2 \right\} R_p = 0,$$

(2.15)

here the primes indicate differentiation with respect to time. The roots of its characteristic polynomial furnish the eigenvalue of eq. (2.15), $c_o = -\beta_o \pm i \omega_o$, written in terms of the dimensionless resonance frequency, $\omega_o$ (or the oscillation period, $T_o$) and damping, $\beta_o$ of the isolated bubble,

$$T_{o,\infty} = \frac{2\pi}{\omega_{o,\infty}} = \frac{2\pi}{\left[ 3\gamma (P_b + 2) - 2 - 4 \, \text{Oh}^2 \right]^{1/2}} = \frac{2\pi}{\left[ 3\gamma \left( \frac{P_b^*}{\sigma^2/R_b^*} + 2 \right) - 2 - \frac{4\mu^2}{\rho \sigma^2 R_b^*} \right]^{1/2}}, \quad \beta_o = 2 \, \text{Oh}$$

(2.16)

The subscript "o" indicates that the corresponding variables refer to the mode preserving spherical symmetry, often called the breathing or the zeroth mode, while the subscript "\infty" indicates that the bubble is isolated. These expressions demonstrate that the dimensionless damping rate is proportional to $\text{Oh}$, while the period decreases with the dimensionless ambient pressure and the Ohnesorge number approximately as $P^{-1/2}$ and $\text{Oh}$, respectively, when these dominate the rest of the terms in the denominator of eq. (2.16) or that it is approximately inversely proportional the liquid viscosity and increases with the bubble radius in a more complicated manner.

The corresponding eigenmode analysis which allows even for deformations of the bubble surface is quite more involved. Miller and Scriven 1968 have thoroughly examined the more general problem of a deformable spherical globule composed of any type of fluid and
immersing in another immiscible fluid which extends to infinity. They have shown that the vorticity and the radial velocity of the linearized equations maybe expressed in terms of spherical harmonics and generalized radial functions and proceeded to provide expressions to determine the eigenvalues of the system. In the limit of inner to outer fluid density and viscosity ratios approaching zero the problem of an isolated bubble is recovered. In this case, the dimensional eigenvalues \( c^* \) are given by the following closed-form but implicit expression,

\[
\frac{\omega_{\text{osc}}^2}{c^*^2} = \frac{l + 2}{\omega^* R_b^*/2} \left[ \frac{(2l + 1)\omega^* R_b^*/2 - 2(l - 1)(l + 1)(2l + 1 - \omega^* R_b^*/l_{1/2})}{2l + 1 - \omega^* R_b^*/l_{1/2} + \omega^* R_b^*/l_{3/2}/2} \right] - 1, \quad l = 2, 3, \ldots, \tag{2.17}
\]

where \( \omega^* = \sqrt{c^* \rho^* / \mu^*} \) has units of inverse length, is related to the unknown \( c^* \) and is introduced only for convenience, while \( \omega_{\text{osc}}^* = \left( \frac{\sigma^* (l + 1)(l - 1)(l + 2)}{R_b^3 \rho^*} \right)^{1/2} \) is the frequency of oscillation, if the surrounding liquid is assumed to be inviscid and the gas in the bubble does not contribute to the dynamics of the problem, as we have already assumed; see Rayleigh 1917; Tsamopoulos and Brown 1983. Finally, \( Q^{(i)}_{l_{1/2}} = \frac{H^{(i)}_{l_{1/2}}(\omega^* R_b^*)}{H^{(i)}_{l_{1/2}}(\omega^* R_b^*)} \), where \( H^{(i)}_{l_{1/2}} \) and \( H^{(i)}_{l_{3/2}} \) are the half-integral-order Hankel functions of the first kind. In these expressions, \( l \) corresponds to the index of the Legendre polynomial characterizing the shape of the bubble. The analytical solution does not apply for volume oscillations of the bubble \( (l = 0) \) or bubble translation \( (l = 1) \). Here again writing \( c_l = -\beta_l \pm \mathbf{i} \omega_l \) one obtains the decay factor as the real part of \( c_l \), while its imaginary part is the angular frequency of the \( l^{th} \) mode.

Next, the oscillation frequencies and decay factors computed numerically with our code will be compared to their values calculated by solving eq. (2.17) using standard software for the \( l \geq 2 \) modes and directly from eq. (2.16) for the \( l = 0 \) mode. Typically, properties of pure water at ambient temperature 20°C and pressure 1 bar are used, i.e. \( \rho^* = 10^3 \text{ kg/m}^3 \), \( \mu^* = 10^{-3} \text{ Ns/m}^2 \), \( \sigma^* = 0.0727 \text{ N/m} \). When these are combined with the bubble size, they yield the particular Ohnesorge number and dimensionless pressure. Table 2.1a gives the dimensionless eigenvalues obtained for two equal bubbles with \( R_b^* = R_b^* = 5 \mu m \) in water, hence \( Oh^{-1} = 19.065, \ P = 6.878 \), located at a large distance \( D = 17 \), where it is anticipated that
the bubbles will not interact, at least in the linear limit. Indeed, two identical sets of eigenvalues result for each wavenumber, each set corresponding to each one of the bubbles.

(a) $D = 17$

<table>
<thead>
<tr>
<th>$l$</th>
<th>Miller &amp; Scriven</th>
<th>M3</th>
<th>M4</th>
<th>M5</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$-0.7533 \pm 3.2030i$</td>
<td>$-0.7568 \pm 3.2858i$</td>
<td>$-0.7551 \pm 3.2447i$</td>
<td>$-0.7543 \pm 3.2268i$</td>
</tr>
<tr>
<td>3</td>
<td>$-1.3166 \pm 5.8695i$</td>
<td>$-1.3192 \pm 5.9312i$</td>
<td>$-1.3179 \pm 5.9004i$</td>
<td>$-1.3173 \pm 5.8871i$</td>
</tr>
<tr>
<td>4</td>
<td>$-2.0104 \pm 8.7725i$</td>
<td>$-2.0128 \pm 8.8243i$</td>
<td>$-2.0116 \pm 8.7984i$</td>
<td>$-2.0111 \pm 8.7872i$</td>
</tr>
<tr>
<td>5</td>
<td>$-2.8326 \pm 11.9223i$</td>
<td>$-2.8349 \pm 11.9681i$</td>
<td>$-2.8337 \pm 11.9452i$</td>
<td>$-2.8332 \pm 11.9354i$</td>
</tr>
</tbody>
</table>

(b) $D = 5$

<table>
<thead>
<tr>
<th>$l$</th>
<th>$c_j$ (in phase)</th>
<th>$c_j$ (out of phase)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$-0.7529 \pm 3.1981i$</td>
<td>$-0.7537 \pm 3.2085i$</td>
</tr>
<tr>
<td>3</td>
<td>$-1.3166 \pm 5.8683i$</td>
<td>$-1.3166 \pm 5.8709i$</td>
</tr>
<tr>
<td>4</td>
<td>$-2.0104 \pm 8.7722i$</td>
<td>$-2.0105 \pm 8.7728i$</td>
</tr>
<tr>
<td>5</td>
<td>$-2.8327 \pm 11.9223i$</td>
<td>$-2.8327 \pm 11.9225i$</td>
</tr>
</tbody>
</table>

(c) $D = 2.8$

<table>
<thead>
<tr>
<th>$l$</th>
<th>$c_j$ (in phase)</th>
<th>$c_j$ (out of phase)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$-0.7494 \pm 3.1218i$</td>
<td>$-0.7649 \pm 3.3066i$</td>
</tr>
<tr>
<td>3</td>
<td>$-1.3160 \pm 5.8040i$</td>
<td>$-1.3192 \pm 5.9499i$</td>
</tr>
<tr>
<td>4</td>
<td>$-2.0112 \pm 8.7278i$</td>
<td>$-2.0099 \pm 8.8238i$</td>
</tr>
<tr>
<td>5</td>
<td>$-2.8338 \pm 11.8943i$</td>
<td>$-2.8315 \pm 11.9532i$</td>
</tr>
</tbody>
</table>

(d) Characteristics of the three meshes used

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Total number of triangles after local refinement</th>
<th>Number of nodes on each free surface after refinement</th>
<th>$\Delta r_{\text{min}}$ around the free surface after local refinement</th>
<th>$\Delta z_{\text{min}}$ around the free surface after local refinement</th>
</tr>
</thead>
<tbody>
<tr>
<td>M3</td>
<td>15360</td>
<td>641</td>
<td>0.01</td>
<td>0.002</td>
</tr>
<tr>
<td>M4</td>
<td>30720</td>
<td>1281</td>
<td>0.005</td>
<td>0.002</td>
</tr>
<tr>
<td>M5</td>
<td>53760</td>
<td>2241</td>
<td>0.003</td>
<td>0.002</td>
</tr>
</tbody>
</table>

Table 2.1: Eigenvalues for two bubbles of equal radii $R_{bi}^* = 5 \mu m$, immersed in pure water at ambient temperature $T^* = 20 \degree C$ and pressure $P^* = 1 \text{bar}$, hence $Oh^{-1} = 19.065$ and $P = 6.878$ for three different interbubble distances: (a) $D = 17$, (b) $D = 5$, (c) $D = 2.8$ and (d) characteristics of the three meshes that are used.

The eigenvalues obtained with the increased spatial discretization of the meshes M3, M4 and M5 monotonically approach their values calculated using the analytical expressions using eqs. (2.16) and (2.17). This confirms that, in spite of the large distance between the bubbles which
increases the distance between the nodes in the computational mesh, the numerical values are highly accurate even with the coarsest mesh. The characteristics of the mesh are given in Table 2.1d. The eigenfrequencies of the same bubbles when they are closer together at $D=2.8$, are given in the same Table 2.1c. The smaller distance between the two bubbles reduces the total number of mesh nodes required and, hence, it makes the discretization with mesh M3 sufficient. This is the mesh that will be used in the bulk of the remaining calculations. Now, two different sets of eigenvalues arise for each wavenumber, the smaller one corresponding to in-phase oscillations of the bubbles and the larger one to out-of-phase oscillations. Figure 2.2 presents the shapes of the two bubbles obtained from the eigenvector corresponding to $l=2$. In figure 2.2a the two bubbles have identical oblate shapes that very much resemble those obtained from the second Legendre polynomial, while in figure 2.2b the left bubble has an oblate shape and the right one a prolate shape also resembling those obtained from the second Legendre polynomial, but in opposite phase. Similar differentiation of the eigenvalues was obtained by Pelekasis and Tsamopoulos 1993a, where the surrounding the two bubbles liquid was assumed to be inviscid. In Newtonian liquids as well, we find that as $D$ decreases, the eigenvalue corresponding to in-phase oscillations decreases, while the other one increases. This is demonstrated here by comparing in Table 2.1 the eigenvalues for $D=2.8$, 5 and 17, where we see that in smaller distances the deviation between the two sets of eigenvalues is clear, in the intermediate one it occurs in the $3^{rd}$ or $4^{th}$ significant digit of the eigenvalues, whereas there is no deviation in the largest distance.

Figure 2.2 Eigenvectors for $R_{bi}^e = 5\mu m$, $Oh^{-1} = 19.065$, $P = 6.67$, $D = 2.8$ and $l = 2$ corresponding to (a) in-phase oscillations and (b) out-of-phase oscillations.
Subsequently, we will present nonlinear simulations for two interacting bubbles with a wide range of radii \((5 \mu m - 1 mm)\) immersed in pure water, when the ambient pressure increases by up to 100%.

2.4.2 Nonlinear dynamics of equal bubbles

2.4.2.1 Bubbles of 5 \(\mu m\) radius and general characteristics of the motion

First, equal bubbles of a relatively small radius \(5 \mu m\) are examined. The two bubbles are immersed in pure water with far-field pressure at 1 \textit{bar}. The dimensionless numbers that result from this bubble size and liquid properties are: \(Oh^{-1} = 19.065\) and \(P = 6.878\). The disturbance amplitude, \(\varepsilon\), in all the following simulations, except for those in section 4.2.3, where the effect of \(\varepsilon\) is examined, is set to \(\varepsilon = 1\). So, for this case the pressure at the far-field is increased at \(t = 0\) to \(P_\infty = P(1 + \varepsilon) = 13.756\). The initial distance between the centers of mass of the two bubbles is set to \(D = 2.8\), while the outer boundary is set always at \(R_\infty = 30\). This large distance is chosen after trial and error in order not to affect in any way the flow around the two bubbles in any of the simulations presented herein.

\[\begin{align*}
\text{Figure 2.3} & \quad \text{Variation with time of the volume of the left bubble. The two bubbles are equal with } R_{bi}^* = 5 \mu m, \quad Oh^{-1} = 19.065, \quad P = 6.67, \quad D = 2.8.
\end{align*}\]
Figure 2.3 shows the time-variation of the dimensionless volume of the left bubble. Since $R_{bl} = 1$, this volume is $V = 4\pi / 3 \approx 4.1888$ at $t = 0$. Doubling of the far-field pressure quickly reduces the bubble volume below its new equilibrium value, and even to less than half its initial size to $V \approx 1.75$. Subsequently the bubble undergoes damped oscillations because of the fluid viscosity. Similar disturbances in inviscid liquids lead to undamped oscillations of the bubble volume; Pelekasis and Tsamopoulos, 1993a. As will be seen later when $Oh$ decreases, the amplitude of the volume oscillations decreases at a slower rate. The volume of the right bubble varies with time in exactly the same way owing to symmetry. Oscillations of the two bubbles are in phase and their first common period is found to be $T_v = 0.762$, subsequent periods of volume oscillations slowly increase with time: 0.768, 0.778, 0.792. All these are lower than the value predicted by the normal mode analysis for in-phase volume oscillations. Indeed, eq. (2.16) for the above parameter values, gives $T_o, \omega = 1.057$ at $P = 6.878$. This decrease in the period of the nonlinear oscillations is because the zeroth mode that corresponds to the volume oscillations is the one that is mainly affected by changes in pressure. In the current simulation, because of the large disturbance in the pressure, $\varepsilon = 1$, the period is predicted by eq. (2.16) to decrease like $P_b^{1/2}$ and to become $1.058/\sqrt{2} = 0.747$, since in this case $P_b$ is dominant over the other terms in the denominator of this equation. This value is slightly smaller than the numerically calculated ones because not only this is an approximate result, but also nonlinear effects increase the importance of inertia and hence the period of bubble oscillations, see Tsamopoulos and Brown, 1983. As will be seen later, a decrease in the disturbance amplitude leads to larger periods.

Figure 2.4 shows the evolution of the centers of mass of each bubble with time. Their locations, $Z_i$, for each bubble are determined along the common axis of symmetry via

$$Z_i = \frac{\int z \rho(z)^2 dz}{\int \rho(z)^2 dz} = \frac{\int z \rho(z)^2 \frac{dz}{ds} ds}{\int \rho(z)^2 \frac{dz}{ds} ds}, \quad i = 1, 2,$$  \hspace{1cm} (2.18a)

where cylindrical coordinates $(z, \rho)$ have been introduced centered at the common axis of symmetry and in the third ratio of integrals the integration with respect to the axial distance has been transformed into an integration with respect to the arclength along the bubble surface to avoid the multi-valuedness of some bubble shapes, as we will see in the next sections. The combined center of mass, $Z$ is computed via
The two centers of mass are seen to oscillate symmetrically on a fast timescale and keep approaching each other in a slow timescale. The combined center of mass remains at zero owing to symmetry, verifying once again the accuracy of our calculations. The initial distance between the two centers is indeed 2.8, but the final one is less than 2 indicating that the bubble centers are at a distance smaller than the sum of their initial radii. This reveals that the bubbles have approached each other so much that they have squeezed each other attaining a deformed oblate shape. Calculating the average distance between the two bubble centers within each oscillation period and fitting these data to a quadratic polynomial in time, one obtains

\[ D_{\text{average}} = 2.804 - 0.186 \, t - 0.06 \, t^2. \]  

(2.19)

This time-dependence shows that the bubbles accelerate towards each other on average.

In figures 2.5a, b the velocity and acceleration, respectively, of the center of the left bubble are shown and are also oscillatory. These are determined by numerically differentiating with respect to time the instantaneous locations of the bubble centers. This figure and the previous two are given up to \( t = 3.778 \), when the simulations diverged because
the bubble surfaces are too close to each other as will be seen next and the elements are quite distorted. The average velocity over a period of volume oscillations initially increases with time almost linearly, then it increases at a lower rate and finally, at the last stages of the simulations and after the two bubbles have approached each other significantly, it decreases. Apparently the two bubbles have come so close together that their translation along their common axis cannot continue.

Figure 2.5 Evolution with time of (a) the velocity and (b) the acceleration of the left bubble. The two bubbles are equal with parameters those of fig. 2.3.

Figure 2.5b shows that the left bubble spends more time accelerating towards the right one than decelerating away from it. The values of the average acceleration over each period of volume oscillation are: \( \langle g \rangle = 0.248, 0.099, 0.007, 0.089 \) and remain always positive, so that the average force remains attractive until the end of the simulation. Their average value is \( \langle g \rangle = 0.111 \), which is not too different from 0.12, the value predicted by eq. (2.19). Because of this strong time-dependence of the bubble acceleration, from now on, the average acceleration of the bubbles will be measured and reported over the first period of volume oscillations. This seems to be most appropriate since the bubbles deform and approach each other with time, both of which affect their acceleration. The oscillation periods of the velocity are 0.751, 0.766, 0.789, 0.79 and for the acceleration are 0.763, 0.767, 0.786, 0.803. They slowly increase following the same trend of the periods in the volume oscillations. Only the last figure signals a decrease in the amplitude just because the two bubbles are now very close and prevent each other from accelerating further. This increase in the periods is attributed to the slow damping of the nonlinear oscillations, Nayfeh 1979.
Figure 2.6 Contours of (a) $u_{rs}$ (upper half), $u_\theta$ (lower half) and (b) $P$ at $t = 3.73$ for $R_{hi}^* = 5 \mu m$, $Oh^{-1} = 19.065$, $P = 6.67$, $\varepsilon = 1$, $D = 2.8$ and $R_c = 30$. 
Figure 2.6 presents the bubble shapes and contour plots of both velocity components and pressure at \( t = 3.148 \). At this instant the bubbles have approached each other significantly, as their nearby surfaces are at a distance 0.039. This distance still allows us to exclude van der Waals and other surface forces from the present model or consider merging of the bubbles. The field variables are presented with respect to a spherical coordinate centered at the middle of the distance between the initial centroids of the two bubbles. The radial velocity, given in the upper half of figure 2.6a, takes its smallest (negative) values at the rear side of the bubbles, while it takes positive values between the two bubbles. This distribution of \( v_r \) indicates that the two bubbles are in the contracting phase of their radial oscillation but still approach each other, squeezing fluid away from the gap between them. The former can be confirmed by observing in figure 2.3 that the time \( t = 3.148 \) is just after the last maximum in the volume oscillations of the bubbles indicating that the bubble have started their final contraction. The azimuthal velocity, given in the lower half of figures 2.6a, is symmetric with respect to \( \theta = \pi/2 \), because the two bubbles are equal and undergo in-phase oscillations. As the two bubbles contract, the azimuthal velocity takes negative values around the left bubble and positive values around the right bubble, while it takes zero values at \( \theta = 0, \ \theta = \pi \) and \( \theta = \pi/2 \), due to the presence of a plane and an axis of symmetry in this configuration. The pressure field, which is given in figure 2.6b, forms contours surrounding both bubbles very close to them. Apparently, the bubbles being in their contraction phase, have overshoot their new equilibrium position and the pressure near their surface is well below that imposed in the outer boundary. Indeed the pressure just outside the bubbles is 8.859. At a distance less than 7 bubble radii from the center of this coordinate system the pressure attains radial symmetry. Moreover the pressure, which has been set at \( P_\infty = P(1+\varepsilon) = 13.756 \) at \( R_\infty = 30 \), decreases only to \( P = 13.092 \) very close to the bubble, at a distance of approximately \( r \approx 3 \), which verifies once more that locating the outer boundary at \( R_\infty = 30 \) should not affect even the pressure field, which is the most sensitive of the flow variables.

Figure 2.7 shows the time evolution of the coefficient \( C_0 \), of the zeroth degree Legendre polynomial, \( P_0 \), that is associated with volume oscillations and the coefficient \( C_2 \) of the second Legendre polynomial \( P_2 \), of the left bubble. Legendre coefficients are computed with respect to spherical coordinates with origin located at the instantaneous center of each bubble and are given by:

\[
C_{il} = \int_0^\pi f_i(\theta) P_i(\theta) \sin(\theta) d\theta, \quad i = 1,2, \quad l = 0,1,2,3...
\] (2.20)
where, $f_{si}$ is the position of the interface of the $i$ bubble. Figure 2.7a shows that the amplitude of the zeroth mode undergoes damped oscillations in exact correspondence to the volume oscillations reported in figure 2.3. Positive values of the coefficient $C_2$ signify prolate bubble shapes (elongated along the axis of symmetry) whereas negative values oblate bubble shapes (flattened at the bubble poles). Figure 2.7b shows that the two bubbles oscillate initially attaining alternatively prolate and oblate shapes, but eventually they attain only oblate shapes because they have squeezed each other along their common axis. Although the two bubbles have approached each other considerably, as can be seen in figure 2.6, they did not flatten significantly, because of their very small size which makes capillary forces dominant over all other forces, as indicated by the small value of $Oh^{-1}$. For the same reason, all modes higher than $P_2$ have negligible contribution to the bubble shape.

![Figure 2.7](image)

**Figure 2.7** Variation with time of the volume of the left bubble. The two bubbles are equal with the parameters of fig. 2.6.

### 2.4.1.2 Bubbles larger than 5μm: Effect of bubble size and initial distance, $D$

Retaining the initial distance between the two bubbles at $D=2.8$ and the pressure amplitude at $\varepsilon=1$, we increased the bubble radius from 5μm to 10μm and then to 20μm. The period of volume oscillations decreases, as it was expected, from 0.768 that was for the bubbles of 5μm to 0.541 for the bubbles of 10μm and to 0.393 for the bubbles of 20μm. Again these values, due to the large increase of the far-field pressure, are lower than the ones predicted from linear theory. These are 0.784 for the bubbles of 10μm and 0.569 for the
bubbles of 20μm. Due to the smaller period of volume oscillations, it is expected that the average acceleration of the bubbles will increase with their size, and consequently, the time needed to approach each other will decrease. The deformations of the bubble surfaces are expected to be larger since the increased $Oh^{-1}$ signifies less important capillary forces with respect to viscous forces.

Figure 2.8 Time evolution of (a) the centers of mass (b) the coefficient of the Legendre polynomial $P_o$ and (c) the coefficient of the Legendre polynomial $P_2$ for two equal bubbles with $R_{bi} = 10\mu m$ ($Oh^{-1} = 26.551$, $P = 14.185$) and $R_{bi} = 20\mu m$ ($Oh^{-1} = 38.131$, $P = 27.51$), $\varepsilon = 1$, $D = 2.8$ and $R_{\infty} = 30$. 
Indeed from figure 2.8a, where the locations of the centers of mass for \( R_{bi}^* = 10\mu m \) 
\( (Oh^{-1} = 26.551, P = 14.185) \) and \( R_{bi}^* = 20\mu m \) 
\( (Oh^{-1} = 38.131, P = 27.51) \) are given, it is obvious that the larger the bubbles, the less time is needed to approach each other. Again we can calculate the average distance between the two bubble centers within each oscillation period and fit these data to a quadratic polynomial in time. For \( R_{bi}^* = 10\mu m \) this yields,

\[
D_{\text{average}} = 2.778 - 0.222 \cdot t - 0.308 \cdot t^2.
\]

As for the \( R_{bi}^* = 5\mu m \) case, this expression gives approximately the initial interbubble distance and the average acceleration, which here is 0.616, i.e. much larger than in bubbles with \( R_{bi}^* = 5\mu m \). In figure 2.8a we can also see that the final distance between the bubble centers is smaller than the sum of their initial radii and somewhat smaller than for the \( 5\mu m \) bubbles. In figures 2.8b, c the time evolution of the zeroth, \( C_0 \), and second, \( C_2 \), coefficients of the Legendre polynomials, \( P_0 \) and \( P_2 \) respectively, are given for \( R_{bi}^* = 10\mu m \) and \( R_{bi}^* = 20\mu m \).

From figure 2.8b it is clear that the period of the volume oscillations decreases when the size of the bubble increases, while the amplitude of the oscillations increases. The former results from the increased dimensionless pressure, while the latter from the increased inertia. Since the average acceleration increases when the bubble size increases and the bubble interaction becomes stronger, it is expected that the larger bubble will attain more flattened shapes. Indeed, comparing the values of \( C_2 \) in figure 2.8c for the bubbles of \( 10\mu m \) and \( 20\mu m \), it is clear that the shape of the larger bubble is characterized by a more negative coefficient towards the end of the simulations, which signals a flatter bubble. Comparing the oscillation periods of the zeroth \( 0.541, 0.548, 0.562 \) and the second modes, \( 0.528, 0.552, 0.574 \), for example for the \( R_{bi}^* = 10\mu m \) bubbles, we find not only that they both increase in time, but, more importantly, that the periods of these two modes are similar. Given that the linear period \( P_2 \) is 1.901, i.e. very different from the linear period of \( P_1 \) and the above computed periods, this implies that the bubbles are deformed not because of a harmonic or subharmonic resonance of \( P_2 \), but because of the coupling of forces from volume oscillation and linear translation.

Increasing even more the bubble radius to \( 30\mu m \), modes higher than \( P_2 \) start to arise and the two bubbles deform on the side facing away from the direction of average acceleration. Hereafter this side will be called the rear side, while the other side will be called
the front side. Figure 2.9 gives a sequence of bubble shapes at the same initial interbubble distance, but with $R_{bi} = 30 \mu m$ in pure water ($Oh^{-1} = 46.701, P = 41.265$).

The Fourier-Legendre decomposition of these shapes is given in figures 2.10a, b for the coefficients of $P_0$ and $P_2 - P_6$. The zeroth mode is seen to undergo the usual damped oscillations, while among the surface harmonics, the 2nd one is seen to start growing immediately with approximately the same period as the zeroth mode, followed by the 3rd one, then the rest of the higher modes follow. Towards the end of the simulations the 2nd harmonic has the largest amplitude, which has even approached the amplitude of the zeroth mode, followed by the 5th and 6th modes. Table 2.2 presents the eigenvalues of the breathing mode and of the $P_2 - P_6$ modes calculated using eqs (16) and (14), respectively. The same table
presents the corresponding nonlinear periods of the first oscillation as computed from figures 2.10a, b.

Figure 2.10 Time evolution of the coefficients of the Legendre polynomials (a) \( P_6 \) and (b) \( P_2 - P_6 \) for two equal bubbles with the same parameters as in figure 2.9.

<table>
<thead>
<tr>
<th>( l )</th>
<th>( c_l ) (in phase)</th>
<th>( c_l ) (out of phase)</th>
<th>( T_l )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(-0.0357 \pm 11.6850i)</td>
<td>(-0.0764 \pm 16.0745i)</td>
<td>0.332</td>
</tr>
<tr>
<td>2</td>
<td>(-0.3500 \pm 3.3078i)</td>
<td>(-0.3584 \pm 3.5035i)</td>
<td>0.29</td>
</tr>
<tr>
<td>3</td>
<td>(-0.6158 \pm 6.1316i)</td>
<td>(-0.6189 \pm 6.2859i)</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>(-0.9471 \pm 9.2444i)</td>
<td>(-0.9480 \pm 9.3470i)</td>
<td>0.437</td>
</tr>
<tr>
<td>5</td>
<td>(-1.3436 \pm 12.6470i)</td>
<td>(-1.3436 \pm 12.7104i)</td>
<td>0.421</td>
</tr>
</tbody>
</table>

Table 2.2 Eigenvalues \( c_l \) and first periods of the nonlinear oscillations \( T_l \) for equal bubbles with \( R_{bi}^* = 30\mu m \), \( Oh^{-1} = 46.701 \), \( P = 41.265 \) and \( D = 2.8 \).

We observe that the frequency of the \( P_3 \) mode is almost half the frequency of the breathing mode, while the frequencies of the \( P_5 \) and \( P_6 \) modes are close to its value. Hall & Seminara, 1980, have shown that, when the frequency of the radial motion of a single bubble happens to be twice the linear frequency of a Legendre mode and sufficiently large perturbations are applied, subharmonic excitation of the later mode occurs. Moreover, when the frequency of the radial motion happens to be equal to the linear frequency of a Legendre mode, harmonic resonance can arise. The former should arise first, as it is inversely proportional to the square
of the excitation amplitude followed by the latter, as it is inversely proportional to the excitation amplitude, when this amplitude is up to one. This is exactly what is observed in figure 2.10b. The dominance of the $P_2$ mode throughout and more so towards the end of the simulations and its oscillation with a frequency similar to that of the breathing mode verifies that it is generated by the combined oscillation and linear translation of the bubbles and the eventual squeezing that they apply to each other, but not by some type of resonance. In other words this mode is excited here by the same mechanism it was excited in the smaller bubbles. The fact that the surface harmonics appear only at the rear side of both bubbles is a result of a Rayleigh-Taylor instability, which occurs at a fluid/fluid interface when inertia overcomes the stabilizing capillary forces. More specifically, as the bubbles accelerate towards each other, the fluid that surrounds them has to accelerate in the opposite direction, in order to conserve mass. The instability will appear on the side of the bubble where fluid acceleration is directed from the lighter fluid towards the heavier one. In all these cases of the accelerating bubbles, this is their rear side. Further increasing the bubble size to $R_{bi} = 1mm$ gives rise to even higher modes, but the bubbles always deform at their rear side and flatten at their front side.

Retaining the size of the bubbles at $R_{bi} = 30 \mu m$ in water, we increase the initial distance between their centers of mass from $D = 2.8$ to $D = 5$. Since the bubbles are now further apart their interaction will be weaker and their average acceleration is expected to decrease. Hence, the time needed for the two bubbles to approach each other will be increased and larger shape deformations are expected to arise, since there will be more time for the two bubbles to oscillate and accelerate. Figure 2.11 presents the time-evolution of the acceleration of the center of the left bubble for $D = 2.8$ and $D = 5$. Indeed the average acceleration over the first period of volume oscillation is $\langle g \rangle = 1.231$ for $D = 2.8$, but decreases to $\langle g \rangle = 0.529$ for $D = 5$. However, as time proceeds and the bubbles approach each other, the amplitude of their periodic acceleration in each period of volume oscillation increases monotonically and eventually approaches the value of the initial acceleration of the bubbles at the smaller initial distance of $D = 2.8$. In the same figure we observe that, for both distances, the periods of the acceleration are in the range 0.308-0.328, which is close to the nonlinear period of the breathing mode. In other words, these periods are governed by the volume oscillations, providing another indication that the linear acceleration is generated by the volume oscillation and it is not significantly affected by bubble deformation, at least when this is not too large.
Figure 2.11 Time evolution of the acceleration of the left bubble for two different distances $D = 2.8$ (---) and $D = 5$ (--). The two bubbles are equal with $R_{in} = 30 \mu m$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$ and $R_{\infty} = 30$.

Figure 2.12 shows the location of the centers of mass for $D = 2.8$ and $D = 5$. As we anticipated, the time needed for the two bubbles to approach each other increases with the distance. When the initial distance, $D$, is set at $2.8$ simulations stop at $t = 0.914$, while when $D = 5$, simulations stop at $t = 2.61$. In both cases the bubbles have approached each other so much that the computations fail to converge. Figure 2.13 presents the evolution of the coefficients of the $P_2 - P_6$ Legendre polynomials for $D = 5$. These may be compared to the coefficients of the modes for $D = 2.8$, which were given in figure 2.10b. Examining the evolution of the coefficients of $P_2$, $P_3$ and $P_4$ makes plain that the final bubble shapes are less squeezed when they are initially closer together, although their initial acceleration is higher, and their deformations described by higher modes, such as $P_3$ and $P_4$, are less significant too, since there was not enough time for them to increase.
Figure 2.12 Time evolution of the location of the centers of mass for two different distances $D = 2.8$ (---) and $D = 5$ (—). The two bubbles are equal with $R_{hi}^* = 30\mu m$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$ and $R_\infty = 30$.

Figure 2.13 Time evolution of the coefficients of the Legendre polynomials $P_2 - P_6$ for two equal bubbles with $R_{hi}^* = 30\mu m$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 5$ and $R_\infty = 30$.

Keeping the initial distance at $D = 5$ and increasing the bubble size to $R_{hi}^* = 100\mu m$ and even more to $R_{hi}^* = 1mm$, results in even more deformed shapes. The deformations are limited
again in the rear bubble side, while the front side remains almost spherical. Such shapes have also been reported by Pelekasis and Tsamopoulos 1993, and have called spherical-cap shapes, because of the resemblance of their front side at least to the classical spherical-cap shapes reported by Davis and Taylor 1950. Computations now fail before the two bubbles come very close together due to the large amplitude deformations. Figure 2.14a shows selected shapes of the two bubbles for the case with $R^*_m = 1 \text{mm}$ in water ($Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 5$), while figure 2.14b shows the time evolution of the coefficients corresponding to the Legendre polynomials $P_2$, $P_4$, $P_5$, $P_{12}$, and $P_{13}$. The lowest surface mode $P_2$ is again the dominant one throughout the simulation but after $t \cong 0.13$ even higher modes start to arise and finally $P_{12}$ and $P_{13}$ dominate the shape of the bubble. This can be verified by noticing the 13 lumps that have developed in the shapes of the two bubbles in figure 2.14a. Linear frequencies of the breathing mode and of the $P_{12}$ and $P_{13}$ modes are $\omega_0 = 76.05$, $\omega_{12} = 44.857$ and $\omega_{13} = 50.332$, respectively, showing that subharmonic excitation of these modes can occur and dominate the shape of the bubbles.
Figure 2.14 (a) Spherical cap shapes of the bubbles at $t = 0.15, 0.165, 0.18, 0.187$ and (b) time evolution of the Legendre polynomials $P_2, P_4$ and $P_5$ for two equal bubbles with $R_{bi} = 1mm$, $Oh^{-1} = 269.63$, $P = 1375.51$, $c = 1$, $D = 5$ and $R_{\infty} = 30$.

In an attempt to explain the formation of the so-called “bubble grapes”, it has been shown by Peleaksis et al 2003 and Mettin 1997, that bubbles at very large distances from each other in an oscillatory pressure field can accelerate towards or away from each other or remain at a constant distance after a very large number of cycles of volume oscillations. One of the basic assumptions made in these studies was that the bubbles could retain their spherical shape and weak viscous effects were introduced, in the form of boundary layers around each bubble in the first of the above studies. To test the viability of large bubbles to retain their spherical shapes while they undergo volume oscillations and accelerate along their common axis we examined bubbles of radius of $1mm$ and increased their initial distance $D$ to $9.9$. The bubble size is larger whereas their distance is smaller, than those examined in these papers. Hence their interaction and acceleration will be stronger here, which should lead to shape instabilities faster. On the other hand, we have included in the present model viscous forces in full and examine a step change in pressure and not an oscillatory one, which could lead to resonance with the forcing frequency as well. This large interbubble distance requires more elements to be used in order to retain the accuracy of our computations. Unfortunately, this distance cannot be increased further, given our hardware/software configuration, without
compromising accuracy. Fairly soon the bubbles are seen to develop spherical-cap shapes and short waves on their back side, although one would have expected that viscous damping could prevent the higher modes from growing. The computations fail before the interbubble distance decreases even to 9. Due to the corrugated surfaces and the microflow that arise within each trough we have refined the mesh, but the computations could not proceed much further even with the denser mesh. Selected bubble shapes are given in figure 2.15 for the right bubble, while the left one will be symmetric, as the two bubbles are equal.

Figure 2.15 Spherical cap shapes of the right bubble at $t = 0.19, 0.2, 0.22, 0.226$. The two bubbles are equal with $R'_{ni} = 1\text{mm}, \text{Oh}^{-1} = 269.63, P = 1375.51, \varepsilon = 1, D = 9.9$ and $R_{oo} = 30$. The left bubble is completely symmetric.
Similar shapes for $R_{bi}^* = 1 mm$, at a large initial distance between the two bubbles but for much lower disturbance amplitude have been observed by Pelekasis and Tsamopoulos 1993. It is noteworthy, that due to the absence of viscosity there, the bubble shapes were even sharper and these irregularities arose earlier Pelekasis 1991. On the contrary, the shapes predicted here are much smoother because of the complete accounting of the effect of viscous forces. As can be seen in figure 2.15b, where the evolution with of selected Legendre coefficients is given, $P_2$ is the dominant mode until $t \cong 0.16$. Subsequently, modes higher than $P_{15}$ start to increase abruptly almost simultaneously. At $t \cong 0.2$, figure 2.15a shows that the bubbles tend to return to their spherical shape, as all higher modes become negligible and $P_2$ becomes the dominant mode again. A little later the higher modes increase again. The period of the zeroth mode at the later stages of the simulation is found to be 0.058, figure 2.15b, while $P_{19}$ oscillates with a period 0.0256 and modes $P_{19} - P_{15}$ and $P_{20}$ are oscillating with a frequency 0.032 approximately. This points to subharmonic resonance of all these modes with the breathing mode, although their eigenfrequencies cannot all be twice the eigenfrequency of the breathing mode.

In order to extract a more general rule governing the force that develops between the two bubbles and examine weather the Bjerknes prediction that this force is inversely proportional to the square of the bubble distance still holds, we performed a number of computations with $R_{bi}^* = 35 \mu m$, $R_{bi}^* = 100 \mu m$, $R_{bi}^* = 500 \mu m$ and $R_{bi}^* = 1 mm$, when this distance is $D = 2.8$, 3.5, 4, 5, 8 and 9.9, while remains $\varepsilon = 1$. The average acceleration is obtained as before over the first period of the particular volume oscillations. Figure 2.16 shows the resulting linear acceleration $\langle g \rangle$ values versus $1/D^2$ for all the above cases and the linear best fits to approximate the three data sets. The expressions for these lines along with the correlation coefficient, $C$, and the standard deviation, $SD$, are,

\[
\begin{align*}
R_b^* = 30 \mu m, & \quad \langle g \rangle = 0.104 + 10.123/D^2, & C = 0.983, & \quad SD = 0.092 \\
R_b^* = 100 \mu m, & \quad \langle g \rangle = 0.312 + 37.896/D^2, & C = 0.994, & \quad SD = 0.203 \\
R_b^* = 500 \mu m, & \quad \langle g \rangle = 0.995 + 205.887/D^2, & C = 0.994, & \quad SD = 1.067 \\
R_b^* = 1 mm, & \quad \langle g \rangle = 2.892 + 404.137/D^2, & C = 0.995, & \quad SD = 0.2
\end{align*}
\] (2.22)

It can be safely concluded that indeed the average acceleration, $\langle g \rangle$, scales linearly with $1/D^2$, even in when the viscosity of water is account for. This acceleration increases
dramatically with the bubble size. According to Bjerknes prediction:

\[ F_1^* \sim V_1^* \left( \frac{V_2^*}{D^2} \right) \sim V_1^* \left( \frac{R_{b2}^* + \varepsilon \sin \omega t^*}{D^2} \right)^3 \sim V_1^* \left( \frac{R_{b2}^* \varepsilon^2 \sin^2 \omega t^*}{D^2} \right), \]

the average acceleration, \( \langle g \rangle \), is proportional to \( R_b^* \) and \( \varepsilon^2 \). From equations (2.22) can be seen, that as the size of the bubbles increases, the slope is proportional to \( R_b^* \) for two bubbles of equal size, while it deviates at smaller bubbles, because of the different viscous drag applied to bubbles of different size and deformation from the spherical shape.

![Figure 2.16 Variation of the average acceleration of the left bubble with the initial distance between the two centers of mass for \( R_{bi} = 30 \mu m \) (●), \( R_{bi} = 100 \mu m \) (▲), \( R_{bi} = 500 \mu m \) (●) and \( R_{bi} = 1 mm \) (■) and \( \varepsilon = 1 \). The two bubbles are equal.](image)

2.4.2.3 Effect of the disturbance amplitude, \( \varepsilon \)

Next we examine the importance of the magnitude of the step change in pressure to initiate bubble attraction in a viscous liquid. In typical experiments values smaller than \( \varepsilon = 1.2 - 1.4 \) have been employed, so it reasonable to examine smaller values than those in the previous sections. As discussed in section 4.2.1, decreasing the disturbance amplitude, increases the period of volume oscillations, because the pressure at infinity will increase less than before; see eq. (2.16). This should lead to a decrease in the average acceleration of the bubbles and consequently to an increase in the time needed for the two bubbles to approach.
each other. First, cases of bubbles up to $80 \mu m$ in water and initial distance $D = 2.8$ are examined. When $\varepsilon = 1$, it was shown that bubbles larger than $30 \mu m$ deform at their rear side. Decreasing the amplitude $\varepsilon$ to 0.2, the bubbles remain almost spherical until the end of the simulations even when their initial radius is $80 \mu m$. Figure 2.17 shows the coefficients $C_0$ and $C_2$ of the $P_0$ and $P_2$ Legendre polynomials, respectively, which compose the bubble surface for bubble radius $40 \mu m$ in water ($Oh^{-1} = 53.926, P = 55.02$), at an initial distance 2.8 with a disturbance amplitude 0.2 and 1.

![Figure 2.17](image)

Figure 2.17 Time evolution of the coefficients of the Legendre polynomials (a) $P_0$ and (b) $P_2$ for two different disturbance amplitudes, $\varepsilon = 0.2$ (---) and $\varepsilon = 1$ (—). The two bubbles are equal with $R_{bi} = 40 \mu m$, $Oh^{-1} = 53.926$, $P = 55.02$, $D = 2.8$ and $R_\infty = 30$.

Clearly, the $C_0$ coefficient, which is related to volume oscillations, demonstrates that when $\varepsilon$ is decreased to 0.2 the period of volume oscillations increases, while their amplitude decreases, in comparison to the case with $\varepsilon = 1$. It is also noteworthy that for $\varepsilon = 0.2$, the value of the period is very close to the one predicted from the linear theory. More specifically, linear theory predicts that for the above parameters, $T_\infty = 0.407$ while from the nonlinear simulations this value is 0.409 for $\varepsilon = 0.2$. When $\varepsilon$ increases to 1 the period decreases to 0.285. Moreover, the coefficient of the $P_2$ mode makes clear that the bubble retains a more spherical shape until the end of the simulations when $\varepsilon$ is decreased to 0.2, although it alternates between oblate and prolate configurations with a constant trend towards an oblate one. Figure 2.18 shows the evolution of the centers of mass of the two bubbles for the same
two cases. We find that the time needed for the two bubbles to approach each other increases, in the case of $\varepsilon = 0.2$, allowing the simulations to proceed to much longer times. The average acceleration over the first period of volume oscillations decreases dramatically from 2.068 when $\varepsilon = 1$ to 0.135 when $\varepsilon = 0.2$, while the best fits to the bubble distances with time give,

\begin{align*}
D_{\text{average}} &= 2.864 - 1.47 t - 0.326 t^2, \quad \varepsilon = 1 \quad (2.23a) \\
D_{\text{average}} &= 2.822 - 0.076 t - 0.052 t^2, \quad \varepsilon = 0.2 \quad (2.23b)
\end{align*}

Figure 2.18 Evolution of the centers of mass for two different disturbance amplitudes, $\varepsilon = 0.2$ (---) and $\varepsilon = 1$ (—). The two bubbles are equal with $R_{\mu} = 40 \mu m$, $Oh^{-1} = 53.926$, $P = 55.02$, $D = 2.8$ and $R_{\infty} = 30$.

In order to examine whether the dependence of the acceleration on the disturbance still follows our prediction for inviscid liquids (Pelekasis and Tsamopoulos 1993a), i.e. that it increases proportionately to $\varepsilon^2$, we also carried out simulations for $\varepsilon = 0.1$, 0.3 and 0.5. Figure 2.19 shows that indeed the average acceleration follows this dependence, while the linear expression that best fits these data points is

$$\langle g \rangle = 0.028 + 1.913 \varepsilon^2$$

(2.24)

This occurs as in Pelekasis and Tsamopoulos 1993a, in spite of the fact that the bubble radii are very small here. In order to directly compare with the results in fig. 9 of Pelekasis and Tsamopoulos 1993a, we increased the bubble radii to 1 mm ($Oh^{-1} = 269.63$, $P = 1375.51$), set
their initial distance at 2.5 and the amplitude to 0.3. In this earlier work, the average acceleration over the first period of volume oscillations was found to be 7.198, whereas it decreases, as it should, to 6.72, because of the viscous damping in the present simulations.

![Figure 2.19](image)

**Figure 2.19** Variation of the average acceleration of the left bubble with the disturbance, $\varepsilon$, for $R_\infty = 40\mu m$, $Oh^{-1} = 53.926$, $P = 55.02$, $D = 2.8$ and $R_\infty = 30$.

Retaining all the physical parameters to their previous values, except for the initial interbubble distance, which we increase to 2.8, we find that the two bubbles deform at their rear side and flatten at the front, an image similar to this of $\varepsilon = 1$. Due to the lower disturbance at the pressure at infinity and as expected, the time needed for the two bubbles to approach increases relative to the case that $\varepsilon = 1$, the average acceleration decreases and consequently the deformations of the bubble surfaces are less intense. If the initial distance between the two bubbles is increased further to 9.9 while the size of the bubbles remains at 1 mm and $\varepsilon$ at 0.3, the average acceleration decreases from 5.503 that was for $\varepsilon = 1$ to 0.698 for $\varepsilon = 0.3$. Now the bubble shapes that arise towards the end of the simulations are wavy in both their front and rear sides. Such shapes were named “globally deformed shapes” by Pelekasis and Tsamopoulos 1993a and are clearly distinct from the “spherical-cap” predicted above when $\varepsilon = 1$ (figure 2.15). The smaller disturbance amplitude combined with the viscous resistance to flow, produce this decrease in the average acceleration, which, in turn, is not sufficient to stabilize the front bubble surface as it did in the spherical cap shapes. Figure
2.20a shows the evolution of the shape of the right bubble for these parameters. As the time needed for the two bubbles to approach increases due to the large distance and the small disturbance, there is enough time for even higher and higher modes to arise. The Legendre decomposition of the shape of the bubbles shows significant growth of high modes, figure 2.20b. Until \( t = 0.45 \) \( P_2 \) is the only mode that is can be seen. After \( t = 0.45 \) higher modes start to appear and finally \( P_{10} \) and \( P_{11} \) become dominant in the bubble shape due to subharmonic resonance with the zeroth mode. Indeed, the eigenvalues are \( c_0 = -0.0074 \pm 76.05i \), \( c_{10} = -1.013 \pm 34.55i \) and \( c_{11} = -1.204 \pm 39.59i \), indicating a very slow damping of the zeroth mode, but also that its eigenfrequency is two as that of these two higher modes.
Figure 2.20 (a) Shapes of the right bubble at $t = 0.5, 0.55, 0.6, 0.651$ and (b) time evolution of the coefficients of the Legendre polynomials $P_2$, $P_{10}$ and $P_{11}$. The two bubbles are equal with $R_{bi}^* = 1 mm$, $Oh^{-1} = 296.63$, $P = 1375.51$, $\varepsilon = 0.3$, $D = 9.9$ and $R_{\infty} = 30$. At the later stages of the simulation globally deformed shapes arise.

Pelekasis and Tsamopoulos 1993a, determined that the appearance of the two distinct types of bubble shapes that they observed in their inviscid simulations, namely “spherical cap shapes” and “globally deformed shapes” depended on the Bond number, $Bo = (gR_{bi}^*\rho^* / \sigma^*)$, which measures the relative importance of buoyancy and surface tension. When the ambient pressure was 1 atmosphere, they found that when $Bo > 1.5$, spherical-cap shapes appear, whereas when $Bo < 1$ the entire interface deformed. For a pair of equal bubbles and following the present characteristic scales $Bo$ is identical to the average acceleration $\langle g \rangle$. So it we can readily examine weather a similar rule applies when viscous forces are included in the model. Table 2.3 presents most of the cases which we have run until either the bubbles came too close to each other or computations failed to converge and the final shapes we observed in each case.
Table 2.3 Observed final bubble shapes depending on the bubble size, distance and disturbance amplitude.

<table>
<thead>
<tr>
<th>( R_{\text{so}} )</th>
<th>( D )</th>
<th>( \varepsilon )</th>
<th>( \langle g \rangle )</th>
<th>Bubble shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 ( \mu \text{m} )</td>
<td>2.8</td>
<td>1</td>
<td>0.078</td>
<td>almost spherical</td>
</tr>
<tr>
<td>10 ( \mu \text{m} )</td>
<td>2.8</td>
<td>1</td>
<td>0.256</td>
<td>almost spherical</td>
</tr>
<tr>
<td>20 ( \mu \text{m} )</td>
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<td>1</td>
<td>0.724</td>
<td>oblate</td>
</tr>
<tr>
<td>35 ( \mu \text{m} )</td>
<td>2.8</td>
<td>1</td>
<td>1.265</td>
<td>spherical cap</td>
</tr>
<tr>
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<td>1</td>
<td>0.543</td>
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</tr>
<tr>
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<td>0.2</td>
<td>0.137</td>
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</tr>
<tr>
<td>100 ( \mu \text{m} )</td>
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<td>1</td>
<td>1.975</td>
<td>spherical cap</td>
</tr>
<tr>
<td>1 \text{mm} )</td>
<td>2.8</td>
<td>1</td>
<td>51.188</td>
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</tr>
<tr>
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<td>0.3</td>
<td>6.028</td>
<td>spherical cap</td>
</tr>
<tr>
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<td>5</td>
<td>1</td>
<td>20.376</td>
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<tr>
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<td>1</td>
<td>5.503</td>
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</tr>
<tr>
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<td>9.9</td>
<td>0.3</td>
<td>0.698</td>
<td>globally deformed</td>
</tr>
</tbody>
</table>

Only in one simulation with large bubbles of 1 \text{mm}, resulting in a large \( Oh^{-1} \), i.e. negligible viscous effects, when they are far apart and under a small pressure perturbation, we predict globally deformed shapes. Clearly, all these factors allow high surface modes to appear and remain after extended oscillation and interaction between the bubbles. As the bubble size decreases, \( Oh^{-1} \) decreases and \( P \) increases leading to higher viscous and capillary forces and as the disturbance amplitude increases, the bubble interaction time decreases. All these favor the formation of bubbles that are either slightly deformed or have spherical cap shapes. Thus, the classification of the bubble shapes in inviscid liquids according to their acceleration only, does not seem to extend to viscous ones.

2.4.3 Bubbles of unequal size

When the two bubbles are unequal, the normal mode analysis shows that two sets of eigenmodes are involved even for in-phase oscillations. More specifically, the first set of breathing and surface modes involve deformations of the left bubble with eigenfrequencies that closely correspond to eigenfrequencies of an isolated bubble of the same size, while the right bubble remains nearly spherical. In the other set of eigenmodes the opposite situation
arises. As we will demonstrate next, the same principle arises in the nonlinear oscillations of unequal bubbles; primarily each bubble oscillates with its own zeroth mode frequency.

Figure 2.21a shows the time-variation of the volume of two unequal bubbles immersed in pure water, where the left one has radius $30 \mu m$ and is twice the radius of the right bubble, $R_{b2} = 0.5$. In all the simulations to follow the left bubble will be the larger one, hence $R_{b2} < 1$ and its radius will still provide the characteristic length for our simulations. Hence, in the present case $Oh^{-1} = 46.701$ and $P = 41.265$. The initial interbubble distance is $D = 2.8$ and the pressure in the far field increases by 100%, $\varepsilon = 1$. As already mentioned in the case of equal sized bubbles, viscosity causes a decrease in the amplitude of volume oscillation and an increase in the period. Coupling these effects with the nonlinear dynamics makes quite difficult the clear identification of a unique period. A closer look at figure 2.21a reveals that two maxima in volume oscillations of the larger (left) bubble and three maxima in volume oscillations of the smaller (right) bubble arise in about the same time interval. Calculating the linear periods for the two bubbles, we find $0.435$ and $0.214$ for the right and the left bubble, respectively, i.e. the period of the larger bubble is almost twice the period of the smaller one, a relation that is preserved in the nonlinear oscillations, explaining the observation in figure 2.21a. Figure 2.21b shows the evolution of the centers of mass with time. Again, the two bubbles attract each other subjected to the same attractive force. Then the right bubble accelerates much more towards the left than the other way around, just because its volume (added mass) is eight times smaller. Even in this aspect the interacting bubbles follow the rules of universal attraction. The combined center of mass, as it is calculated from eq. (2.18b), is not stationary any more, but it fluctuates around its value at $t = 0$. The best fit to the average interbubble distance with time now is

$$D_{\text{average}} = 2.778 - 0.222 t - 0.308 t^2$$  \hspace{1cm} (2.25)

Figures 2.21c, d show the velocities and the accelerations of the centers of mass of each bubble to undergo a rather complex oscillatory motion. The primary extrema in velocity and acceleration of the left bubble arise at times corresponding to the extrema in the volume oscillations of the right bubble and vice versa, demonstrating that the linear motion of one bubble is induced by the volume oscillations of the other one. The velocity and, especially, the acceleration of the smaller bubble seem to develop also a second twice as high frequency. As already mentioned in relation to figure 2.21a, two maxima in the volume oscillations of the left bubble take about the same time as three maxima of the right bubble and form a repeatable cycle of their combined motion. So, we calculate the average acceleration of each
bubble in the respective time interval and it to be 0.389 and 0.582, respectively. As already explained, the smaller bubble is moving faster compared to the larger one. When the two bubbles were equal, the average acceleration under the same conditions, was 1.23, i.e. greater than both values of acceleration when the right bubble has half the radius of the left. This is attributed to the fact that the interaction force is proportional to the volume of either bubbles and when even the right bubble alone decreases this force decreases as well.
Figure 2.21 Variation with time of the (a) volume (b) centers of mass, (c) velocity and (d) acceleration of both bubbles. The two bubbles are unequal with $R_{b1}^* = 30 \mu m$, $R_{b2} = 0.5$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 2.8$ and $R_\infty = 30$.

Figure 2.22a presents the time-evolution of the $C_2$, $C_3$ and $C_4$ coefficients of the corresponding Legendre polynomials, while Table 2.4a presents the eigenvalues of each bubble. The breathing frequencies are 13.406 and 27.284 for the left and the right bubble, respectively. Comparing these values, we conclude that the left bubble may undergo subharmonic resonance with its $3^{rd}$ and even its $4^{th}$ shape modes, while the right bubble may undergo subharmonic resonance with its $3^{rd}$ mode and harmonic resonance with its $4^{th}$ mode. Indeed, the evolution of the Legendre coefficients in figure 2.22a and of the shapes of the bubbles in figure 2.22b show that the left bubble remains almost spherical until $t \approx 0.8$ with a very small contribution from the $2^{nd}$ mode and, subsequently, the $3^{rd}$ and the $4^{th}$ modes arise almost simultaneously. As for the right bubble, the $2^{nd}$ mode prevails at the beginning of the simulations, while after $t \approx 0.7$, the $3^{rd}$ and somewhat later the $4^{th}$ start to arise also and
eventually dominate its shape. It may come as a surprise that the subharmonic resonances of the left bubble require more time to appear and are much less intense than even the harmonic resonance of the right bubble. The reason for that is the higher frequency of the right bubble, which introduces twice as many breathing cycles to it in comparison to the left.

Figure 2.22 (a) Time evolution of the coefficients of the Legendre polynomials $P_2$, $P_3$ and $P_4$, and (b) bubble shapes at $t = 0.738$, $0.886$, $1.034$, $1.287$ for two unequal bubbles with $R_{\text{b1}} = 30 \mu m$, $R_{\text{b2}} = 0.5$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 2.8$ and $R_{\text{s}} = 30$. The smaller (right) bubble is deformed.

Figure 2.23 presents contour plots of both velocity components and pressure at $t = 1.034$ in the same coordinate system used in figure 2.6. Since the two bubbles are not
equal any more, none of the three variables take the same values around them. According to figure 2.21a, at this time instant both bubbles happen to be in their expansion phase. This is confirmed by looking at the radial velocity, shown in the upper half of figure 2.23a. It is positive all around the deformed bubbles and larger in the segments of their surfaces facing away from each other. In the segments facing each other they are quite smaller, apparently because of the indentation of the smaller bubble at the axis of symmetry which is moving to the right and the linear velocity of both bubbles towards each other. The azimuthal velocity shown in the lower half of figure 2.23a is not symmetric with respect to the line $\theta = \pi/2$ originating from the center of this coordinate system, because of the inequality of the bubbles. The azimuthal velocity takes zero values at the axis of symmetry, $\theta = 0$ and $\theta = \pi$, as it should and at a line extending from the larger bubble to infinity at an angle $\theta = \pi/2$, also because both bubbles are expanding. The complicated motion of the deformed bubble shapes prevents a direct interpretation of the variation of the azimuthal velocity on the bubble surfaces.
Figure 2.23 Contours of (a) $u_\alpha$ (upper half), $u_\theta$ (lower half) and (b) $P$ at $t = 1.034$ for $R_{b1}^* = 30\mu m$, $R_{b2} = 0.5$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 2.8$ and $R_\infty = 30$.

The pressure field, shown in figure 2.23b, with respect to both velocities, takes much larger values here in comparison to figure 2.6b, because the dimensionless pressure is proportional to the bubble size, which is now larger. Moreover the pressure is larger near the smaller bubble in comparison to those near the larger just because of capillarity. In spite of all these asymmetries, the pressure reaches spherical symmetry at a distance of about 10 bubble radii from the center of the present coordinate system. At this distance its value is already quite close to the far field pressure, which is 82.53.

As explained above, increasing the radius of the right bubble to $R_{b2} = 0.75$, increases the average acceleration of both bubbles. Up to the instant that the computations diverged, the deformations for both bubbles are less significant than before and $P_2$ becomes the dominant
mode throughout the simulation. Keeping $R_{b2}$ to 0.75, but increasing the initial distance $D$ between the two bubbles to 5, will decrease again the average acceleration for both bubbles, giving time to higher shape modes to arise. The breathing frequencies, calculated using eq. (2.16), are 13.406 and 19.36 for the left and the right bubble, respectively. The most relevant eigenvalues for each mode are given in table 2.4b. So, for the left bubble the $P_3$ and $P_4$ modes are expected to arise via subharmonic resonance with the zeroth mode, while for the right bubble the $P_3$ mode is expected to arise. Figure 2.24 presents shapes of the two bubbles at selected times.

Figure 2.24 Bubble shapes at $t = 1.575, 1.674, 1.772, 1.907$ for two unequal bubbles with $R_{b1}^* = 30 \mu m$, $R_{b2} = 0.75$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 5$ and $R_c = 30$. The bigger (left) bubble is deformed.
In contrast to shapes given in figure 2.22b, now the left (larger) bubble is the one that deforms the most with $P_3$ the clearly dominant mode after $t \approx 0.9$. At the last stages of the simulation $P_4$ also increases for the left bubble while computations fail before the right bubble starts to deform because of the last distortions of the left bubble. Apparently, the larger size of the right bubble has two effects in comparison to the previous case: (i) the breathing frequencies of the bubbles are closer and can undergo about the same number of volume oscillations until the shape deformations become prohibitive and (ii) the stabilizing capillary force remains more significant in the smaller (right) bubble keeping the left bubble more susceptible to shape deformations. It is noteworthy, that in figure 2.22b up to the end of the simulations at $t=1.307$ the left bubble was only slightly deformed, whereas in figure 2.24 it gets highly deformed much later, at $t=1.937$. In both cases we have kept the same size for the left bubble resulting in the same characteristic time scale.

If the size of the left bubble is now increased to $100 \mu m$ and for all the cases mentioned above the observations remain quite the same. The average acceleration increases with the size of the right bubble and decreases with the distance. Since now $Oh^{-1}$ increases to 85.26 and $P$ to 137.55 the deformations of the bubble shapes become more significant. When the radius of the right bubble is half that of the left one $R_{b2}=0.5$ and $D=2.8$, the smaller bubble is the one that deforms significantly, while the larger one remains almost spherical until the time computations fail to converge. When the initial distance is set to $D=5$ and $R_{b2}=0.5$ still the smaller bubble is the one that deforms and as can be seen from figure 2.25. The breathing frequencies that linear theory predicts are 24.17 and 48.6 for the left and the right bubble respectively, while the eigenmodes for each bubble are given in Table 2.4c. As can be seen in figure 2.25, the left bubble does not deform before the end of simulations, while in the right bubble subharmonic resonance with the fourth mode causes the increase of $P_4$, which finally dominates its shape and leading to failure of convergence of our computations. This picture is inverted when the size of the right bubble is increased to 0.75. As in the case of $R_{b1}^{c}=30 \mu m$, the left bubble is the one that deforms the most.
Figure 2.25 Bubble shapes at \( t = 0.45, 0.47, 0.49, 0.505 \) for two unequal bubbles with \( R_{61} = 100 \mu m, R_{62} = 0.5, Oh^{-1} = 85.26, P = 137.55, \varepsilon = 1, D = 5 \) and \( R_\infty = 30 \). The smaller (right) bubble is deformed, while the bigger one (left bubble) remains almost spherical.
(a) $R_{b1}^* = 30\mu m$, $R_{b2} = 0.5$, $Oh^{-1} = 46.701$, $P = 41.265$ and $D = 2.8$

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(b) $R_{b1}^* = 30\mu m$, $R_{b2} = 0.75$, $Oh^{-1} = 46.701$, $P = 41.265$ and $D = 5$

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(c) $R_{b1}^* = 100\mu m$, $R_{b2} = 0.5$, $Oh^{-1} = 85.26$, $P = 137.55$ and $D = 5$

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Table 2.4 Eigenvalues $c_l$ and first periods for unequal bubbles.
2.5 Conclusions

The motion of two equal or unequal gas bubbles immersed in pure water and subjected to a step change in ambient pressure at the far field was studied. The present study covered a wide range of bubbles sizes, $5\mu m - 1 mm$. In contrast to previous works, viscous forces were fully accounted for and shape deformations were allowed. Our newly developed finite element methodology based on generating the computational mesh to follow the large deformations of the bubbles and to become finer near the bubble surfaces in order to resolve the sharp boundary layers that may arise there proved to be accurate, robust and versatile.

The step change in pressure induces volume oscillations on the two bubbles. The volume oscillations of one bubble generate a secondary pressure field to the ambient liquid which accelerates the other bubble along their common axis of symmetry. This acceleration is known as ‘Bjerknes effect’ and in neglecting viscosity and bubble deformations it has been shown to follow a law similar to Newton’s law of universal attraction, i.e. it is proportional to the volume of the two bubbles and inversely proportional to the distance of their centers:

$$F_i \sim V_i \left(g_t \sim V_i \left(\frac{V_i}{D}\right)\right).$$

The two bubbles may attract or repel each other depending on their driving frequency, but in the case of a step change in pressure they always attract each other. Both volume oscillations and translational motion cause deformation of the bubble shapes.

With the present study, we have demonstrated that the principle of the ‘Bjerknes law’ still applies for viscous fluids and deformable bubbles as well, but there are certain new aspects to it: (i) The constant of proportionality in this law depends strongly on the viscous drag, (ii) the bubble deformation seems to be the rule rather than the exception for bubbles with $R_{bi} \geq 100\mu m$ and, most probably, it will lead to their breaking up in spite of the stabilizing of short waves by capillary and viscous forces, and (iii) their interaction force increases and, hence, the time needed for the two bubbles to approach each other decreases with $Oh^{-1}$, with the ambient pressure $P$ and the increase applied to it $\varepsilon$ to set them in motion, all three of these parameters decrease the period of the breathing mode.

More specifically, as the size of the bubbles increases and consequently $Oh^{-1}$ increases, surface modes arise of order which depends on their spectrum of eigenvalues, which, in turn, depends on their size and applied disturbance in pressure. The interbubble distance affects bubble deformation by giving more or less time to these to develop. When the two bubbles are equal and their initial distance is quite small, they remain almost spherical.
until the end of the computations when their size is very small (5 μm), or they take an oblate shape for 5 μm < \( R^*_b \leq 20 \mu m \), or finally deformations arise and are kept at their rear side for \( R^*_b > 20 \mu m \). Increasing their initial distance \( D \) and the bubbles are relatively large \( R^*_b \geq 100 \mu m \) these Rayleigh-Taylor-type instabilities increase substantially and the computations fail to converge after some time. When the two bubbles are set far enough from each other globally deformed shapes appear. Decreasing the disturbance amplitude, \( \varepsilon \), the time needed for the deformations to appear increases while the bubbles remain almost spherical till the end of the computations even for \( R^*_b = 80 \mu m \). With unequal bubbles, the ratio of their radii \( R_{b1} / R_{b2} \) and their initial distance seems to determine whether the smaller or the larger bubble will deform. When \( R_{b1} / R_{b2} = 2 \), the smaller bubble is the one that deforms independently of the initial distance between the two bubbles. As the ratio \( R_{b1} / R_{b2} \) decreases, deformation of the smaller, the larger or of both bubbles depends on their initial distance and the Oh number. As with equal bubbles, higher modes arise as \( Oh^{-1} \) increases.
CHAPTER 3

Viscous Effects On Two Interacting And Deformable Bubbles Under An Oscillatory Pressure Field

3.1 Introduction

The principle of the primary Bjerknes forces on bubbles was first formulated by Bjerknes (1906, 1909). These forces are active in any pressure field containing a pressure gradient. Therefore, in a focused acoustic field, if the forcing frequency is below the resonance frequency for volume pulsations of the bubbles, they will travel to the focal pressure antinode, whereas if the forcing frequency is larger than the resonance frequency for volume pulsations of the bubbles, they will travel away from the focus. The first who gave the satisfactory explanation of the origin of this phenomenon was Blake (1949). Since then, there have been several associated observations of interest. Miller (1977) describes how large bubbles move to pressure nodes in a standing-wave field. Crum and Eller (1969) used photographic techniques to measure translational bubble speeds in a stationary-wave field. Experiment and theory agreed for rectilinear motion, but the bubble translation became erratic above a threshold acoustic pressure, which appeared to coincide with the threshold for the erratic dancing motion of bubbles trapped by radiation forces close to the pressure antinode.

Bjerknes also discovered that when two bubbles are pulsating in an acoustic field, another one force also arises from the pressure field radiated from one pulsating bubble acting on the other one. This force is known as mutual or secondary Bjerknes force. When two bubbles are driven by a soundfield, it will tend to lock the two bubbles to a certain phase difference: if both bubbles are larger or both smaller than the resonant size corresponding to the frequency of the applied soundfield, they will tend to oscillate in phase and to attract each other. On the contrary, if one bubble is larger and the other smaller, they oscillate out of phase and repel each other. Pelekasis and Tsamopoulos (1993b) simulated bubbles of 1mm, equal and unequal, in water, under a variety of forcing frequencies, \( \omega_f \), and for amplitude, \( \varepsilon \), relative small, \( \varepsilon = 0.3 \). They found agreement with the Bjerknes theory on both equal and unequal bubbles. Also, they observed either a tendency towards bubble breakup due to intense shape oscillations or violent collapse while maintaining their spherical shape due to transient
cavitation, as the amplitude of the sound wave increases. More details about the primary and secondary Bjerknes force are given in chapter 2, where the motion of two bubbles due to a step change in pressure is studied.

Other experimental observations under very high amplitude of the acoustic pressure, have revealed the formation of bubble grapes or acoustic streaming. In the first one a number of bubbles are seen to arrange themselves forming structures reminiscent of bunches of grapes while in the second one bubbles are generated at certain points in the liquid, move along paths towards a focal point, where they seem to rearrange forming larger or smaller bubbles. In both cases the interbubble distance seems to remain approximately constant. This cannot be directly attributed to one of the Bjerknes forces, since it seems that it requires that the direction of the Bjerknes force changes in time or with interbubble distance. In an attempt to explain it, Oguz and Prosperetti (1990) argued that this is possible when the forcing frequency lies outside the range of the eigenfrequencies resulting in bubble attraction, but its second harmonic, which becomes important at high amplitudes, lies between this range, resulting in bubble repulsion. This idea offer an explanation, but has at least two weaknesses: (i) The amplitude of the second harmonic is necessarily smaller than that of the first harmonic and (ii) it is also possible that the third and higher harmonics with frequency again outside the range of eigenfrequencies will arise inducing bubble attraction once more. An alternative explanation and numerical simulations to support it has been offered by Mettin et al. (1997). They studied the interaction between two spherical bubbles whose separation distance remains much larger than their radius, of the order of 100 radii. They observed that a sign inversion in the Bjerknes force arise, as the distance between the two bubbles decreases. Barbat et al. (1999) observed in their experiments that two bubbles in an incompressible liquid can undergo stable, periodic translational motion. However, all the above researchers have considered both inviscid liquid and irrotational flow and large initial distance between the bubbles compared to their radii. More recently, Pelekasis et al. (2004) included viscous boundary layers around each bubble which remained spherical because they maintained the large interbubble distance and carried out very extensive numerical experiments. They found that for bubbles up to 100μm in water, increasing the amplitude, ε, the translational velocity of the two bubbles can change sign, from repulsive to attractive, primarily when conditions are close to those of the Blake threshold.

In the present study, we examine the motion of two initially static and spherical bubbles induced by an acoustic field, including both viscous forces and bubble deformation and translation. In § 3.2 we give a brief account of the specific features of the problem treated
here. The formulation of the problem, the governing equations and the solution method are given in detail in chapter 2. In § 3.3.1 and § 3.3.2 we give results of equal and unequal size bubbles, respectively. Finally, conclusions are drawn in § 3.4.

3.2 Problem Formulation

The flow field examined here is similar to that in chapter 2 with the exception of the initial disturbance. More specifically, we study the motion of two gas bubbles in water. The two bubbles are initially spherical of radii $R_{b1}$ and $R_{b2}$ for the left and right bubble respectively and located initially at a distance $D$ between their two centers of mass. All lengths are scaled with the radius $R_{b1}$ of the left bubble, while surface tension $\sigma^*$ and liquid density $\rho^*$ are used for making velocity, pressure, time and forcing frequency dimensionless.

The dimensionless number that arises is the Ohnesorge number, $Oh = \left( \frac{\mu^2 R_{b1} \sigma}{\rho^2 \rho^* R_{b1} \sigma} \right)^{1/2}$, measuring the ratio of viscous to inertia and capillary forces. That importance of the latter also arises in the value of the dimensionless pressure because of the way it has been made dimensionless.

At time $t \geq 0$, an acoustic pressure field is applied at infinity and given in dimensionless form by

$$P_\infty = P \left(1 + \varepsilon \cos \omega_f t \right)$$

(3.1)

where $\varepsilon$ is the measure of the disturbance and $\omega_f$ the forcing frequency. Because of the small bubble size and interbubble distance, we will assume that the initial and the applied pressure field are uniformly distributed in space. For air bubbles in viscous liquids the linear resonance frequencies for volume oscillations are given by Minnaert’s (1933) formula, corrected to include viscous effects due to the normal stress at the bubble’s interface,

$$\omega_{io}^* = \frac{1}{R_{io}^* \sqrt{\rho^*}} \left[ 3 \gamma \left( P^* + \frac{2\sigma^*}{R_{io}^*} \right) - \frac{4 \mu^*}{\rho^* R_{io}^*} \right]^{1/2}.$$  

(3.2)

In the following, the modes corresponding to the natural volume or radial oscillations of each bubble (zeroth mode) will be referred to as breathing modes. The rest of the eigenmodes inducing deformations to the bubble shapes, and for this reason called shape modes, will be represented by the Legendre modes obtained through Fourier decomposition of the shape in a spherical coordinate system based on the instantaneous center of mass of each bubble.
The full Navier-Stokes equations are solved, neglecting gravitational effects. These are negligible because of the small bubble size resulting in a very small gravitational Bond number which is a measure of the relative importance of buoyancy and surface tension and given by \( Bo = \frac{(g^* R_b^2 \rho^*)}{\sigma^*} \). For gas bubbles with radius of the order of 1 mm, which are the bigger bubbles that studied here, surrounded by water at 20°C, the gravitational Bond number is 0.135 and thus gravity can be neglected. The two gas-liquid interfaces are treated as moving surfaces subject to a local force balance between capillary forces, viscous stresses in the liquid and pressure difference between the gas in the bubble and the surrounding liquid and moving according to the usual kinematic condition. All equations are solved by a finite element/ Galerkin method coupled with the implicit Euler for time integration. The highly deforming interfaces are accurately computed by a block-structured mesh, which closely and accurately follows the deformation of their surfaces. At each time step, the flow equations are solved along with the mesh equations using Picard iterations.

More details about the problem, the finite element/Galerkin method and the mesh equations are given in chapter 2.

3.3 Results

In order to thoroughly examine the importance of the large number of parameters arising in this problem and try to identify conditions that do not follow the Bjerknes principle we have carried out a very large number of extremely time-consuming simulations. Most cases requires between 2 and 6 weeks of real time in our dual-core Xeon cluster. Moreover, to make these calculations affordable without any compromise in the accuracy we had to keep the interbubble dimensionless distance below 10. A very crucial parameter is the forcing frequency because it can induce very different responses to this system. This depends on whether its value is below in between or above the range of the two eigenfrequencies of the breathing mode of each bubble and on whether it can induce harmonic or subharmonic resonance with them or with one of the two infinite but countable arrays of eigenfrequencies of the shape modes of each bubble. Luckily, capillary and viscous forces cutoff and damp, respectively, the large wavenumber disturbances on the bubble surfaces. Indeed in our simulations we did not predict shape modes corresponding to Legendre polynomials larger than \( P_{20} \). To ease the presentation we will discuss our predictions with an increase forcing of the forcing frequency.
First, equal size bubbles in an acoustic field will be studied in §3.3.1. In this case the two bubbles will always attract each other since only in phase oscillations can occur. Following this, unequal bubbles will be studied in §3.3.2. In this case the two bubbles can attract or repel each other depending on whether they oscillate in or out of phase respectively. In what follows, the two bubbles are immersed in water at $T^* = 20^\circ C$ temperature and $P^* = 1\, \text{bar}$ pressure. Hence the liquid properties relevant for this study are $\rho^* = 10^3\, \text{kg m}^{-3}$, $\mu^* = 10^{-3}\, \text{N s m}^{-2}$, $\sigma^* = 0.0727\, \text{N m}^{-1}$. The outer boundary is set always to $R_\infty = 30$, after trial and error and in order not to affect the flow around the two bubbles.

3.3.1 Bubbles of equal size

3.3.1.1 Larger bubbles, $R^* = 1\, \text{mm}$

In chapter 2 it was found that when bubbles of $1\, \text{mm}$ radius in water are set in oscillation by a step change in the far field pressure with amplitude $\varepsilon = 1$, spherical cap shapes start to arise at $t \approx 0.178$ when the two bubbles are initially at a distance $D = 9.9$. Turning now to a disturbance in pressure that oscillates with $\omega_r = 3.5$, and $\varepsilon = 1$, it is found that spherical cap shapes arise also but a little later, at $t \approx 0.182$. This delay in the excitation of the modes as compared with the case of a step change in pressure is because, on average, the periodic forcing provides less energy to the system. At $t = 0.239$ and before the external pressure completes a period $T_f = \frac{2\pi}{\omega_r} \approx 1.8$, calculations fail to converge due to the large deformations of the bubble surfaces that cause the growth of higher modes. Although the forcing frequency is very close to the frequency of the second shape mode ($c_z = -0.078 \pm 3.458i$), harmonic resonance does not have enough time to arise. Instead, the external forcing sets the bubble volume in oscillation with frequency not that of the forcing, but its own eigenfrequency which is much larger and hence it is excited first ($\omega_{0,i} = 76.05$, $i = 1, 2$). Subsequently, growth of the higher modes is caused by resonance with this zeroth mode and not with the second. This is something that should be expected since subharmonic resonance becomes evident when $t = O(1/\varepsilon)$, whereas harmonic resonance occurs when $t = O(1/\varepsilon^2)$, Hall and Seminara 1980. Figure 3.1 shows a sequence of shapes of the right
bubble at $t = 0.19$, $0.21$, $0.23$ and $0.239$. As the two bubbles are of equal size, the shapes of the left bubble are mirror images to those of the right one.

![Shapes of the right bubble for $R_y = 1\, mm$, $Oh = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 9.9$, $R_x = 30$ and $\omega_f = 3.5$ at $t = 0.19$, $0.21$, $0.23$, $0.239$. The two bubbles are equal and the left bubble is completely symmetric.](image)

**Figure 3.1** Shapes of the right bubble for $R_y = 1\, mm$, $Oh = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 9.9$, $R_x = 30$ and $\omega_f = 3.5$ at $t = 0.19$, $0.21$, $0.23$, $0.239$. The two bubbles are equal and the left bubble is completely symmetric.

![Variation with time of selected Legendre coefficients (a) $C_0$ and (b) $C_2$, $C_{18}$, $C_{19}$ of the shape of the bubbles. The two bubbles are equal while $Oh = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 9.9$, $R_x = 30$ and $\omega_f = 3.5$.](image)

**Figure 3.2** Variation with time of selected Legendre coefficients (a) $C_0$ and (b) $C_2$, $C_{18}$, $C_{19}$ of the shape of the bubbles. The two bubbles are equal while $Oh = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 9.9$, $R_x = 30$ and $\omega_f = 3.5$. 
Figure 3.2 shows the evolution of the zeroth $C_0$, the second, $C_2$, the 18th, $C_{18}$, and the 19th, $C_{19}$, coefficients of the respective Legendre polynomials. Both figures 3.1 and 3.2 demonstrate that the $P_{18}$ and $P_{19}$ modes become dominant on the bubble shape during the last stages of the simulation. Before computations fail to converge the $C_{18}$ and $C_{19}$ coefficients oscillate with periods 0.038 and 0.028 respectively, while $C_0$ with 0.055, indicating once more that the very early appearance of the zeroth mode due to its very small period is followed by subharmonic excitation of these two shape modes.

A similar pattern appears if we increase the forcing frequency, $\omega_f$, to 6.3 which is now close to the frequency of the third mode $P_3$ $(c_3 = -0.1382 \pm 6.3344i)$. Again, spherical cap shapes arise that dominated by $P_{18}$ and $P_{19}$ before simulations fail to converge at $t = 0.284$. Looking at the evolution of the center of mass of the right bubble (figure 3.3) for $\omega_f = 0, 3.5$ and 6.3 it is obvious that the higher the forcing frequency is, the smaller the acceleration of the two bubbles towards each other and consequently even more time is needed for shape oscillations to arise.

![Figure 3.3](image.png)

**Figure 3.3** Evolution with time of the center of mass of the right bubble for $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 9.9$, $R_e = 30$ and three different forcing frequencies. The two bubbles are equal.
Moreover, the period of the oscillations increases with $\omega_f$, and an indication of period doubling exist when the frequency is increased to $\omega_f = 6.3$. More specifically, the last two periods of the oscillation of the center of mass observed for $\omega_f = 3.5$ tends to merge to one for $\omega_f = 6.3$. Period doubling in spherosymmetric oscillations of a single bubble has been predicted by Lauterborn, 1976 and Lauterborn & Cramer, 1981. Moreover the amplitude of volume oscillations is changing with time and is modulated by the forcing frequency. This can be observed in figure 3.4, which gives the evolution of volume of the right bubble for $\omega_f = 0, 3.5$ and 6.3.

Figure 3.4 Time evolution of the volume of the right bubble for $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 9.9$, $R_\infty = 30$ and three different forcing frequencies. The two bubbles are equal.

Here as $\omega_f$ increases, the maxima in the volume of each bubble increases as well and consequently more time is needed for the bubbles to complete a period of volume oscillation. It is also noteworthy that when $\omega_f = 6.3$ the period of volume oscillations and consequently that of $P_0$ increases from 0.053, as found from first interval, to 0.07 in the last interval, denoting once again the tendency of period doubling. In contrast to the case of the step change in pressure, $\omega_f = 0$, where the average acceleration was calculated mainly over the
first period of volume oscillations in order to provide a more representative property of each simulation, in the case of the oscillatory pressure it is calculated now over each period of the breathing mode and it is found that for \( \omega_f = 3.5 \) it is: \( \langle g \rangle = 5.47, 5.3, 4.69, 13 \), while for \( \omega_f = 6.3 \) it is: \( \langle g \rangle = 5.43, 4.79, 3.31, 2.7 \). In both cases over the first period of the breathing mode, the average acceleration is very close to its value for \( \omega_f = 0 \), which is \( \langle g \rangle = 5.5 \), but still below it. This is attributed to the fact that when the energy is varying in the far field the available energy in the system oscillates as well and on average it is less. Consequently, any long-time effect that is about to evolve in one direction during the first half of the period of the external forcing is reversed in the second half, thus generating a weaker net effect than in the case of the step change in pressure. As mentioned in chapter 2, the dimensionless average acceleration, \( \langle g \rangle \), coincides with the Bond number, \( Bo = (gR_{bi}P^* / \sigma^*) \), for a pair of equal bubbles. Pelekasis & Tsamopoulos (1993a) have shown that for ambient pressure 1 atm, when \( Bo \) is over 1.5, spherical cap shapes arise, whereas globally deformed shapes arise when \( Bo \) is below 1.0. In chapter 2 we found that this law was followed for large bubbles of 1 mm, where \( Oh^{-1} \) is large too and, consequently, viscous effects are negligible, although the discriminating value of \( Bo \) was found to be larger. In the case of the oscillatory pressure and for large bubbles, it seems that this principle is followed too, at least for the cases that studied above, considering that the observed shapes are smooth on their front and deformed on their back. It is noteworthy however, that the overall shape is not squeezed to resemble the typical spherical caps reported by Davies and Taylor (1950).

\[ 3.3.1.2 \text{ Smaller bubbles, } R^* = 30 \mu m \]

In order to study the effect of the oscillatory pressure and compare it to that of the step change in pressure for smaller bubbles we examined with parameters identical to a case that was studied in chapter 2. The size of the bubbles is reduced to 30 \( \mu m \) \((Oh^{-1} = 46.701, P = 41.265)\). The initial distance between their centers of mass is set at 5 and the disturbance \( \varepsilon \) at 1. When the two bubbles oscillate under a step change to far-field pressure with amplitude \( \varepsilon = 1 \), it was found in chapter 2, that the simulations failed to converge at \( t = 2.61 \) and after the bubbles have approached so much that coalescence seemed imminent. Additionally, according to figure 2.15 of chapter 2, the two bubbles assume an oblate shape, with \( P_2 \) the dominant mode throughout the simulation, while \( P_3 \) and \( P_4 \) start to grow at the
later stages of the simulation. Retaining all the other parameters the same and applying at the far-field pressure disturbance with frequency, $\omega_f = 3.5$, which is very close to the frequency of the second mode $P_2^\prime$ ($c_2 = -0.3524\pm3.3935i$), the behavior of the two bubbles is completely different. Figure 3.5 shows the evolution of the centers of mass of the two bubbles with time.

![Figure 3.5](image)

Figure 3.5 Evolution of the centers of mass with time of two equal bubbles with $R_m^* = 30\mu m$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 5$, $R_w = 30$ and $\omega_f = 3.5$.

In contrast to the case of the step change of the zeroth mode in pressure at infinity (figure 2.14 of chapter 2) where the two centers of mass follow a constant and oscillatory acceleration, here the two bubbles deviate very little from their centers of mass for a long time, but after $t > 1.38$ they start to accelerate abruptly towards each other. A little later and just before the far-field pressure completes a period, at $t = 1.576$, computations fail to converge. At this instant, the volume of each bubble, after having completed a period and started to increase abruptly at $t = 0.532$, reaches 9.3 times the initial volume of the bubbles at $t = 1.26$ and then drops rapidly, figure 3.6a. The interval between the second and the third maxima in volume oscillations is 0.914 denoting subharmonic excitation between the forcing frequency and the zeroth mode and explaining the rapid growth and collapse of the bubbles. No modes greater
than the third seem to be excited during the motion, figure 3.6b. Figure 3.6c gives shapes of the two bubbles at selected times.

Figure 3.6 (a) Evolution with time of the volume of the right bubble, (b) variation with time of $C_2$, $C_3$ and $C_4$ Legendre coefficients of the right bubble and (c) bubble shapes of the two bubbles at $t = 1.28$, $1.526$, $1.565$, $1.575$ for $R_{bi} = 30 \mu m$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 5$, $R_o = 30$ and $\omega_f = 3.5$. The two bubbles are equal.

As can be seen $P_0$ and $P_2$ are the dominant polynomials throughout the simulation, while $P_3$ starts to grow after $t \approx 1.56$. Apparently, towards the end of the rapid bubble collapse a strong
pressure change is felt in each bubble because of the collapse of the other one. This causes a quick and intense acceleration of both bubbles inducing a strong deformation at the rear side of the bubbles starting at $t = 1.565$ and ending a little later when the computations fail to converge. Figure 3.6c seems to indicate the formation of a jet emanating from the rear side of each bubble and rapidly moving towards its front side and could lead to the formation of a toroidal bubble. The first phase of rapid bubble growth and collapse is called transient cavitation and is often observed in cavitation experiments (Neppiras 1969). The second phase of jet formation from the bubble surface away from a solid wall and accelerating towards its opposite surface has been predicted in single bubble simulations (Blake 1949). Figure 3.7 presents contour plots of both velocity components and pressure at $t = 1.477$. The results are given in spherical coordinates with center located at the middle of the distance between the initial centroids of the two bubbles.
Figure 3.7 Contours of (a) $u_r$ (upper half), $u_\theta$ (lower half) and (b) $P$ at $t=1.477$ for $R_{bi} = 30 \mu m$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 5$, $R_o = 30$ and $\omega_f = 3.5$.

The radial velocity, which is given in the upper half of figure 3.7a, takes its highest and negative values at the rear side of the bubbles, while it takes positive values between the two bubbles, indicating that the two bubbles are simultaneously contracting and approaching each other. The azimuthal velocity, which is given in the lower half of figure 3.7a, is symmetric with respect to $\theta = \pi / 2$, as it should, since the two bubbles are equal and undergo in phase oscillations. Moreover, it takes negative values around the left bubble and positive ones around the right bubble, since the two bubbles contract, while it takes zero values at $\theta = 0$, $\theta = \pi$ and $\theta = \pi / 2$, because of the symmetries with respect to existing axis and plane of symmetry. The pressure field, which is given in figure 3.7b, forms contours lines around each bubble which turn into contour lines around both bubbles. It attains radial symmetry at a
distance equal to 8 radii from the center of this coordinate system, verifying that the locating
the outer boundary at 30 radii away does not affect the flow around them.

3.3.2 Bubbles of unequal size

3.3.2.1 Larger bubbles, $R^* = 1mm$

First we present cases where the radius of the left bubble is $1mm$. Therefore, $Oh^{-1}$ is
269.63 and the dimensionless pressure is 1375.51. The right bubble is considered to be
initially at a distance $D = 8$ away from the left and its radius to be 25% smaller than that of
the left bubble, i.e. $R_{b_2} = 0.75$. The forcing frequency is set at 6, which is close to the
frequency of the second mode of the right bubble, $\omega_{2,2} = 5.344$, and to the third mode of the
left bubble, $\omega_{3,1} = 6.334$, while $\varepsilon = 1$. Therefore, this value of the forcing frequency can cause
harmonic resonance with the 2nd mode of the right bubble and either subharmonic resonance
with the 3rd mode of the left bubble, since $\omega_{3,1} = 3.47$, or harmonic resonance with its 3rd
mode. However, none of these effects is observed, since other interactions evolve faster. More
specifically, the oscillatory pressure excites immediately volume oscillations of both bubbles.
Then, the $P_{10}$ ($\omega_{0,2} = 52.4$) and $P_{11}$ ($\omega_{1,2} = 60.05$) modes of the right bubble get excited
owing to subharmonic resonance with the breathing mode ($\omega_{0,2} = 101.4$) of the same bubble.
This leads to the globally deformed shapes with 10 lumps that can be seen in figure 3.8 where
shapes of the two bubbles are shown at $t = 0.19$, 0.2, 0.22 and 0.237.

Figure 3.8 Shapes of two unequal bubbles at $t = 0.19$, 0.2, 0.22, 0.237 for $R^*_b = 1mm$, $R_{b_2} = 0.75$, $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 8$, $R_e = 30$ and $\omega_f = 6$. 
Computations fail to converge at the next time step due to the large and global deformation of the right bubble and before the far field pressure completes even a period of oscillation. The larger size of the left bubble leads to a larger period of its breathing mode and, hence, to slower excitation of its shape modes. Indeed, it deforms globally later and with less intensity than the left bubble but seems to tend to return to its spherical shape just before computations fail to converge. As in the case of equal bubbles of size 1\,mm, harmonic resonance of the shape modes directly with the forcing does not have enough time to evolve, but resonance with the zeroth mode prevails.

Decreasing the initial distance between the two bubbles to half its previous value, $D = 4$, and keeping all the other parameters the same, is expected to change the excited shape modes and decrease the time needed for them to arise. This is because the secondary Bjerknes force increases, increasing the acceleration of the two bubbles. Indeed, figure 3.9a shows shapes of the two bubbles at selected times. The bubbles start to deform earlier than when the bubbles are equal, at $t = 0.17$, while computations fail to converge at $t = 0.194$ due to the growth of the high Legendre modes $P_{18}$, $P_{19}$, and $P_{20}$ of the left bubble. Figure 9b shows that these modes start oscillating with periods 0.037, 0.045 and 0.033 respectively, while the zeroth mode of the left bubble oscillates with period 0.06 implying subharmonic resonance between the breathing mode and the $P_{18}$-$P_{20}$ modes. As for the right bubble, counting the peaks in the variation of the $P_0$ in figure 9c, we find that they occur at $t = 0$, 0.039 and 0.071, indicating that no subharmonic resonance between the breathing mode and the forcing frequency exists as well. Moreover, given the period of oscillation of the other modes that could arise in this bubble, it does not seem that they can resonate either with the breathing or the forcing frequency. Calculating the average acceleration of the right bubble over the first four maxima in volume oscillations we find it to become very large, 19.73, indicating that the smaller interbubble distance makes the acceleration of the right bubble the dominant effect. Its $Bo$ number is 11.1, well above the critical range, for spherical cap shapes to arise. So, in this case, the larger (left) bubble is the one that deforms globally in shorter time, while the right one deforms only at its rear side remaining nearly spherical and its front side.
Figure 3.9 (a) Shapes of two unequal bubbles at $t = 0.17$, 0.18, 0.19, 0.194, (b) evolution with time of $P_0$, $P_2$, $P_{18}$, $P_{19}$, $P_{20}$ Legendre coefficients for the left bubble and (c) evolution with time of the Legendre coefficients $P_0$, $P_2$, $P_3$, $P_4$ for the right bubble and parameters $R_{91}^* = 1mm$, $R_{02} = 0.75$, $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 4$, $R_{\infty} = 30$ and $\omega_f = 6$. 
Next we decrease the radius of the right bubble to half that of the left one ($R_{b1}/R_{b2} = 2$). The initial distance between the bubbles is retained at $D = 4$, the forcing frequency is increased to 10.5, which is close to the frequency of the second mode of the right bubble, $\omega_{2,2} = 9.674$ and to the fourth mode of the left bubble ($\omega_{4,1} = 9.502$), and $\varepsilon = 1$.

Due to the high amplitude, $\varepsilon$, in pressure at infinity and the small initial distance of the two bubbles, acceleration becomes the dominant effect and eliminates any possibility for subharmonic resonance. The acceleration $\langle g \rangle$ for the right bubble is 2.26 over the first two periods of its volume oscillations occurring in the interval $t = 0 - 0.0488$, and increases to 5.73 over the next two periods, $t = 0.0488 - 0.10304$, while for the left bubble $\langle g \rangle$ is 1.819 and 3.63 over the first and the second periods of volume oscillation, respectively, occurring over the time intervals $t = 0 - 0.0507$ and $t = 0.0507 - 0.1082$, respectively. Since $\langle g \rangle$ is well above the critical range for both bubbles, spherical cap shapes should arise for both bubbles. Shapes of the two bubbles are shown in figure 3.10.

Due to the higher frequency of the breathing mode and higher acceleration of the smaller bubble, this is the one that deforms while the bigger one remains nearly spherical until computations fail to converge. The right bubble deforms mainly at the side that faces the left bubble, which should imply that it accelerates away from it. Instead, the smaller bubble undergoes large amplitude motion towards and away from the left bubble, which on average
result in bubble attraction. This can be seen in figure 3.11. Its deformation on its front side is in contrast to what we have seen so far and is initiated during a repulsion phase which starts at $t \approx 0.08$ and ends at $t \approx 0.1$. Subsequently, the deformation at its front side increases, although it has reversed its direction of linear motion, as seen in figure 3.11. These deformations are intense and computations fail to converge a little later at $t = 0.122$.

![Figure 3.11](image)

**Figure 3.11** Evolution with time of the centers of mass of the two bubbles for $R_{b1}^* = 1 \text{ mm}$, $R_{b2} = 0.5$, $O h^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 8$, $R_{\infty} = 30$ and $\omega_f = 10.5$.

Increasing the initial distance between the two bubbles to $D = 8$ and keeping all the other parameters the same, the smaller (right) bubble is again the one that deforms, while the left one remains almost spherical throughout the simulation. However, due to the smaller acceleration of the two bubbles, higher shape modes have time to arise and subharmonic resonance between the breathing mode ($\omega_{0,2} = 152.18$) and mode $P_8$ ($\omega_{8,2} = 70.14$) prevails deforming the right bubble globally, as seen in figure 3.12. Simulations fail to converge a little later than $t = 0.217$ due to exponential growth of the $P_8$ mode of the right bubble. On the other hand, in the left bubble, $P_2$ remains the dominant mode until the end of the simulation.
Figure 3.12 (a) Shapes of two unequal bubbles at $t = 0.18, 0.19, 0.2, 0.217$ and (b) evolution of the Legendre polynomials $P_2$ and $P_8$ of the right bubble with time for $R_{b1}^* = 1 \text{mm}$, $R_{b2} = 0.5$, $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 1$, $D = 8$, $R_\infty = 30$ and $\omega_f = 10.5$.

Next, we decrease the amplitude of the oscillatory pressure to 0.3, while the size of the left bubble remains at 1 mm. The initial distance between the centers of mass of the two bubbles is set at $D = 4$ and the radius of the right bubble is such that $R = 0.7$. According to Eq. (3.2) the breathing frequencies are 76.05 and 108.67, for the left and the right bubble, respectively. The forcing frequency is increased to 40 which is almost half the breathing
frequency of the left bubble, while superharmonic resonance between the breathing mode of the left bubble and the forcing frequency is expected. Using the properties of pure water the dimensionless numbers that arise are: $Oh^{-1} = 269.63$ and $P = 1375.51$. This is a case that was studied also by Pelekasis & Tsamopoulos (1993b) (see fig.15 of that ref.), the only difference being that, with our characteristic scales, their dimensionless pressure is slightly lower, 1333.32. This slightly increased pressure in the present simulation leads to slightly smaller periods of volume oscillations and, hence, should cause a slightly faster appearance of the bubble deformations. Indeed, comparing the shapes and the times of fig. 15 of Peleaksis & Tsamopoulos (1993b) with our results shown in figure 3.13a, it is clear that there is very good agreement between the them, although in our case the same shapes appear a little earlier in time. Moreover, because of including liquid viscosity, the present deformations are not as severe as in the case of the inviscid fluid in Pelekasis & Tsamopoulos (1993b). Unfortunately, simulations fail to converge early on and the larger bubble deformations of Pelekasis & Tsamopoulos (1993b) could not be reached. As can be seen in figure 3.13b, the amplitude of the volume oscillations of the left bubble increases significantly while the three maxima appear at $t = 0.09$, 0.175 and 0.261 denoting superharmonic resonance between the forcing frequency and the breathing mode. The severe oscillations of the left bubble force the right one to accelerate faster and spherical cap shapes arise, while the left one does not have enough time to develop shape oscillations until the time the computations fail to converge and remains nearly spherical.
In order to study further the effect of viscosity on the shapes and the other characteristics of the bubbles, another case of Pelekasis & Tsamopoulos (1993b) is simulated. All the model parameters are kept the same, except for the forcing frequency, which is set to 90, i.e. it is now between the breathing frequencies of the two bubbles. In this case the two bubbles should repel each other. In figure 3.14 we compare the evolution of the centers of mass of the two bubbles resulting from our simulation with the corresponding predictions of Pelekasis & Tsamopoulos (1993b), given in their fig. 18. The increased here pressure in the surrounding liquid brings about an earlier evolution of the centers of mass, but our computations fail to converge before the bubbles establish a clear direction in their motion. Moreover, the period of the oscillations of the centers of mass slightly decreases when viscous forces are included. Figure 3.15 gives shapes of the two bubbles at the same times given in fig. 19 by Pelekasis & Tsamopoulos (1993b). Unfortunately, computations fail to converge a little after $t = 0.193$. Comparing the two sets of shapes we find very good agreement as well.

Figure 3.13 (a) Shapes of two unequal bubbles at $t = 0.265$, 0.28, 0.295, 0.304 and (b) evolution of the volume of the left and right bubble with time for $R_{b1}^* = 1 \text{mm}$, $R_{b2} = 0.7$, $Oh^{-1} = 269.63$, $P = 1375.51$, $\epsilon = 0.3$, $D = 4$, $R_c = 30$ and $\omega f = 40$. 
Figure 3.14 Comparison of the location of the centers of mass of the two bubbles between the current simulation (—) and the simulation of Pelekasis & Tsamopoulos (−−−) (fig. 18 of Pelekasis and Tsamopoulos 1993b) for $R_{b1}^* = 1 \text{mm}$, $R_{b2} = 0.7$, $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 0.3$, $D = 4$, $R_{\infty} = 30$ and $\omega_f = 90$.

Figure 3.15 Shapes of two unequal bubbles at $t = 0.14$, 0.17, 0.19, 0.193 for $R_{b1}^* = 1 \text{mm}$, $R_{b2} = 0.7$, $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 0.3$, $D = 4$, $R_{\infty} = 30$ and $\omega_f = 90$.

Increasing only $\varepsilon$ to 0.6 and keeping all the other parameters the same, we see that the bubbles deform significantly and early on. Figure 3.16 shows that the centers of mass
have initially the same tendency as in the case of $\varepsilon = 0.3$, namely the two bubbles oscillate around their initial position. However, after $t \approx 0.062$ the force becomes clearly attractive, with the right smaller bubble moving faster towards the left one. This attraction is opposite to what one would expect based on the Bjerknes principle. Nevertheless, at $t \approx 0.09$ the right bubble reverses its direction of motion, while the left one keeps the same direction on average. Unfortunately, a little later, at $t = 0.1041$, computations fail to converge due to the large deformation of both bubbles.

The increased external disturbance, from $\varepsilon = 0.3$ to 0.6, induces a larger amplitude in the volume oscillations (Figure 3.17a), a faster motion to the two bubbles (compare figures 3.14 & 3.16), and an earlier appearance of shape oscillations. In fact, the shapes are completely different now from those in the case of $\varepsilon = 0.3$. As already discussed the larger (left) bubble undergoes larger volume variations inducing higher acceleration on the right one. On the other hand, the smaller (right) bubble has a higher frequency inducing faster changes in the direction of motion to the left one. The higher acceleration of the right bubble leads to the earlier formation of spherical cap shapes as seen in figure 3.17b. The right bubble starts to deform at $t \approx 0.085$. Looking at the evolution of its center of mass, figure 3.16, at this time the right bubble moves towards the left and deformations appear at its rear side, which eventually lead to the formation of jet piercing this bubble as time increases. Figure 3.17b demonstrates that at $t \approx 0.095$ the volume of the left bubble has decreased and has almost
reached its maximum value, whereas that of the right one keeps on increasing. Subsequently, the volume of the left bubble increases very fast, but the expansion of its front side is opposed by the rapidly approaching and still expanding right bubble. This leads to its deformation, very clearly seen at $t = 0.104$. Actually, a closer look at figure 3.16, shows that the two bubbles are repelling each other very briefly at $t \approx 0.095$. Computations fail to converge at $t = 0.1041$ while both bubbles are penetrated by rapidly accelerating jets emanating from their right side. This combined deformation is a very unusual.

Figure 3.17 (a) variation of the volume of the left and the right bubble with time for $\varepsilon = 0.3$ and $\varepsilon = 0.6$ and (b) shapes the two unequal bubbles at $t = 0.085, 0.09, 0.095, 0.104$ for $R_{\infty}^* = 1\text{mm}, R_{\theta_2} = 0.7, Oh^{-1} = 269.63, P = 1375.51, \varepsilon = 0.6, D = 4, R_w = 30$ and $\omega_f = 90$. 

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Increasing the initial distance slightly to $D = 5$ and retaining all the other parameters the same, the two bubbles attract each other for a long time before the right one starts to move away from the left. Again, computations fail to converge early on and before it becomes clear whether attractive or repulsive forces will prevail eventually. However, since the acceleration of both bubbles decreases because of the larger distance between them, more time is provided for shape oscillations to arise. The volume of the left bubble expands significantly during the second period of its oscillations causing the right one to deform. The left bubble does not have the time to deform and remains almost spherical until computations fail.

Next, we examine an arrangement in which the forcing frequency is set at the average value defined by the eigenfrequencies of the two breathing modes, $\omega_{0,1}$ and $\omega_{0,2}$, to 115. Here again the size of the left bubble remains at $1\text{mm}$ and its breathing frequency at 76.05, while the size of the right bubble is decreased to 0.5 and so, its breathing frequency increases to 152.18. The initial distance between the two bubbles is set at $D = 4$ while $\varepsilon$ at 0.6. The dimensionless numbers are the same as in the previous cases. In contrast to the previous cases, where it was not clear whether repulsive or attractive forces prevail, here, after a short oscillatory interval, the force between the two bubbles is mainly repulsive, as seen in figure 3.18.

![Graphs showing the evolution of the centers of mass of the two bubbles](image)

Figure 3.18 Evolution with time of the centers of mass of the two bubbles for $R_{b1}^\infty = 1\text{mm}$, $R_{b2} = 0.5$, $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 0.6$, $D = 4$, $R_\infty = 30$ and $\omega_f = 152.18$.

Unfortunately, simulations fail to converge again rather early. As the forcing frequency is almost twice the frequency of the breathing mode of the left bubble, superharmonic resonance
between them is anticipated. However, due to the moderate amplitude, $\varepsilon$, and the small distance between the bubbles, their acceleration is very large and becomes the dominant effect. More specifically, the acceleration, as it is calculated over the first period of volume oscillations, is 26.12 and 50.62 for the left and the right bubble respectively. As the right bubble is the smaller one, it behaves as a body of less inertia compared to the larger one, moves faster away from the left and is the one that deforms the most. As the force between the two bubbles is repulsive the deformation is expected on its side phasing away from the left bubble. This is observed in the shapes of the two bubbles given in figure 3.19. The left bubble is again the one that exhibits the largest volume oscillations, while its deformations are less significant than those of the right bubble. The jet that seems to emanate from the rear side of the right bubble is very broad in this case.

![Shapes of two unequal bubbles](image)

**Figure 3.19** Shapes of two unequal bubbles at $t = 0.095, 0.1, 0.103, 0.107$ for $R_{b1} = 1 \text{mm}$, $R_{b2} = 0.5$, $Oh^{-1} = 269.63$, $P = 1375.51$, $\varepsilon = 0.6$, $D = 4$, $R_\infty = 30$ and $\omega_j = 152.18$.

### 3.3.2.2 Intermediate bubbles, $R^* = 200 \mu m$

Here we will examine bubbles of intermediate size. As such we choose the radius of the left bubble to be $200 \mu m$, resulting in $Oh^{-1}$ and dimensionless pressure, $P$, equal to 120.582 and 275.103, respectively, indicating the increased importance of viscous over
capillary forces. The radius of the right bubble is 30% smaller than the radius of the left bubble, i.e. \( R_{b2} = 0.7 \). The breathing frequencies as calculated by eq. 3.2 are: 34 and 49 for the left and the right bubble, respectively. The initial distance between the two bubbles is set at \( D = 4 \), \( \epsilon = 1 \) and the forcing frequency is lower than both breathing frequencies but close to that of the left bubble, \( \omega_f = 30 \). Since \( \omega_f \) is close to \( \omega_{b,1} \) and \( \epsilon \) is large enough, it is not clear whether the bubbles will repel or attract each other. Figure 3.20 shows the time-evolution of the centers of mass of the two bubbles.

![Figure 3.20](image)

*Figure 3.20* Evolution with time of the centers of mass of the two bubbles for \( R_{b1} = 200 \mu m \), \( R_{b2} = 0.7 \), \( Oh^{-1} = 120.582 \), \( P = 275.103 \), \( \epsilon = 1 \), \( D = 4 \), \( R_o = 30 \) and \( \omega_f = 30 \).

The two bubbles initially oscillate around their center of mass and then attract each other rather abruptly. The volume of both bubbles is expanding significantly, as seen in figure 3.21a, due to the large disturbance amplitude. However, the right bubble shrinks very rapidly after its expansion while the other one remains large until the end of computations. Until \( t \approx 0.228 \) both bubbles remain almost spherical with \( P_o \) to be the dominant mode on the shape of the bubble. At \( t = 0.228 \) the volume of the right bubble assumes its minimum value, \( V_2 = 0.440 \), while the volume of the left bubble is still fairly large, \( V_1 = 14.445 \). This causes the acceleration of the right bubble and its quick deformation at its rear side, see figure 3.21b. Computations fail to converge a little after 0.23 while the shape of the right bubble shows a tendency to break up forming a torus by the penetrating liquid jet. The left bubble does not have time to excite any shape deformations and remains almost spherical.
Figure 3.21 (a) variation with time of the volume of the two bubbles and (b) shapes of two unequal bubbles at $t = 0.22, 0.227, 0.228, 0.23$ for $R_{b1} = 200 \mu m, R_{b2} = 0.7, Oh^{-1} = 120.582, P = 275.103, \varepsilon = 1, D = 4, R_{\infty} = 30$ and $\omega_f = 30$.

3.3.2.3 Smaller bubbles, $R^* = 30 - 100 \mu m$

Finally we consider bubbles in the lower end of sizes of those typically arising in cavitation experiments. To this end, we take the radius of the left bubble to be $30 \mu m$. Then,
Oh$^{-1}$ becomes 46.701 and the dimensionless pressure, $P$, equals to 41.265, increasing further the importance of viscous over capillary forces. The right bubble radius is set again so that $R_{b2} = 0.7$, while the initial interbubble distance and the disturbance amplitude, $\varepsilon$, are the same as in the previous case. The natural frequencies are now 13.4 and 19.3 for the left and the right bubble, respectively. Under similar conditions with the previous case, the behavior of the two bubbles is quite the similar. Namely, we set the forcing frequency, $\omega_f$, at 10, i.e. lower but close to the natural frequency of the left bubble. We observe in figure 3.22 that the two bubbles undergo volume oscillations, while they remain spherical for a long time until the smaller one finally deforms, as it accelerates towards the larger one. The shapes of the two bubbles are very similar to those in the previous case, but more time is needed for disturbances to appear, as it should be expected owing to the higher Ohnesorge number, which, through the increased viscosity, delays bubble deformation.

Figure 3.22 Shapes of two unequal bubbles at $t = 0.64, 0.641, 0.643, 0.645$ for $R_{b1} = 30 \mu m$, $R_{b2} = 0.7$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 1$, $D = 4$, $R_\infty = 30$ and $\omega_f = 10$.

Setting the forcing frequency between the two natural frequencies of the two bubbles, $\omega_f = 17$ and for large disturbance amplitude, $\varepsilon = 1$, the two bubbles, after a short oscillation around their initial positions, quickly approach each other, instead of repelling each other according to the Bjerknes principle, figure 3.23. The simulations can not continue further than
\( t = 0.454 \) and after external pressure has completed only one period \( (T_f = 0.369) \), because the right bubble deforms and tends to form a torus.

Figure 3.23 Evolution with time of the centers of mass of the two bubbles for \( R_{b1}^* = 30 \mu m \), \( R_{b2} = 0.7 \), \( Oh^{-1} = 46.701 \), \( P = 41.265 \), \( \varepsilon = 1 \), \( D = 4 \), \( R_c = 30 \) and \( \omega_f = 17 \).

The volumes of the two bubbles exhibit again violent oscillations, the right bubble is again the one that deforms the most, while the left one remains almost spherical. Since the forcing frequency is higher now the deformations of the bubble shapes appear earlier in time than in the case of \( \omega_f = 10 \). Figure 3.24 shows a sequence of bubble shapes that qualitatively is similar to those in figures 3.21 and 3.22.

Figure 3.24 Shapes of two unequal bubbles at \( t = 0.443, 0.448, 0.453, 0.454 \) for \( R_{b1}^* = 30 \mu m \), \( R_{b2} = 0.7 \), \( Oh^{-1} = 46.701 \), \( P = 41.265 \), \( \varepsilon = 1 \), \( D = 4 \), \( R_c = 30 \) and \( \omega_f = 17 \).
Decreasing the amplitude $\varepsilon$ to 0.6, the resulting smaller bubble-shape disturbances allow the external pressure to complete almost three periods before computations fail to converge. Although, after some initial oscillations about its initial position, the right bubble accelerates abruptly towards the left one for the time interval $t = 0.333 - 0.529$ it seems to partially retract this motion and oscillate around a location that is to the left of its initial position, figure 3.25. On the other hand, the left bubble initially move a little towards the right bubble, but finally it abruptly turns away from it. The interbubble distance at the end of the simulations is slightly larger than that at the beginning, but the motion has not reached a clear direction.

Figure 3.25 Evolution with time of the centers of mass of the two bubbles for $R_{b1}^* = 30\mu m$, $R_{b2}^* = 0.7$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 0.6$, $D = 4$, $R_\infty = 30$ and $\omega_f = 17$.

Since the acceleration of the bubbles has decreased due to the lower disturbance amplitude there is time for any subharmonic resonance to arise. The frequency of $P_4$ for the left bubble, derived from linear theory, is 9.29, while the frequency of $P_3$ of the right bubble is 10.52. Since the two bubbles are quite close and interact, these frequencies will decrease and so, subharmonic resonance between the forcing frequency and the above modes could take place. Figure 3.26a shows the evolution of the $C_2$, $C_3$ and $C_4$ coefficients of the respective Legendre polynomials for both bubbles, while figure 3.26b shows shapes of the two bubbles at four different times, $t = 0.837$, 0.886, 0.935 and 0.984, the last one being just before the end of the simulations. $P_2$ is the only mode that arises even at small amplitudes for both
bubbles right from the beginning of the simulations. At time $t \approx 0.55$ the values of $P_2$ for the right bubble start to increase and the bubble tends to take an oblate shape, while the left one still remains almost spherical. The $P_3$ mode starts to grow a little later in time for the right bubble at $t \approx 0.75$. This is also obvious in figure 3.26b at $t = 0.837$ where the shape of the right bubble seems to have contribution mostly from $P_3$. Later in time $P_2$ prevails again for the right bubble and its volume starts to increase and become larger than the one of the left bubble. The acceleration of the left bubble increases and it starts to deform at the front side showing a tendency of the two bubbles to repel each other. Finally, in contrast to the case with $\varepsilon = 1$, the left bubble is the one that tends to break up.

Figure 3.26 (a) Evolution with time of $C_2$, $C_3$ and $C_4$ Legendre coefficients for the left and the right bubble and (b) shapes of the two bubbles at $t = 0.837$, 0.886, 0.935, 0.984 for $R_{61}^* = 30 \mu m$, $R_{62} = 0.7$, $Oh^{-1} = 46.701$, $P = 41.265$, $\varepsilon = 0.6$, $D = 4$, $R_\infty = 30$ and $\omega_f = 17$.
Pelekasis et al. (2004) found that when the initial distance between the centers of mass of the two bubbles is very large, up to 50 times the larger of the two equilibrium radii and the disturbance amplitude $\varepsilon$ 1 or larger, the force between the two bubbles can change sign as they approach each other irrespective of whether $\omega_f$ stands between or outside the interval defined by $\omega_{0,1}$ and $\omega_{0,2}$. In their simulations they also assumed that the bubbles remain spherical since they are far enough from each other and they included small viscous (damping) forces. In order to examine if their consequents stand when the initial distance between the centers of mass of the two bubbles is much closer, up to 6 radii, we considered, as they did, the case that the left bubble is $100\mu m$, while the right one is either 80, 90 or also $100\mu m$. The amplitude $\varepsilon$ is set to 0.5 and the forcing frequency to $\omega^*/2\pi = 16.8kHz$ so that it stands outside of the interval of $\omega_{0,1}$, $\omega_{0,2}$ in any of the three cases. According to Pelekasis et al. (2004) when the distance $D$ is large, for $R^*_{b_2} = 100\mu m$ attractive forces arise between the two bubbles, for $R^*_{b_2} = 90\mu m$ a stable bubble pair appears after attraction while for $R^*_{b_2} = 80\mu m$ repulsive forces dominate (see fig. 12 of that ref.). In the current simulation that $D = 6$, only attractive forces are observed in all three cases, while the bubbles deformed before they approached each other significantly.

If the initial distance between the two bubbles increased further to 10 radii the results are quite the same. The two bubbles always attract each other and deform before they approach each other. That means that the conclusions by Pelekasis et al. (2004) do not extend to the present situation where the bubbles are initially located closer to each other. The assumption that the bubbles remain spherical for long time does not hold either. From the numerous simulations we have carried out, it seems that even when the bubbles are very far apart, it is inevitable that the large amplitude disturbance will set them in volume oscillation which will subsequently excite one of the shape modes eventually leading to bubble breakup.

The evolution of the centers of mass with time for $R^*_{b_2} = 100$, 90 and $80\mu m$ is given in figures 3.27a, b, c, respectively, while shapes of the two bubbles at selected times are given in figures 3.28a, b, c for $D = 6$ and figures 3.29a, b, c for $D = 10$. Unfortunately the long computational time needed for the simulations to complete together with the high computational cost does not allow us to reach even larger initial distances between the two bubbles.
Figure 3.27 Evolution of the center of mass of the right and the left bubble for (a) 
\( R_{b2}^* = 100\mu m \), (b) \( R_{b2}^* = 90\mu m \) and (c) \( R_{b2}^* = 80\mu m \) for two different distances \( D = 6 \) and 
\( D = 10 \) and \( R_{b1}^* = 100\mu m \) and \( \omega^*_f / 2\pi = 16.8kHz \).
Figure 3.28 Shapes of the two bubbles for $R_{b1}^* = 100\mu m$ and (a) $R_{b2}^* = 100\mu m$ at $t = 0.65, 0.7, 0.72$ and $0.746$ (b) $R_{b2}^* = 90\mu m$ at $t = 0.9, 0.95, 0.97$ and $0.991$ and (c) $R_{b2}^* = 80\mu m$ at $t = 0.9, 0.95, 0.97$ and $0.996$ with $D = 6$ and $\omega_f^* / 2\pi = 16.8 kHz$. 
Figure 3.29 Shapes of the two bubbles for $R_{1}^{*} = 100\mu m$ and (a) $R_{2}^{*} = 100\mu m$ at $t = 0.65$, 0.7, 0.72 and 0.746 (b) $R_{2}^{*} = 90\mu m$ at $t = 0.9$, 0.95, 0.97 and 0.991 and (c) $R_{2}^{*} = 80\mu m$ at $t = 0.9$, 0.95, 0.97 and 0.996 with $D = 10$ and $\omega_{f}^{*} / 2\pi = 16.8 kHz$.

3.4 Conclusions

We have studied the motion and deformation of two equal or unequal bubbles in a viscous liquid extending to infinity and subjected to a uniform acoustic pressure at the far field at $t \geq 0$. The radius of the left bubble ranged from $30\mu m$ to $1\mu m$ while the right bubble
covered a range 70-100% of that of the left bubble. In contrast to previous works, viscous forces and shape deformations were allowed. According to Bjerknes, two bubbles pulsating in an acoustic field will repel each other if the forcing frequency lies in the interval defined by the natural breathing frequencies of the two bubbles. Then they will oscillate out-of-phase. In any other case the two bubbles will repel each other. If the two bubbles are of equal size, they will always attract each other as only in phase oscillations can occur.

Here indeed we found that equal bubbles always attract each other. When they are large, $R_{m}^2 = 1\text{mm}$, oscillate under a forcing frequency related to the second or third Legendre mode of the bubbles, at rather large initial distance between their centers of mass and large external disturbance, $\varepsilon = 1$, resonance between the zeroth mode and higher modes $(P_{18} - P_{20})$ prevails and spherical cap shapes dominated by these modes arise before computations fail to converge. Increasing the forcing frequency $\omega_f$ from 3.5 to 6, shows a tendency for period doubling in the oscillations of the center of mass and the volume. Smaller bubbles located at smaller initial distances and oscillating with a forcing frequency close to the second Legendre mode and $\varepsilon = 1$, allow subharmonic resonance between the zeroth mode and the forcing frequency causing the severe expansion of the volume of the two bubbles. In contrast to the case of the step change in pressure at infinity, under oscillatory pressure, the bubbles oscillate for a long time around their center of mass and then accelerate abruptly due to severe changes of their volumes. This deforms the bubbles significantly before they approach each other appreciably.

If the size of the right bubble decreased to 0.75, while the one of the left is of $1\text{mm}$, and the forcing frequency is set close to the frequency of the lower modes, e.g. $P_2$, $P_3$, of any of the two bubbles, then subharmonic resonance between the breathing mode and higher modes of either of the two bubbles prevails. The initial distance and consequently the acceleration, will define which bubble will deform. Further decrease of the relative size of the right bubble to 0.5, makes the acceleration the dominant effect at small distances, $D = 4$, and eliminates any possibility for subharmonic resonance. The right bubble is the one that deforms due to higher acceleration. At larger initial distances, $D = 8$, subharmonic resonance between the breathing mode and higher modes prevails again. Since the period of the modes that resonate with the breathing mode is larger for the left bubble, the right bubble is the one that deforms the most. If the forcing frequency increases to lie in the interval between the frequencies of the breathing modes of the two bubbles, repulsive forces prevail for small amplitude disturbance, $\varepsilon = 0.3$, as the Bjerknes law predicts. Increasing $\varepsilon$ to $\varepsilon = 0.6$,
acceleration of the two bubbles increases and shape oscillations appear at earlier times. The deformation of both or the one of the two bubbles, depending on their initial distance, leads to failure of the computations, before it becomes clear if repulsive or attractive forces will prevail. In none of the above cases subharmonic resonance between the forcing frequency and shape modes have time to arise.

Decreasing the size of the left bubble to 200$\mu m$ and moreover to 30$\mu m$ the two bubbles attract each other if the forcing frequency lies outside the interval of the breathing frequencies of the bubbles. Under a high amplitude disturbance, $\varepsilon = 1$ the volume of the both bubbles expands significantly, while the right bubble is the one that deforms due to the higher acceleration. In the case that the forcing frequency lies in the interval of $\omega_{b,1}$, $\omega_{b,2}$ computations fail early in the case of high $\varepsilon$ and before become clear if attractive or repulsive forces prevail. At lower amplitude disturbances, $\varepsilon = 0.6$, the two bubbles show a tendency of repulsion but again it does not become clear before the end of the simulations.

Finally, it is done a try to examine the consequences of Pelekasis et al. (2004). They assumed that the bubbles retain their spherical shape when they are far apart from each other, up to 50 radii and also found that the Bjerknes law may change sign as the bubbles approaching each other and certain conditions. It was found that their conclusions do not extend in the case that the two bubbles are located initially up to 10 radii apart. Unfortunately the long computational time needed for the simulations to complete together with the high computational cost does not allow us to reach even larger initial distances between the two bubbles.
CHAPTER 4

Steady bubble rise, deformation and entrapment in Bingham fluids

4.1 Introduction

The motion of a bubble in viscous liquids has attracted the interest of many researchers because of its numerous practical applications and scientific challenges. Over many years people have examined the flow and deformation of a single or multiple bubbles theoretically, experimentally and numerically in various flow fields; see, for example, the reviews by Harper (1972), Clift, Grace and Weber (1978), and Magnaudet and Eames (2000). However, a large number of materials such as suspensions, emulsions, slurries, foams, fermentation broths and polymer solutions deviate from the Newtonian law. These materials are called viscoplastic and behave differently in different physical regions depending on the local level of stress. The first constitutive law used to describe their behaviour was proposed by Bingham (1922):

\[
\tau^* = \left( \mu_o + \frac{\tau_y}{\gamma^*} \right) \gamma^*, \quad \text{for} \quad \tau^* > \tau_y^*
\]

\[
\dot{\gamma}^* = 0, \quad \text{for} \quad \tau^* \leq \tau_y^*
\]

(4.1a, 4.1b)

where \( \dot{\gamma}^* = \nabla \dot{v}^* + \nabla \dot{v}^{*T} \) is the rate of strain tensor and \( \tau^*, \gamma^* \) are the second invariants of the respective tensors, defined as:

\[
\tau^* = \left[ \frac{1}{2} \tau^* : \tau^* \right]^{1/2}, \quad \gamma^* = \left[ \frac{1}{2} \dot{\gamma}^* : \dot{\gamma}^* \right]^{1/2}
\]

(4.2)

and \( \mu_o \) and \( \tau_y^* \) are the plastic viscosity and the yield stress, respectively. The superscript * indicates that the corresponding variable is dimensional. As (4.1) indicate, when the second invariant of the stress exceeds \( \tau_y^* \), the material flows with a non-Newtonian viscosity, \( \mu_o + \tau_y^*/\gamma^* \), whereas when it does not exceed it, the material behaves as a solid. The motion of a bubble through a viscoplastic material exhibits new and interesting aspects, which cannot be directly deduced from the corresponding laws for Newtonian liquids. For example, bubbles may become entrapped indefinitely in a viscoplastic material when their buoyancy is
sufficiently small compared to $\tau_y^*$, owing to their inability to break the weak physical bonds in the material. However, bubbles may attain shapes that are non-unique, which further complicates the study of their entrapment in a viscoplastic fluid. This behavior directly affects the quality of a product. For example, aerated chocolate has a taste different from solid chocolate and cosmetic and food products have different appeal and cost depending on the amount of air in them. Also, it affects the efficiency of a physical, chemical or biochemical process. For example, it is more difficult for gases to diffuse from/to an entrapped bubble, slowing down a fermentation processes, whereas inside an oil well a gas kick in drilling mud may occur, rise upwards and lead to blow out at the surface (Johnson and White, 1990; Terasaka and Tsuge 2001; Dubash and Frigaard 2004, 2006).

Because of the added complexity of a viscoplastic constitutive law and difficulties in observing through such typically opaque materials, the motion of a bubble in them has been studied much less than in Newtonian fluids. A first notable exception is the work of Astarita and Apuzzo (1965) who reported bubble shapes and velocities in viscoplastic (Carbopol solutions) and slightly or highly elastic liquids. They observed that curves of bubble velocity vs. bubble volume for viscoplastic liquids had an abrupt change in slope at a critical value of bubble volume that depended on the solution concentration of Carbopol in the solution, i.e. the yield stress of the material. The solution concentration also affected the very slow bubble velocities at small bubble volumes and the rate of their increase with bubble volume. The bubble shapes in Carbopol solutions exhibited the usual deformations found in Newtonian fluids, passing from spherical to oblate ellipsoid and finally to spherical caps as their volume increased. Dubash and Frigaard (2007) verified experimentally the observations of Astarita and Apuzzo (1965) on the existence of a critical bubble radius required to set it in motion, but the bubble shapes they observed in different Carbopol solutions inside a vertical pipe were different and resembled an inverted teardrop. Another notable observation was that surface tension significantly affects the bubble stopping conditions. Earlier, the same authors estimated the conditions under which bubbles should remain static using variational principles (Dubash and Frigaard, 2004). The bounds they obtained based on either strain minimization or stress maximization for any type of viscoplastic fluid were characterized as conservative, in the sense that they provide a sufficient but not necessary condition. However, they concluded that in general “if a big bubble does not move nor will a small one”. The mobilization of bubbles in a yield-stress fluid by setting them into pulsation was the subject of Stein and Buggish’s (2000) research who presented analytical solutions and experimental data to
support them. Apparently larger bubbles rose faster than smaller ones at similar pressure amplitudes. Finally, Terasaka and Tsuge (2001) presented bubble shapes developed by a bubble forming at a nozzle in a yield-stress fluid and provided an approximate model for bubble growth. On the other hand, Dimakopoulos and Tsamopoulos (2003b, 2006) simulated the formation and expansion of a long ‘open’ bubble during the displacement of viscoplastic liquids by pressurised air from straight, suddenly constricting and expanding cylindrical tubes for a wide range of Bingham (i.e. the dimensionless yield stress) and Reynolds numbers, providing details about the topology of the unyielded regions and their effect on the shape of the long bubble.

The corresponding problem of a solid sphere translating in a Bingham fluid has been studied more extensively. Beris et al. (1985), verified earlier estimations, based on variational inequalities, of the dependence of the drag force on the sphere in an unbounded medium as on the yield-stress. They solved the governing equations with (4.1) as a constitutive model under creeping flow conditions using an algebraic mapping of the yield surfaces to fixed spherical ones and finite elements. They found that the sphere falls within an envelope of fluid, the shape and location of which depends on the yield stress and that unyielded material arises around the stagnation points of flow at the poles of the sphere. Finally, they obtained the critical yield-stress value beyond which the sphere is immobilized by combining asymptotic scalings derived from the plastic boundary-layer theory with numerical calculations. Similar results have been reported by Liu, Muller and Denn (2002). Blackery and Mitsoulis (1997) extended this study, including the effect of the tube diameter to the sphere diameter ratio when the sphere is moving inside a cylindrical tube, using Papanastasiou’s (1987) viscoplastic model. This model holds in both the yielded and unyielded material regions:

\[
\tau^* = -\left[\mu_o + \tau_y \frac{1-e^{-\gamma^*}}{\gamma^*}\right] \gamma^* \tag{4.3}
\]

where the stress growth exponent, \( n \), must assume large enough values, depending on the particular flow, in order that the original Bingham model is approached; see Dimakopoulos and Tsamopoulos (2003b, 2006) and Burgos, Alexandrou and Entov (1999).

Out of the very extensive literature on bubble motion in viscous liquids, we will mention here only papers that are more relevant to the present work or will be used to compare our predictions to established experimental and theoretical data and demonstrate ways in which the viscoplastic fluids deviate from Newtonian ones. Early on, Haberman and Morton (1954) measured bubble rise velocities as a function of bubble size for various liquids.
and introduced a new dimensionless number for the description of their results, the Morton number, $Mo$, which depended on the liquid properties only. Hnat and Buckmaster (1976) experimentally determined the physical conditions under which either spherical caps arise or bubbles develop very thin, long and rounded ‘skirts’ from their sides. Bhaga and Weber (1981), carried out extensive experiments to determine the physical conditions under which bubbles assume spherical, oblate ellipsoidal, deformed ellipsoidal, spherical cap or skirted shapes, steady or unsteady. They presented these conditions in a map of bubble shapes with the Reynolds vs. Eötvos numbers as parameters. In their photographs of bubble motion in aqueous sugar solutions, they quite clearly visualized the streamlines around and in the wake of these bubbles. Aware of the importance of surface impurities while carrying out experiments with water, Duineveld (1995) used ‘hyper clean’ water and very accurately determined the velocity and the shape of bubbles, with an equivalent radius of 0.33-1.00 mm or Reynolds numbers in the range $100 \leq Re \leq 700$. Finally, Maxworthy et al. (1996), extended such experiments using clean mixtures of triple distilled water and pure, reagent grade, glycerine. Hence, they covered a wider range of the relevant parameters and provided plots of the drag coefficient $C_d$ and the bubble terminal velocity versus the diameter of an equal spherical bubble.

The early theoretical studies assumed that the bubble remained spherical in an infinite medium and first predicted its drag coefficient under creeping flow conditions, (Rybszynski 1911; Hadamard 1911). The corresponding analysis for large but finite Reynolds numbers was first attempted by Levich (1949) who argued that the velocity field around the spherical bubble differed only slightly from the inviscid solution. He evaluated the drag force from energy dissipation based on the irrotational solution, to find that the drag coefficient based on the bubble diameter is $C_d = 48 / Re$. Later Moore (1963) performed a very elegant boundary layer analysis to determine the structure of the flow around the bubble and the wake behind it and calculated the next-order correction to this formula. Small bubble deformations in creeping flow were examined by Taylor and Acrivos (1964), who studied the importance of surface tension. Deformation at high Reynolds numbers was examined by Moore (1965), who assumed that the bubble had an oblate spheroidal shape and derived the boundary layer solution for it. Since then, the high-Reynolds number flow around oblate ellipsoidal bubbles has been examined to investigate among other things the range of Reynolds numbers in which recirculation arises behind the bubble (Blanco and Magnaudet 1995).
Solution of the general problem, depending solely on fluid properties and bubble size and dropping any *a priori* assumption about bubble shape or range of the Reynolds number, demands the use of advanced numerical methods, because of the large and complicated bubble deformations and flow structure around them. This became possible in the middle 1980s. First, Miksis, VanDen-Broeck and Keller (1982) assumed potential flow, included only viscous forces in the normal force balance and calculated shapes of rising bubbles using boundary elements, but inherently flow separation could not be predicted. Then Ryskin and Leal (1984) used finite differences and an orthogonal two-dimensional transformation, to solve the Navier-Stokes equations and obtained bubble shapes for Reynolds numbers up to 200 and Weber numbers up to 18. They also predicted accurately the flow recirculation behind the bubble and suggested that the mechanism of eddy formation behind the bubble is the competition between the rate of vorticity production on the free surface and the rate of vorticity convection downstream. Subsequently, Christov and Volkov (1985) used finite differences with a quite restrictive one-dimensional mapping to obtain such solutions in a narrower parameter range. Numerical methods that do not solve for the bubble shape simultaneously with the flow field, but calculate it *a posteriori* by defining an appropriate function, such as volume tracking and level set, have also being used. Their disadvantage of decreased accuracy can be counterbalanced by their ability to predict more complicated bubble shapes and bubble breakup. Some notable examples are the papers by Unverdi and Trygvasson (1992), Bonometti and Magnaudet (2006, 2007) and Hua and Lou (2007).

We will solve this free-boundary problem, assuming axial symmetry and steady state, with the very accurate and versatile numerical algorithm that we developed recently for such problems (Dimakopoulos and Tsamopoulos 2003a). It is based on a quasi-elliptic set of equations for generating a discretization mesh that conforms to the entire fluid domain outside the bubble. Key ideas for the success of the transformation are limiting the orthogonality requirements on the mesh and employing an improved node distribution function along the deforming boundary. A non-orthogonal mesh is allowed since we will solve the entire equation set by finite elements. The retained orthogonal term eliminates the discontinuous slopes of the coordinate lines that are normal to the free surface. These usually arise owing to the harmonic transformation around highly deforming surfaces. This procedure produces meshes of higher density where necessary; stagnation points of flow, equatorial plane and wake behind the bubble. We have applied this method to a number of free- or moving-boundary steady or transient problems, such as displacement of a Newtonian or viscoelastic fluid from a tube (Dimakopoulos and Tsamopoulos 2003c, 2004), transient squeezing of a
viscoplastic material between parallel disks (Karapetsas and Tsamopoulos 2006) and deformation of several bubbles during filament stretching (Foteinopoulou et al. 2006).

In § 4.2 we present the governing equations and boundary conditions of this problem. In § 4.3 we give some basic ideas of our body-fitted coordinate transformation and the key features to implement the finite-element algorithm for solving this problem. We present our results in terms of bubble shapes, yield surfaces, flow structure and conditions for bubble entrapment depending on fluid parameters and bubble size in § 4.4. Conclusions are drawn in § 4.5.

4.2 Problem formulation

We consider the flow of a bubble of volume $V_b^*$ rising at a constant velocity $U_b^*$ through a viscoplastic fluid, with a constant yield stress, $\tau_y^*$ and upon yielding a constant dynamic viscosity, $\mu_0^*$. We assume axial symmetry and that the fluid is incompressible with constant density, $\rho^*$ and a constant interfacial tension with gas in the bubble, $\gamma^*$, whereas the viscosity and density of the gas in the bubble are assumed to be zero. Figure 4.1 illustrates the flow geometry examined herein. The motion of the bubble is driven by gravity which is aligned with the z-axis. We select a reference frame moving with the bubble and locate the origin of the spherical coordinate system at the centre of mass of the bubble. Hence, the bubble becomes stationary and the surrounding fluid moves downwards with velocity $U_f^* = -U_b^*$. Henceforth, we will denote by $U^*$ the magnitude of these velocities.

We scale all lengths with the equivalent radius, $R_b^*$, of a spherical bubble with the same volume, $V_b^*$, as the bubble under study: $R_b^* = \left(4V_b^*/3\pi\right)^{1/3}$. We scale velocities by balancing buoyancy and viscous forces, i.e. with $\rho^* g^* R_b^* {R_b^*}^2 / \mu_0^*$, where $g^*$ is the gravitational acceleration, because: (i) we would like to follow as closely as possible typical experimental procedures which are carried out using the same fluid while varying the bubble size, while the steady rise velocity is measured a posteriori and (ii) we would like to determine conditions under which the bubble velocity can approach zero resulting in an entrapped bubble. Then the bubble velocity will be calculated as part of the solution, not imposed beforehand, and will be followed by determination of the values of the dynamic parameters, such as the Reynolds number, $Re = 2R_b^* \rho^* U^* / \mu_0^*$ and the Weber number, $We = 2R_b^* \rho^* U^* 2 / \gamma^*$. Pressure and
stresses are scaled with $\rho^* R_b^* g^*$. Thus, the dimensionless groups that arise are the Archimedes number, $Ar = \rho^* g^* R_b^* \mu^*/\mu_o^*$, which is related to the Galileo number; the Bond number, $Bo = \rho^* g^* R_b^* \gamma^*/\gamma$, often called the Eotvos number and the Bingham number, $Bn = \tau^*/\rho^* g^* R_b^*$, which is the dimensionless yield stress.

Figure 4.1 Schematic of the flow geometry and coordinate system.

The flow is governed by the momentum and mass conservation equations, which in their dimensionless form are:

$$Ar \nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{\sigma} - e_z = 0 \quad (4.4)$$

$$\nabla \cdot \mathbf{v} = 0 \quad (4.5)$$

where $\mathbf{\sigma}$ is the total stress tensor,

$$\mathbf{\sigma} = -P \mathbf{I} + \mathbf{\tau}, \quad (4.6)$$

$\mathbf{v}$, $P$ are the axisymmetric velocity vector and the pressure respectively, while $\nabla$ denotes the gradient operator. To complete the description, a constitutive equation that describes the rheology of the fluid is required. In the present study we employ the continuous constitutive equation proposed by Papanastasiou (1987) which was mentioned in the introduction and in dimensionless form is:

$$\tau = -\left[1 + Bn \frac{1-e^{-N\dot{\gamma}}}{\dot{\gamma}}\right] \dot{\gamma} \quad (4.7)$$
where $N$ is the dimensionless stress growth exponent given by $N = n \rho^* g^* R_h^* / \mu^*$. In the simulations to be presented in this paper and after careful evaluation, we have chosen the value of $N$ up to $5 \times 10^4$ in order to neither affect the yield surface by overly decreasing $N$ nor produce numerical instabilities or stiff equations by increasing it.

Along the free surface of the bubble, the velocity field should satisfy a local force balance between capillary forces, viscous stresses in the liquid and pressure inside the bubble:

$$n \cdot \sigma = -P_b n + \frac{2H}{Bo} n,$$

where $P_b$ is the pressure inside the bubble, $n$ is the outward unit normal to the free surface and $2H$ is its mean curvature which is defined as:

$$2H = -\nabla_s \cdot n, \quad \nabla_s = (I - nn) \cdot \nabla$$

We cannot define simultaneously both the volume of the bubble and its pressure. Thus, the latter is calculated as part of the solution by imposing that the dimensionless bubble volume remains constant irrespective of bubble deformation and velocity:

$$\int_0^\pi R_f^3 \sin \theta \, d\theta = 2$$

where $R_f(\theta)$ is the radial position of the bubble interface.

On the axis of symmetry ($\theta = 0$ and $\theta = \pi$) we apply the usual symmetry conditions:

$$v_\theta = 0$$

$$\frac{\partial v_r}{\partial \theta} = 0.$$ (4.11)

Very far from the bubble, theoretically at infinite distance, the fluid moves in the gravity direction with respect to the stationary bubble and with a uniform dimensionless velocity, $U$:

$$v_\theta = -U \sin \theta$$

$$v_r = U \cos \theta.$$

In our numerical implementation of this condition we will truncate the region around the bubble by a spherical surface at a distance $r = R_\infty$. The value of $R_\infty$ will be determined so that it does not affect the solution. As we will see, this is more crucial for a Newtonian fluid, than a viscoplastic one, where the material behaves as a solid at a finite distance from the bubble. The magnitude of the far-field velocity, $U$, is unknown, but is determined as part of the solution by requiring that the bubble centre of mass remains at the origin of the spherical coordinate system:
\[
\int_0^{\pi} R_f^4 \sin \theta \cos \theta \, d\theta = 0
\] (4.15)

The model is completed by setting the datum pressure of the fluid far from the bubble at the equatorial plane \((r = R_c, \theta = \pi/2)\) equal to zero.

### 4.3 Numerical Implementation

In order to solve numerically the above set of equations we have chosen the mixed finite element method to discretize the velocity and pressure fields, combined with an elliptic grid generation scheme for the discretization of the deformed physical domain.

#### 4.3.1 Elliptic grid generation

The grid generation scheme that has been employed consists of a system of quasi-elliptic partial differential equations, capable of generating a boundary-fitted discretization of the deforming domain occupied by the liquid; see Dimakopoulos and Tsamopoulos (2003a). There it was shown that this scheme is superior to previous ones, since it takes into consideration all the intrinsic features of the developing surface and the deforming control volume. Here we will only present our adaptation of its essential features to the current problem. The interested reader may refer to Dimakopoulos and Tsamopoulos (2003a) for further details on all the important issues of the method. With this scheme the physical domain \((r, \theta)\) is mapped onto computational one \((\xi, \eta)\). A fixed computational mesh is generated in the latter domain while, through the mapping, the corresponding mesh in the physical domain follows its deformations. As computational domain we choose here the volume that would be occupied by the fluid if the bubble remained spherical. This mapping is based on the solution of the following system of quasi-elliptic partial differential equations

\[
\nabla \cdot \left( \epsilon_1 \frac{r^2 + r^2 \theta^2_\eta}{r^2_\xi + r^2_\theta^2_\xi} + (1 - \epsilon_1) \right) \nabla \eta = 0
\] (4.16)

\[
\nabla \cdot \nabla \xi = 0
\] (4.17)

where the subscripts denote differentiation with respect to the indicated variable and \(\epsilon_1\) is a parameter that controls the smoothness of the mapping relative to the degree of orthogonality of the mesh lines. This is adjusted by trial and error; here it is set to 0.1. In order to solve the above system of differential equations, appropriate boundary conditions must be imposed. On the fixed boundaries, we impose the equations that define their position, and the remaining...
degrees of freedom are used for optimally distributing the nodes along these boundaries with the assistance of the penalty method. In addition, along the moving interface we impose the no-penetration condition:

$$\mathbf{n} \cdot \mathbf{v} = 0$$

(4.18)

together with a condition that imposes the desired distribution of nodes along the free surface.

The computational domain is discretized using triangular elements by appropriately splitting into two triangular elements each rectangular element generated by our mesh generation method. This splitting is preferred, because triangles conform better to large deformations of the physical domain and can sustain larger distortions than the rectangular ones. In order to illustrate the quality of the mesh produced following our method we present in figure 4.2a a blowup of the physical domain close to the bubble, along with the entire mesh around the bubble in figure 4.2b. For clarity in this figure, we show the nearly rectangular elements before splitting them into triangular ones in a case with only 80 radial and 90 azimuthal elements. As we can see, the mesh becomes smoothly denser where this is most needed, around the bubble surface and near its equatorial plane and its poles, because unyielded regions or flow recirculation are expected to arise there. In order to compute accurately the large deformations of the physical domain, even under the axial symmetry assumption, we used, in most cases, the type of mesh shown in figure 4.2b, but with 120 elements on the $\xi$-direction (radial) and 100 elements on the $\eta$-direction (azimuthal), resulting in 24 000 triangular elements and 205 985 unknowns including the two coordinates of each grid point. An alternative mesh that was employed in order to use the highest value of the stress growth exponent ($5 \times 10^4$), without running into numerical problems, is shown in figure 4.2c. Here we started with 70 radial and 50 azimuthal equidistant elements far away from the bubble, but for $2 \leq \xi \leq 3$ we split each rectangle into four rectangles using a strip of rectangle elements around the bubble that were split to three transition triangular elements to connect the two regions. In this way we quadruple the elements in both $\xi$- and $\eta$-directions. We perform another similar refinement through element splitting in the region $1 \leq \xi \leq 2$. In this way we achieved a much finer mesh near the bubble where it is most needed as we will see shortly, while we actually reduced the computational time and computer memory requirements. For example, at the bubble surface this approach results in 200 elements in the azimuthal direction, while the total number of unknowns has now decreased to 185 223, although the mesh is denser near and all around the bubble and in both directions. With both mesh generation methods, we ensured that there were at least two mesh nodes in any thin
boundary layer that could arise at the bubble surface at large Reynolds numbers, as discussed by Blanco and Magnaudet (1995).

Figure 4.2 Typical mesh, always conforming to the bubble boundary, for $Bn = 0.1$, $Ar = 500$, $Bo = 50$. For clarity we show rectangular elements only and (a) a region near the bubble and (b) the entire physical domain which in this case extends to $R_e = 10$. (c) Alternative mesh for the highest value of the stress growth component, showing triangular elements.

4.3.2 Mixed finite element method

We approximate the velocity vector as well as the position vector with 6-node Lagrangian basis functions, $\phi^i$, and the pressure with 3-node Lagrangian basis functions, $\psi^i$. We employ the finite element/Galerkin method, which after applying the divergence theorem results in the following weak forms of the momentum and mass balances:

\[
\begin{align*}
\int_{\Omega} \left[ Ar \nabla \cdot \nabla \phi^i + \nabla \phi^i \cdot \sigma - \phi^i e_z \right] d\Omega - \int_{\Gamma} \left[ n \cdot \sigma \right] \phi^i d\Gamma &= 0 \\
\int_{\Omega} \psi^i \nabla \cdot \nu d\Omega &= 0
\end{align*}
\]
where \( d\Omega \) and \( d\Gamma \) are the differential volume and surface area respectively. The surface integral that appears in the momentum equation is split into four parts, each one corresponding to a boundary of the physical domain, and the relevant boundary condition is applied. In order to avoid dealing with the second-order derivatives that arise in the boundary integral of the interface, through the definition of the mean curvature, \( H \), we use the following equivalent form:

\[
2Hn = \frac{dt}{ds} - \frac{n}{R_2}
\]  

(4.21)

where the first term describes the change of the tangential vector along the free surface, \( t \), and \( R_2 \) is the second principal radius of curvature, \( R_2 = \frac{r\sqrt{r^2 \theta^2 + r_n^2}}{r\theta - r_n \cot \theta} \).

The weak form of the mesh generation equations is derived similarly by applying the divergence theorem:

\[
\int_{\Omega} \left( \frac{\varepsilon_1}{2} \frac{r^2 \theta^2 \eta^2}{r^2 \varepsilon^2 + r^2 \theta^2 \varepsilon^2} + (1 - \varepsilon_1) \right) \nabla \eta \cdot \nabla \phi^i \, d\Omega + L \int_{\partial \Omega} \frac{\partial \phi^i}{\partial \eta} \sqrt{r^2 \theta^2 + r^2 \theta^2 \eta^2} \, d\eta = 0
\]  

(4.22)

\[
\int_{\Omega} \nabla \xi \cdot \nabla \phi^i \, d\Omega = 0
\]  

(4.23)

where the penalty parameter, \( L \), is in the range \( 10^3 - 10^5 \) and the line integral is along the free surface.

The resulting set of algebraic equations is solved simultaneously for all variables using the Newton-Raphson method. The Jacobian matrix that results after each Newton iteration is stored in Compressed Sparse Row (CSR) format and the linearized system is solved by Gaussian elimination using PARDISO, a robust, direct, sparse-matrix solver, Schenk and Gärtner (2004, 2006). The iterations of the Newton-Raphson method are terminated using a tolerance for the absolute error of the residual vector, which is set at \( 10^{-9} \). The code was written in Fortran 90 and was run on a workstation with dual-core Xeon CPU at 2.8 GHz in the laboratory of Computational Fluid Dynamics, Patras. Each calculation typically required 2-5 hours to complete.

### 4.3.3 Yield surface determination

There are two different criteria that have been employed by several researchers in the past for determining the location of the yield surface: the first as the location where \( \dot{\gamma}^* = 0 \),
and the second as the location where $\tau^* = \tau^*_{\gamma}$. Although these criteria are equivalent according to the Bingham model, they are not equivalent when the Papanastasiou model is used. In fact, only the second criterion may be used, i.e. that the material flows when the second invariant of the extra stress tensor exceeds the yield stress. This criterion in its dimensionless form becomes:

Yielded material: $\tau > Bn$  
Unyielded material: $\tau \leq Bn$  \hfill (4.24)

Near the yield surface, i.e. for small $\dot{\gamma}$, this is equivalent to:

$$\dot{\gamma} \approx \frac{Bn}{1 + NBn} \rightarrow \frac{1}{N},$$

for large $N$ values, which should substitute the first criterion as shown by Dimakopoulos and Tsamopoulos (2003b).

Consequently, in order to determine the yield surface, the second invariant of the stress tensor must be calculated and this includes the computation of the velocity gradient tensor. As mentioned earlier however, the velocity field is discretized using Lagrangian basis functions, which means that the velocity gradient tensor is not continuous on the element sides and, hence, the direct computation at the nodes of the stress tensor is not possible. The most appropriate way to do this is to find a continuous approximation of the extra stress tensor by using the Galerkin projection method, that is:

$$\int_{\Omega} \phi^i(T - \tau) d\Omega = 0$$ \hfill (4.26)

where $T = \tau$ denotes the continuous approximation of the extra stress tensor $\tau$. Having calculated the nodal values of the extra stress tensor, the position of the yield surface can be easily determined. A similar procedure is followed to obtain contour lines of $\dot{\gamma}$.

**4.4 Results and discussion**

First we need to demonstrate that our numerical algorithm predicts accurately bubble shapes and velocities and flow field structure of earlier studies. Such detailed studies exist only for Newtonian fluids. In the process, we will show that our algorithm can extend the parameter values for which converged and accurate solutions can be obtained even for Newtonian fluids. Then, we will present results for bubble rise velocity, deformation and entrapment in a viscoplastic fluid depending on the fluid parameters and bubble volume. All our results are based on the assumptions of axial symmetry and steady state. Clearly,
obtaining such a solution does not assure that it is stable; this would require a separate
stability analysis. Conversely, not obtaining such a solution does not imply that a non-
axisymmetric or time-dependent solution does not exist, for the same parameter values.

4.4.1 Comparison with previous experimental and numerical results for Newtonian fluids

First, we compare our results with the experimental observations by Duineveld (1995)
who measured bubble rise velocities as a function of bubble size in ‘hyper clean’ water and by
Maxworthy et al. (1996) who conducted the same experiments using mixtures of distilled
water with glycerin to produce more viscous liquids. The physical properties of these liquids
are shown in table 4.1. The Morton number, which is given also in table 4.1, depends only on
physical properties of each liquid and is defined as:

\[
Mo = \frac{g \mu_0^4}{\rho \sigma^3} = \frac{Bo^3}{Ar^2}
\]  

(4.27)

<table>
<thead>
<tr>
<th></th>
<th>( \rho^* ) (kg/m(^3))</th>
<th>( \eta^*_0 ) (Ns/m(^2))</th>
<th>( \sigma^* ) (N/m)</th>
<th>Mo</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>1000</td>
<td>(10^{-3})</td>
<td>0.0727</td>
<td>2.722 \times 10^{-11}</td>
</tr>
<tr>
<td>b</td>
<td>1153.8</td>
<td>(9.45 \times 10^{-3})</td>
<td>0.06782</td>
<td>2.174 \times 10^{-7}</td>
</tr>
<tr>
<td>c</td>
<td>1208.5</td>
<td>0.0601</td>
<td>0.0655</td>
<td>3.769 \times 10^{-4}</td>
</tr>
</tbody>
</table>

Table 4.1 Physical properties of experimental data by Maxworthy et al. (1996).

Figure 4.3 compares our predictions for the rise velocity as a function of bubble diameter with
three sets of experimental data, each one related to three values of \( Mo \), which cover what are
typically called fluids with ‘very low’ \( Mo \) values of order \(10^{-11}\) up to fluids with ‘high’ \( Mo \)
values of order \(10^{-4}\). In figure 4.3, \( d \) is the diameter in mm of a corresponding spherical
bubble of the same volume and \( U^* \) is the magnitude of the dimensional rise velocity of the
bubble in mm/s. For the two higher values of \( Mo \), which correspond to more viscous fluids,
we observe very good agreement between our predictions and the data of Maxworthy et al.
(1996). For the lowest value, \( Mo = 2.722 \times 10^{-11} \), attained using pure water, we have excellent
agreement between our predictions and the experimental data of Duineveld (1995). Even
Moore’s (1965) analytical predictions, based on the assumptions that the bubble retains an
oblate spheroidal shape and that non-separated flow takes place that can be calculated using
boundary layer analysis, are in excellent agreement, except for the largest bubbles where bubble shapes deviate from the assumed symmetric shape and flow separation becomes possible.

On the other hand, bubble velocities measured by Maxworthy et al. (1996) are consistently lower, especially for the smaller bubbles. This has been attributed by Maxworthy et al. (1996) to a very small amount of impurities that is still present in their fluids, which is known to affect the smaller bubbles more substantially. For all values of $Mo$ we observe that, as the size of the bubble increases from its smallest value, its rise velocity increases, owing to the increased buoyancy. The less viscous the liquid, the higher the rise velocity is, as the resistance to flow decreases. Moreover, the rate of increase of $U^*$ is larger for the fluid with the smallest $Mo$. In the same fluid with $Mo = 2.7 \cdot 10^{-11}$, a maximum velocity is achieved at a certain bubble size, beyond which the velocity decreases and, then, it increases again. The interplay of the forces on the bubble at different sections of this curve has been analyzed by Maxworthy et al. (1996). The maximum in the bubble velocity vs. bubble diameter corresponds to the minimum in a drag coefficient vs. Reynolds number curve that has been

Figure 4.3 Comparison of our predictions for the dimensional bubble rise velocity vs. bubble diameter in a Newtonian liquid for three selected values of $Mo$ with experiments reported by Duineveld (1995), Maxworthy et al. (1996) and theory by Moore (1965).
reported for these and other low-\( Mo \) fluids in the literature. The shape of this curve becomes for large \( Mo \), exactly as we predict in figure 4.3. For the lower bubble diameters for all three curves the bubbles are nearly spherical. As the bubble diameter increases, they first become oblate spheroidal and then asymmetric having a flatter front side in the two curves with lower \( Mo \) or a flatter rear side for the curve with the highest \( Mo \).

Figure 4.4 Comparison of our predictions for \( We \) vs. bubble aspect ratio, \( \chi \), in pure water with results by Duineveld (1995) and Moore (1965).

In figure 4.4 we compare the predictions of our simulations to the experimental observations of Duineveld (1995) for the Weber number dependence of the bubble deformation expressed by the ratio between the longer and the smaller axes of the bubble, \( \chi \). In both the experiments and our study, \( We \) can be obtained after computing the magnitude of the bubble rise velocity, \( U \), since it is related to it and the dimensionless numbers we have defined by the expression:

\[
We = \frac{2R_b \rho^* U^2}{\sigma^*} = 2ArBoU^2. \quad (4.28)
\]

Clearly, numerical and experimental results are in excellent agreement. In the same figure, we include Moore’s predictions, which require a consistently larger bubble deformation for a given \( We \) (i.e. bubble rise velocity) owing to their inability to predict flow separation.
To further validate our new algorithm we compared the predicted drag coefficient for a steadily rising bubble with that calculated by Ryskin and Leal (1984, referred to herein as RL) for different values of $Re$ and $We$. The Reynolds number and the drag coefficient are defined as:

$$Re = \frac{2R_b^* \rho^* U^*}{\mu^*} = 2ArU$$  \hspace{1cm} (4.29)

$$C_d = \frac{2F^*}{\rho^* U^* R_b^*} = \frac{2F}{\pi ArU^2}$$  \hspace{1cm} (4.30)

where $F$ is the dimensionless drag force, defined in terms of $\tau$ and the dynamic pressure, $P_{dyn}$:

$$F = 2\pi \int_0^\pi \left( -\frac{P_{dyn}}{\rho} + \tau \right) \cdot e_j R_j^2 \sin \theta d\theta$$  \hspace{1cm} (4.31)

where $P_{dyn}$ includes the gravitational potential. Having calculated the magnitude of the bubble velocity, $U$, we readily determine the values of $C_d$, $Re$ and $We$. However, it is not obvious how to get the same parameter values for $Re$ and $We$ as those reported by RL. To this end, we had to rely on trial and error, choosing values of $Ar$ and $Bo$, to prepare table 4.2, which demonstrates that the drag coefficients we calculated are in very good agreement with those of RL and, in this range of $Re$, they decrease with it.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$Re$ & $We$ & $C_d$ (Present work) & $C_d$ (Ryskin & Leal) \\
\hline
1 & 0.003 & 17.43 & 17.35 \\
10 & 0.02 & 2.39 & 2.38 \\
20 & 15 & 3.53 & 3.57 \\
100 & 2.1 & 0.53 & 0.54 \\
101 & 0.14 & 0.37 & 0.39 \\
\hline
\end{tabular}
\caption{Comparison of the drag coefficient calculated herein to that calculated in RL.}
\end{table}
To set the stage for the presentation of bubble shapes in viscoplastic fluids, it is useful to examine first the effect of fluid properties and bubble size on the shape of the bubble when it is steadily rising in a Newtonian fluid. In figure 4.5 we show a map of bubble shapes as a function of $Bo$ and $Ar$. The corresponding $Mo$ is given in table 4.3 and remains the same in the similar shape maps for Bingham fluids, to be presented in § 4.4.2. For easy reference and comparison to previous studies, underneath each shape we give the corresponding $Re$ and $We$. We have obtained steady solutions for $4 \times 10^{-14} \leq Mo \leq 1.25 \times 10^5$ which is a much wider range of $Mo$ than has been available up to now, and for $Bo$ as high as 50. Results for $Ar = 0$ and any $Bo$ are not shown, because according to (4.28) and (4.29), this leads to $Re = We = 0$ and, of course, to a perfectly spherical bubble in a Newtonian fluid; see also RL. However, as $Ar$ and $Bo$ increase, the importance of gravitational and inertia forces increases and affects the shape of the bubble. For $Ar \leq 500$, on increasing $Bo$, the shape of the gas bubble changes from spherical to oblate-spheroid and to more complicated ‘oblate’ shapes with an indentation and/or flattening of their rear side. For $Bo \geq 20$, it seems that for the same $Ar$ the overall shapes do not change much, except that they become more pointed at their rim. It is known that for even higher values of $Bo$, skirted bubbles develop, which demand a much finer discretization. For $Ar = 5000$, on increasing $Bo$, the bubble first flattens at its top side, then for $3.7 \leq Bo \leq 8.8$ steady solutions could not be obtained with this procedure. The shape we managed to compute for $Bo = 10$ is obtained by parameter continuation in $Ar$, not by increasing $Bo$. It required special attention to be captured accurately.

<table>
<thead>
<tr>
<th>$Bo$</th>
<th>$Ar$</th>
<th>$10^{-6}$</th>
<th>$10^{-5}$</th>
<th>$10^{-4}$</th>
<th>$10^{-3}$</th>
<th>$10^{-2}$</th>
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<td>$10^{-4}$</td>
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<td>$10^{-2}$</td>
<td>$10^{-1}$</td>
<td>$10^{0}$</td>
<td>$10^{1}$</td>
<td>$10^{2}$</td>
</tr>
<tr>
<td>5</td>
<td>0.1</td>
<td>$4 \times 10^{-4}$</td>
<td>$4 \times 10^{-5}$</td>
<td>$4 \times 10^{-6}$</td>
<td>$4 \times 10^{-7}$</td>
<td>$4 \times 10^{-8}$</td>
<td>$4 \times 10^{-9}$</td>
<td>$4 \times 10^{-10}$</td>
<td>$4 \times 10^{-11}$</td>
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<tr>
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<td>$4 \times 10^{-3}$</td>
<td>$4 \times 10^{-4}$</td>
<td>$4 \times 10^{-5}$</td>
<td>$4 \times 10^{-6}$</td>
<td>$4 \times 10^{-7}$</td>
<td>$4 \times 10^{-8}$</td>
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</tr>
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<td>$4 \times 10^{-6}$</td>
<td>$4 \times 10^{-7}$</td>
<td>$4 \times 10^{-8}$</td>
</tr>
</tbody>
</table>

Table 4.3 Morton number for the values of Archimedes and Bond numbers shown in figures 5 and 10.
Figure 4.5 Map of bubble shapes in a Newtonian fluid as a function of the Bond and Archimedes numbers. Underneath each figure we give the corresponding Reynolds and Weber numbers \((Re, We)\).

In particular, we had to remove the outer boundary very far away from the bubble in order not to affect the flow in any way, \(R_\infty = 100\), and we had to increase the radial elements to 180, while keeping the azimuthal elements at 100 with the mesh shown in figure 4.2b. This steady shape is qualitatively different from all others reported heretofore, exhibiting an upward indentation of the bubble outer edge and flatter rear side, resembling a hat. As we start to increase \(Bo\), the bubble becomes a spherical cap again. Comparing our bubble shapes for various \(Re\) and \(We\) when such shapes are also available in RL we find very good agreement.

We should mention that we managed to compute steady bubble shapes for larger \(Re\) and \(We\) than in RL. For example, \(Ar = 5000\) and \(Bo = 0.01\) correspond to \(Re = 984\) and \(We = 0.97\), while \(Ar = 50\) and \(Bo = 20\) correspond to \(Re = 43\) and \(We = 36.5\). We had no difficulty to reach to even higher values of \(Ar\), but it is known that beyond a critical value of \(Re\) and \(We\) number time-dependent solutions prevail.

We have captured accurately not only the bubble shapes, but also the details of the flow around them and the recirculation behind them, as shown in figure 4.6, which compares the experimental observations in Hnat and Buckmaster (1796, referred to herein as HB), left-hand side of each plot, to our predictions, right-hand side, for three cases given in that reference. In
all three cases of spherical-cap shapes, these shapes and the streamline pattern including flow separation and wake formation compare extremely well. This flow separation from a smooth fluid/fluid interface has now been reported in numerous theoretical and numerical studies, e.g. RL and HB. The indentation in the rear of the bubble is not visible in the photograph by HB, but can be visualized by the dotted line we have drawn from the bubble tip towards the axis of symmetry in our results. A larger indentation in the rear of the bubble arises in figure 4.7, which compares our predictions to the experimental observations by Bhaga and Weber (1981, referred to herein as BW), who unfortunately did not show streamlines. Again the agreement is extremely good. The excellent agreement holds for $5 \times 10^{-3} \leq Mo \leq 10^3$ and $Re$ up to $\sim 100$, which is the entire range reported by BW. This is shown in figure 4.8 where we compare some of the geometric characteristics of the flow concerning bubble and wake shapes, to our predictions. These characteristics were introduced and measured by BW and are defined in figure 4.8a. In figure 8b, we clearly see that increasing $Re$ increases the bubble width and in figure 4.8c that it decreases the bubble height for the entire range of Morton numbers shown. Moreover, increasing $Re$ increases both the width (figure 4.8d) and length (figure 4.8e) of the wake and moves its centre behind the bubble further away from the bubble (figure 4.8f).

![Figure 4.6 Comparison of bubble shapes and flow streamlines observed by HB (left half) with our predictions (right half): (a) $Re = 19.62, We = 15.64$, (b) $Re = 32.69, We = 31.72$ and (c) $Re = 50.18, We = 58.04$.](image-url)
Figure 4.7 Comparison of the bubble shapes observed by BW on the left with our predictions on the right: (a) $Re = 2.44, We = 16.11$ and (b) $Re = 3.78, We = 21.69$.

(a)

(b)
Figure 4.8 Geometric characteristics of the bubble and the vortex behind it as observed in the experiments by BW (open symbols) and predicted by our code (filled symbols) as a function of Re:

(a) definitions of bubble characteristics, (b) dimensionless width of the bubble, (c) dimensionless height of the bubble, (d) dimensionless width of the vortex, $w_v$, (e) dimensionless height of the vortex, $h_v$, and (f) dimensionless location of the stagnation ring of the vortex, $h_s$. (BW: $\bigcirc$ Mo = 711, $\square$ Mo = 55.5, $\triangle$ Mo = 4.17, $\lozenge$ Mo = 1.03, $\triangledown$ Mo = 0.108, $\leftdownarrow$ Mo = 5.48×10^{-3}, present work: ■ Mo = 2.5×10^{-3} − 5×10^{-3}, ● Mo = 3.2×10^{-2}, ▲ Mo = 0.4, ▼ Mo = 1, 3.2, ◇ Mo = 25.6, 40, ★ Mo = 125, 320, ▶ Mo = 10^3 − 1.25×10^3).
4.4.2 Bubble shapes in Bingham fluids

First, we will present some of the convergence tests we have performed to verify that our results have converged with the exponent $N$ of the Papanastasiou model. We have also undertaken the usual convergence tests with just mesh refinement, but we will not report them here for conciseness. The issue of convergence of results with $N$ is often raised, when Papanastasiou’s or any other of the so-called regularization models are used. All these models depend on some regularization parameter to avoid the discontinuity introduced by the original Bingham model. To verify convergence, Beris et al. (1985, referred to herein as BTAB), having modified the discontinuous Bingham model by introducing the regularization parameter suggested by Becovier and Engelman (1980) and Glowinski, Lions and Tremolieres (1981), carried out such a convergence study and verified that their results approached an asymptotic value as this regularization parameter reached very large values. Moreover, Smyrnaios and Tsamopoulos (2001) studied the squeeze flow of a Bingham plastic between two parallel disks using either the same regularization parameter as BTAB or Papanastasiou’s exponential model. They demonstrated that not did only did each model converge as the each regularization parameter took very large values, but that they converged to the same result. In all cases very sensitive variables for convergence are the rate of strain tensor and the location of the yield surface. On the other hand, Frigaard and Nouar (2005) examined the convergence of regularized models to those of the corresponding exact (discontinuous) model. For the Papanastasiou model they showed that the $H_1$ norm of the velocity vector converged with increasing $N$ like $N^{-0.5}$, whereas no explicit form was derived for the convergence of the norm of the stress tensor. Nevertheless, it was determined that convergence deteriorated as the second invariant of the stress approached the yield stress, i.e. critical conditions for the entire yielded material. We have carried out repeated tests to verify that the results in this study are independent of the exponent $N$. One such study is shown in table 4.4, for two sets of parameters for which we predict that the bubble is about to become entrapped in the material, i.e. near critical conditions, where the velocities have decreased considerably. We calculated the Euclidian norm of the deviation of a solution with $N=100, 500, 1000$ and $5000$ from the solution with $N=10000$ for the velocity and the stress components and the pressure. Here we have used a mesh of the type in figure 4.2(a,b). We can clearly see that the computations converge with increasing $N$, faster for the velocities than the stresses or the pressure, with an exponent that is always larger in absolute value than $0.5$ and that the difference between values computed with $N=5000$ and those computed
with \( N = 10000 \) is fairly small. Consequently, we can generally consider that our results have converged with \( N \) when we take \( N = 10000 \) and that the \textit{a posteriori} calculated yield surfaces are reasonably accurate.

<table>
<thead>
<tr>
<th>Variable</th>
<th>( v_r )</th>
<th>( v_\theta )</th>
<th>( \tau_{rr} )</th>
<th>( \tau_{r\theta} )</th>
<th>( \tau_{\theta\theta} )</th>
<th>( P )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case B(_1)</td>
<td>–0.685</td>
<td>–0.689</td>
<td>–0.648</td>
<td>–0.635</td>
<td>–0.598</td>
<td>–0.502</td>
</tr>
<tr>
<td></td>
<td>( (1.3 \times 10^{-5}) )</td>
<td>( (1.5 \times 10^{-5}) )</td>
<td>( (5.2 \times 10^{-5}) )</td>
<td>( (3.6 \times 10^{-5}) )</td>
<td>( (3.0 \times 10^{-5}) )</td>
<td>( (2.3 \times 10^{-5}) )</td>
</tr>
<tr>
<td>Case B(_2)</td>
<td>–0.867</td>
<td>–0.870</td>
<td>–0.721</td>
<td>–0.751</td>
<td>–0.584</td>
<td>–0.701</td>
</tr>
<tr>
<td></td>
<td>( (7.4 \times 10^{-6}) )</td>
<td>( (8.2 \times 10^{-6}) )</td>
<td>( (3.9 \times 10^{-5}) )</td>
<td>( (3.0 \times 10^{-5}) )</td>
<td>( (1.9 \times 10^{-5}) )</td>
<td>( (1.1 \times 10^{-4}) )</td>
</tr>
</tbody>
</table>

Table 4.4 Least squares fit of the exponents, \( \beta \), in the expression \( \| \text{dev} \| = A \| N \|^{\beta} \), where ‘dev’ stands for the deviation of the indicated variable of each of the solutions with \( N = 100, 500, 1000 \) and \( 5000 \) from the solution with \( N = 10000 \). Below each value and in parentheses we give the norm of the ‘dev’ between the two larger values of \( N \), 5000 and 10000. In case \( B_1 \), the parameter values are \( Ar = 1, Bo = 20, Bn = 0.14 \) and the mesh has 100 radial and 120 azimuthal nodes, whereas in case \( B_2 \), \( Ar = 1, Bo = 5, Bn = 0.1 \) and the mesh has 90 radial and 80 azimuthal nodes. In both cases the mesh is of the type shown in figure 4.2(a,b).

Next we will discuss the effect of increasing the Bingham number on bubble shapes and yield surfaces. Figure 4.9 shows the dependence of the bubble shape and the yielded (white) and unyielded regions (grey) on \( Bn \) for two quite distinct cases of \( Ar \) and \( Bo \). The dimensionless distance of the outer boundary from the bubble centre is always \( R_\infty = 10 \), except for the first case in figure 4.9b where \( R_\infty = 15 \), in order to include the outer yield surface in each case. In the first set of bubbles (Figure 4.9a), where the gravitational forces balance viscous forces (\( Ar = 1 \)) and capillarity is rather weak (\( Bo = 50 \)) we see that inside the cavity that exists at the rear of the bubble, even for a Newtonian fluid, the stresses fall below the yield stress and a very small region of unyielded material is formed for \( Bn = 0.01 \). Of course, stresses monotonically decrease away from the bubble and unyielded material exists there also. The yield surface is nearly symmetric around the bubble, but slightly closer to it around the poles. A similar shape of the yield surface was obtained for the creeping flow of a sphere in a Bingham fluid in BTAB. At higher \( Bn \), \( Bn = 0.05 \), the material around the bubble
“freezes” closer to the bubble surface and the yield surface retains the previously described shape. The bubble elongates a little, and the size of the rear indentation decreases and does not provide enough space for slow enough flow there. Hence the unyielded region at the rear of the bubble disappears. At even higher $Bn$ ($Bn = 0.14$), the bubble elongates further and unyielded material arises in contact with it around its equatorial plane. BTAB have shown that unyielded material arises around the poles of a solid sphere in a region that increases with $Bn$. On the contrary in a bubble, the zero-shear-stress condition applied on its entire surface forces it to move with the surrounding liquid. Moreover, bubble deformability makes it elongated-developing a small region around its equatorial plane that is parallel to the z-axis with a locally uniform azimuthal velocity. Around this portion of the bubble surface velocity variations decrease and the material can become unyielded. As $Bn$ increases further, $Bn = 0.19$, the area of the unyielded material at the equatorial plane increases and the unyielded material away from the bubble comes closer to it. Eventually these two unyielded areas will merge, the velocity all around the bubble will drastically decrease and the bubble will be entrapped in the material. We will discuss this further in § 4.4.4.
Figure 4.9 Dependence of the bubble shape and the yielded (white) and unyielded (grey) domains on $Bn$ for $N=10^4$ and (a) $Ar=1$, $Bo=50$, (b) $Ar=50$, $Bo=10$, for $Bn=0.01$, 0.05, 0.14, and 0.19; $R_s=10$ in all cases except for the first one in (b) where $R_s=15$.

In the second case (figure 4.9b) where the gravitational forces are more important compared to viscous forces ($Ar=50$) and capillarity is not so weak ($Bo=10$), we observe some distinct changes at small $Bn$, $Bn=0.01$ and $Bn=0.05$, but nearly the same bubble shapes at the larger $Bn$. At $Bn=0.01$, the bubble has an oblate ellipsoidal shape with a flatter rear side, not very different from its Newtonian counterpart, but completely different from that in case (a). Unyielded material exists at the rear surface of the bubble as in (a), but more importantly the rising bubble generates a vortex behind it and enhances the rate of strain there so that unyielded material appears further away from the bubble at its rear than at its front side. Thus, the unyielded surface around the bubble does not have a fore-aft symmetry any longer. At $Bn=0.05$ the shape of the bubble is still different from that in case (a), being flatter underneath, and the unyielded region around the bubble tends to become symmetric. At even higher $Bn$, both the shape of the bubble and the unyielded areas are much like those in case (a).

In figure 4.10 we show how the map of bubble shapes, given in figure 4.5, evolves as $Bn$ increases. The corresponding Morton numbers are given in table 4.3 and the $Re$ and $We$ values underneath each bubble shape. The bubble rise velocity decreases with the Bingham
number and that is reflected in the decreasing Reynolds and Weber numbers. We show the unyielded material in grey. For $Bn \leq 0.1$ we show only the unyielded material, when it arises, on the bubble surface, because unyielded regions around the bubble are too far to be included in this figure. For larger $Bn$ we also show the unyielded material around the bubble. Even a small $Bn$ introduces qualitative changes in certain bubble shapes. For example, when $Ar = 0$, $Bn = 0.01$ (figure 4.10a) and $Bo$ is high enough, the bubble is no longer spherical because a small cavity at its rear side has been formed, while when $Bn = 0.05$ (figure 4.10b) and $Bo \geq 5$, the shape is again not spherical, but slightly elongated and at its rear side flatter or with a small indentation. Papanastasiou’s (and every other) viscoplastic model, is nonlinear. This, for finite Bond numbers, i.e. deformable bubbles, the characteristic Newtonian property at $Ar \to 0$ of fore-aft symmetry in the bubble shapes and the flow field is broken. The break-up of the flow fore-aft symmetry in inelastic non-Newtonian fluids has been also experimentally observed in the case of the flow around a settling sphere even at small Reynolds numbers, (Gueslin et al. 2006). Moreover, the measured rate of strain near the bubble and at the equatorial plane has very small values and consequently the effective viscosity of the material is high there. On the contrary, near the poles the measured rate of strain is higher and the effective viscosity is smaller. As a result, the bubble tends to deform preferentially in the direction of its poles, taking an elongated shape. The elongation of the bubble becomes more prominent as the yield stress over the capillary forces increase and the bubble has to squeeze through the material. In certain cases that the Newtonian fluid recirculates very slowly at the rear of the bubble, the stress in a viscoplastic fluid is small, with $\|\tau\| \leq \tau_y$, and so the material in this region is unyielded. One such case is shown in figure 4.10a, but such cases populate the entire corner of the map with large Bond and Archimedes numbers as $Bn$ increases to 0.05 (figure 4.10b) and the effective viscosity increases. Here the unyielded area behind the bubble increases and the bubble deformation from spherical decreases compared to that for a Newtonian fluid. A shape with flatter front side does not arise in the map with $Bn = 0.05$, in which every location is occupied by a converged solution.

Dubash and Frigaard (2007) have studied experimentally the motion of air bubbles rising under gravity in a column filled with Carbopol solutions. The yield stress of the material they used was $\tau_y^* = 2.2 - 2.3 \text{ Pa}$ and its other properties and bubble sizes were such that $Bn = 0.0104 - 0.022$, $Ar = 0.466 - 4.31$ and $Bo = 15 - 66$. This range of parameter values is covered in figure 4.10a,b. Unlike our predictions, the bubble shapes they observed resembled an inverted teardrop. We tried to reproduce these shapes numerically, first using
the Papanastasiou model and then using the Herschel-Bulkley model which is more appropriate for the Carbopol solutions used in these experiments, by assuming either shapes closer to the experimental ones as initial bubble shapes to start the Newton-Raphson iterations or higher \( Bn \). Our iterations never converged to such shapes, but to the shapes given in figure 4.10a,b. We could attribute the inverted teardrop shape to a number of reasons: (i) Carbopol solutions have a small elasticity which may be important at the rear of the bubble where slower flow takes place and closer to the axis of symmetry the flow is elongational. It is well-known that bubbles assume inverted teardrop shapes in viscoelastic fluids; Astaritta and Apuzzo (1965), Pilz and Benn (2007), Malaga and Rallison (2007). (ii) Another reason could be that Carbopol is thixotropic, which could introduce phenomena that cannot be predicted by viscoplastic models, Gueslin, et al. (2006). (iii) A third reason could be that, in the experiments by Dubash and Frigaard (2007), the bubbles were rising in a tube with diameter not much larger than a typical bubble diameter. In such a narrow tube the fluid must flow downwards closer to the bubble surface giving it a prolate shape. If this deformation is large enough for a liquid drop in creeping flow, Koh and Leal (1989) have shown that the drop shape becomes time-dependent, forming a tail that may constantly elongate and even break. They have also shown that the larger the initial deformation, the smaller the capillary number required for this instability to arise and that this occurs for a wide range of viscosity ratios between the drop and the host liquid. Presumably this could also takes place in a rising bubble and, when the host liquid is viscoplastic, the tail can be ‘frozen’, so that a stationary shape is obtained. Moreover, Terasaka and Tsuge (2001) have observed that the bubble assumes inverted teardrop shapes when it is formed at a nozzle and this shape is ‘frozen’ owing to the material’s yield stress. Finally, we should mention that experiments with different Carbopol solutions have also been reported by Astarita and Apuzzo (1965) who observed shapes of unconfined bubbles similar to the ones we predict, whereas they observed teardrop shapes in other fluids which were clearly viscoelastic.

As \( Bn \) increases to \( Bn = 0.1 \) (figure 4.10c), the shape of the bubble has changed in all cases for \( Bo \geq 0.1 \), for reasons that we have mentioned already. For small Bond numbers the bubble remains almost spherical, as surface tension is very important. For \( Bo \geq 5 \) gravitational forces become dominant over surface tension, the effective viscosity around the equatorial plane is higher than that at the poles and the bubble starts to take a bullet-like shape. The bubble retains a flatter rear side than the front side and an indentation for large Bond and Archimedes numbers. As the rate of strain is low enough around the equatorial plane, unyielded material exists there. The sizes of the two unyielded regions, the one far
from the bubble and the other around the equatorial plane, increase as $Bn$ increases to 0.14 (figure 4.10d). For $Bo < 5$ where the bubble in nearly spherical the two unyielded regions are considerably larger than for $Bo \geq 5$. At $Bn$ greater than 0.14 and depending on the value of the Bond number, the two regions will start merging, and then the bubble is immobilized and all the material becomes unyielded. For this reason, in figure 4.10e, where $Bn = 0.19$, we show cases with $Bo \geq 10$ only, so that, although $Bn$ approaches its critical value, the more deformable bubble can take a nearly symmetric prolate shape or a bullet-like shape while rising in the material, irrespective of the values of the other parameters. An envelope of yielded material still completely surrounds the bubble and flow continue to take place. For $Bo < 10$ the flow has stopped and the bubble has been immobilized.
### (b)

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<th>10</th>
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<td>(7.941, 0.630)</td>
<td>(6.976, 2.433)</td>
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<td>(6.742, 9.955)</td>
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<td>(6.680, 22.31)</td>
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<td>(44.85, 2.013)</td>
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<td>(100.8, 10.16)</td>
<td>(100.6, 20.25)</td>
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### (c)

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<td>(3.171, 2.012)</td>
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<td>(3.128, 4.893)</td>
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<td>(16.28, 1.325)</td>
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<td>(13.87, 9.615)</td>
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<td>(158.7, 0.252)</td>
<td>(93.45, 0.873)</td>
<td>(55.13, 2.121)</td>
<td>(61.70, 3.806)</td>
<td>(57.99, 6.725)</td>
<td>(54.93, 12.07)</td>
<td>(54.20, 14.69)</td>
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</table>
Figure 4.10 Map of bubble shapes in a Bingham fluid as a function of the Bond and Archimedes numbers. Underneath each figure we give the corresponding Reynolds and Weber numbers ($Re, We$): (a) $Bn = 0.01$, (b) $Bn = 0.05$, (c) $Bn = 0.1$, (d) $Bn = 0.14$ and (e) $Bn = 0.19$. Unyielded material is shown black, and always when it arises in contact with the bubble, but away from the bubble only when it is close enough, $Bn \geq 0.14$. 

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Figure 4.11 quantifies the bubble shapes by showing their aspect ratio \( \chi = \frac{h}{w} \), where \( h \) and \( w \) are defined in figure 4.8a, as a function of \( Bo \) for the entire range of \( Ar \) we studied and \( Bn = 0.01, 0.1, 0.14 \). At the smallest \( Bn \) and for \( Ar = 1 \), the aspect ratio remains very close to unity as \( Bo \) increases, since for such materials the bubble remains almost spherical. For larger \( Ar \), the aspect ratio decreases from unity, more so at a larger \( Ar \), until it reaches a plateau, as the bubble assumes an oblate spheroidal shape. In the line with-largest Archimedes number, \( Ar = 5000 \), and for \( 4.5 \leq Bo \leq 9 \) there is a discontinuity in the curve of the aspect ratio because stationary bubble shapes could not be calculated there but the bubble shapes changed abruptly there, see figure 4.10a. For \( Bn = 0.1 \) and as \( Bo \) increases, the aspect ratio decreases below 1 for \( Ar \geq 500 \) and increases above 1 for \( Ar \leq 50 \) as the bubble assumes a prolate spheroidal shape. For the highest \( Bn \), changes in \( Ar \) have a small effect on the aspect ratio as long as \( Bo \leq 1 \). Beyond this \( Bo \) value the aspect ratio increases and, above a particular value of \( Bo \) which is in the range \( 10 \leq Bo \leq 20 \), it decreases, more so for the larger \( Ar \), trends which are opposite to those for \( Bn = 0.01 \). Summarizing, bubbles with small \( Bn \) will be either spherical or oblate, but with large \( Bn \) they will be either spherical or prolate.

Figure 4.12 gives the definitions of the width and the height of the unyielded region at the rear side of the bubble and shows that they increase monotonically with the Bond number, the width more so. Such regions arise mainly when \( Bn = 0.05 \) and they increase with \( Ar \), which generally produces spherical cap shapes, and with \( Bo \), which increases bubble deformability. Given a \( Bo \) value, larger inertia produces a flatter bubble shape which provides a larger shield behind it for unyielded material to exist there. As soon as unyielded material is formed, its size first increases abruptly with \( Bo \), but then both its height and width reach an asymptote which usually do not exceed the radius of the equivalent spherical bubble.
Figure 4.11 Bubble aspect ratio vs. $Bo$, for various $Ar$ values and (a) $Bn = 0.01$, (b) $Bn = 0.1$ and (c) $Bn = 0.14$.

Figure 4.12 Dimensionless width (dashed line) and height (solid line) of the unyielded region behind the bubble vs. $Bo$, for various $Ar$ values and $Bn = 0.05$. In an inset we show the definitions of these geometric characteristics.
4.4.3 Flow field in Bingham fluids

Figure 4.13 illustrates the flow field around the bubble in a viscoplastic fluid. Capillary forces are rather weak, $Bo = 30$, while the gravitational forces balance the viscous forces, $Ar = 1$. We show contour plots of radial velocity, on the left half, and azimuthal velocity on the right half of each figure, for low $Bn = 0.01$ (figure 4.13a) and for high $Bn = 0.19$ (figure 4.13b). The total number of equidistant contour lines in this and all other similar plots is 20, unless otherwise mentioned. The outer boundary has been chosen at such a distance that it does not affect the results in any way. For these two cases we have used $R_\infty = 10$, but for clarity in the figures we present a square of side length 10 only. The radial velocity takes its lowest and negative values at the upper side far from the bubble, as the fluid flows downwards, and its highest and positive values at the far lower side of the bubble, while it is zero at the equatorial plane. As mentioned earlier, a boundary condition sets the radial and azimuthal velocities far from the bubble to vary like $\cos(\theta)$ and $\sin(\theta)$ respectively. Our computations show that this dependence remains throughout the unyielded material but not in the yielded material and especially as the bubble surface is approached and $Bn$ increases (see § 4.4.4), indicating that the far-field unyielded material behaves as solid. The values of the radial velocity are quite large for small $Bn$, $Bn = 0.01$ (left side of figure 4.13a) where the fluid still behaves similarly to a Newtonian one. As a reminder, the dimensionless far-field ($r \to \infty$) velocity of a spherical bubble in a Newtonian fluid for $Re = 0$ is $U = 1/3$. However, we can see in figure 4.13a that even for this small $Bn$ the far-field ($r = 10$) velocity has decreased to $U = 0.224$. This is a consequence of the viscoplasticity of the fluid and of the shape of the bubble. At higher $Bn$, $Bn = 0.19$, viscoplasticity will further decrease the velocity field around the bubble. Indeed, in figure 4.13c the radial velocity is two orders of magnitude smaller, but still varies away from the bubble following the cosine function. The shape of the bubble is very different in these two cases, as discussed in § 4.4.2. The azimuthal velocity, for both values of $Bn$, is zero at the axis of symmetry as it should, while it has its largest values at the equatorial plane. The azimuthal velocity is almost zero inside the indentation that arises at the rear of the bubble for $Bn = 0.01$. Increasing the $Bn$ to 0.19, the magnitude of the azimuthal velocity also decreases by 2 orders of magnitude. Here an area of nearly uniform azimuthal velocity arises at the equatorial plane and in contact with the bubble surface. Indeed the contour lines of the azimuthal velocity clearly demonstrate that its gradient is much larger at the poles while it decreases to zero at the equatorial plane, where the bubble surface is nearly flat. Figures 4.13b and 4.13d show the pressure field (left side)
and the second invariant of the rate of strain tensor (right side), respectively. For both $Bn$ values, the pressure field varies linearly with the axial distance from the bubble, with negative values above it and positive values below it, as expected. The presence of the bubble affects the pressure field only locally and around it. The rate of strain has a local maximum at the poles, a local minimum around the equatorial plane near the bubble and tends to zero at infinity. Calculating $\dot{\gamma}$ for a spherical bubble moving in a Newtonian fluid, where the analytical solution is known, we find that at $(\theta = \pi/2, \ r = 1)$, $\dot{\gamma} = 0$, whereas $\dot{\gamma} \neq 0$ at $\theta = 0$ and $\theta = \pi$. The existence of even one point on the bubble surface where $\dot{\gamma} = 0$ forces the material to become unyielded there; this slows down the flow field and decreases $\dot{\gamma}$ around it. This eventually leads to the creation of a finite domain in the material that is unyielded. In figure 4.13b, we observe that $\dot{\gamma}$ has a local maximum at the bubble tip at the rear of the bubble and abruptly decreases as we move towards the south pole of the bubble. However, it does not become small enough to allow unyielded material to form inside the small indentation which exists there. This occurs for other parameter values as seen in figures 4.10a,b. On the contrary, in figure 4.13d, the larger $Bn$ reduces the values that $\dot{\gamma}$ takes and gives the bubble a prolate shape without a tip or an indentation. Hence, $\dot{\gamma}$ varies smoothly around the bubble surface and is symmetric with respect to the equatorial plane of the bubble. For both values of $Bn$ the values of $\dot{\gamma}$ where unyielded material exists are smaller by over three orders of magnitude than those in the rest of the material.

In figure 4.14, we show corresponding contours for the same four variables and the same $Bo$, but larger buoyancy with respect to dynamic viscosity, $Ar = 50$. For $Bn = 0.01$ (figure 4.14a,b), the bubble has the shape of a spherical cap with a tip in its rear side. For $Bn = 0.19$ (figure 4.14c,d), the bubble takes a prolate shape and is nearly flat at its equatorial plane. In the smaller $Bn$ case, the radial velocity is larger, but quite symmetric before and after the bubble because of the large vortex that is formed in the bubble wake. The pressure contours remain straight and horizontal away from the bubble and are slightly affected by it and only in its vicinity. The rate of strain has a local sharp maximum at the bubble tip and becomes very low in its wake, but unyielded material does not arise there. On the contrary, for $Bn = 0.19$, the velocity components are much smaller, have a plane of symmetry and the azimuthal velocity is very small at the equatorial plane near the bubble. At this same location, the rate of strain takes its lowest values (smallest by 4 orders of magnitude than its maximum at the poles) giving rise to unyielded material in contact with the bubble.
Figure 4.13 (a, c) Contour plots of the radial, left side, and azimuthal, right side, velocity, and (b, d) contour plots of the pressure field, left side, and second invariant of the rate of strain tensor, right side, for $Ar = 1$, $Bo = 30$, $R_\infty = 10$, $N = 10^4$ and (a, b) $Bn = 0.01$ and (c, d) $Bn = 0.19$. The range of the respective variable is divided into 20 equal intervals.
Selected cases with bubble shapes and streamlines are shown in figure 4.15. The particular values of the stream function are given in each figure. For the lowest Bingham number we examined, $Bn = 0.01$, the streamlines do not deviate appreciably from the corresponding ones for a Newtonian fluid and no unyielded material arises in contact with the bubble. In particular, for $Ar = 1, Bo = 50$ (figure 4.15a) an indentation is formed behind the...
bubble and the streamfunction assumes very small and negative values in this region, indicating flow separation. As the Archimedes number increases to 500 (figure 4.15b), a vortex is formed behind the bubble, which takes an oblate shape with rounded edge for $Bo = 10$ or more pointed edge at higher Bond numbers, $Bo = 40$ (figure 4.15c). At even higher Bond numbers it is possible skirted bubbles could be formed in analogy to those in Newtonian fluids. Figure 4.15d shows a particular bubble shape that arises for $Ar = 5000$ and $Bo = 4.5$ just before the region in which steady bubble shapes could not be computed for this Bingham number or for a Newtonian fluid; see figures 4.5 and 4.10a. Here the bubble edge is smooth but tilted in the upstream direction, the bubble resembles a hat and the vortex behind it is fairly large. A slight increase of the Bingham number to 0.05 eliminates flow separation and the vortex behind the bubble, see figure 4.15e, which is a common feature in general for $Bn \geq 0.05$. Increasing the Bingham number further to 0.1 (figure 4.15f) or 0.14 (figure 4.15g) produces more rounded bubbles with a prolate shape and, hence, streamlines that are less curved around the bubble.
We have measured and depict in figure 4.16, the size and the location of the vortex behind the bubble in a Bingham fluid only for $Bn = 0.01$. These geometric characteristics were defined in figure 4.8a. Figure 4.16a clearly shows that the vortex length and width increases with both the Archimedes and the Bond numbers. Similarly in figure 4.16b, shows that its centre becomes further away from the bubble back side and the axis of symmetry as these dimensionless parameters increase.
Figure 4.16 (a) Length and width of the vortex behind the bubble and (b) distance of its centre from the bubble centre and the axis of symmetry for \( Bn = 0.01 \). (\( Ar = 5 \); \( Ar = 50 \); \( Ar = 500 \); \( Ar = 5000 \)).
4.4.4 Dynamic parameters of flow and critical Bingham number for bubble entrapment

The magnitude of the bubble rise velocities or equivalently the magnitude of the far-field velocities in a frame moving with the bubble is given in terms of the corresponding Reynolds or Weber number as a function of the Bingham number in figure 4.17. Both these dynamic parameters are post-calculated based on the bubble velocity according to (4.2) and (4.3). The Bond number is fixed in figure 4.17a at $Bo = 10$. As $Ar$ increases, $Re$ increases as well, more so for small Bingham numbers. Moreover, as $Bn$ increases $Re$ decreases because the bubble rise velocity decreases and at a critical $Bn$ the bubble stops moving, irrespective of the value of $Ar$ and $Bo$ because all the material is unyielded. The dependence of $We$ on $Bn$ is similar to that of $Re$, as shown in figure 4.17b, for $Ar = 1$ and for different values of $Bo$. The Weber number increases monotonically with $Bo$ and decreases with $Bn$. Apparently, lines of different $Bo$ approach zero for different values of $Bn$, indicating that capillary forces will affect the critical level of yield stress in a material that will cause bubble entrapment. The exact condition for bubble entrapment is not easy to determine from this figure or from plotting the drag force on the bubble as a function of $Bn$, because Papanastasiou’s constitutive equation does not discriminate between yielded and unyielded domains a priori and allows some residual flow even where unyielded material is found a posteriori. So a clear asymptote in the drag force, like the one produced in figure 6 of BTAB, should not be expected.
A first possible determining the conditions for bubble entrapment in a viscoplastic fluid is to perform a plastic boundary layer analysis assuming that the bubble remains spherical, i.e. the Bond and Archimedes numbers are fairly small, parallel to the analysis in BTAB for a solid sphere. Under this assumption, we first examined whether a boundary layer is formed around a bubble and whether the Papanastasiou model can capture it by plotting the radial profile of the azimuthal velocity at the bubble equatorial plane with $Bn$ as a parameter. Unlike the analysis in BTAB, here the bubble rise velocity is determined as part of the solution and decreases with $Bn$, whereas on the bubble surface it is zero, owing to the zero-shear boundary condition applied there. In order to compare the various profiles with each other more easily, we normalized the azimuthal velocity so that it is equal to 1 away from the bubble. The computed profiles are shown in figure 4.18, where we have kept the same low value for the Reynolds number, $Re = 0.04$, in analogy with the creeping flow conditions in BTAB. We observe that the azimuthal velocity for a Newtonian fluid approaches its far-field value monotonically. On the contrary, in a Bingham fluid it exhibits a maximum, which moves closer to the bubble and becomes sharper as the Binghma number increases. This occurs because the outer yield surface moves closer to the bubble decreasing the width of the path through which material can still flow through the equatorial plane. This approach of the velocity maximum to the bubble surface indicates the formation of a boundary layer. At $r = 1$, 

Figure 4.17 Dependence of (a) $Re$ on $Bn$ for $Bo = 10$ and (b) $We$ on $Bn$ for $Ar = 1$. 

![Figure 4.17](image-url)
the location of the bubble surface at the equatorial plane, the azimuthal velocity is not zero as in the case of a solid sphere (see figure 10 in BTAB), but equals the bubble surface velocity there because of the zero-shear condition. As $Bn$ increases, this velocity first increases above its far-field value, $0.04 \leq Bn \leq 0.11$, but then it decreases towards it as critical conditions are approached and the two yield surfaces tend to merge, $Bn = 0.135$. Unfortunately, the inevitable formation of unyielded material around the bubble equator, the shape and size of which depends on $Bn$, makes the necessary scaling arguments very complicated and the outcome of this semi-analytical approach questionable.

Figure 4.18 Radial profiles of the azimuthal velocity at $\theta = \pi / 2$ for different values of $Bn$ and $Re = 0.04$, $Bo = 0.01$.

Instead, it is reasonable to consider that the bubble motion stops and that $Bn$ has reached its critical value when the unyielded area away from the bubble merges with the one around its equatorial plane. Such a situation just before the two yield surfaces merge is shown in figure 4.19 for three different sets of material parameters. If the third decimal place of $Bn$ increases by even one unit in each of the three cases the two yield surfaces will merge. On the left half of each figure we show the bubble and the yielded domains in white and the unyielded domains in grey, while on the right half of each figure we show the second invariant of the rate of strain tensor. In all cases, we see that although the two unyielded regions are about to merge, $\dot{\gamma}$ is nowhere equal to zero, but where unyielded material is
predicted it takes values that are smaller by 3-4 orders of magnitude than in the rest of the material and certainly below the critical value $N^{-1}$ for the Papanastasiou model as explained in § 4.3.3. So even when the two regions have merged, finite motion of the material is predicted, albeit with very large viscosity and, hence, very small velocity.

**Figure 4.19** Yielded (white) and unyielded (grey) domains, left half, and contour plots of the second invariant of the rate of strain, right half, near the critical Bingham number for $N = 10^4$, $R_\infty = 10$, and (a) $Bn = 0.142$, $Ar = 1$, $Bo = 0.1$, (b) $Bn = 0.198$, $Ar = 50$, $Bo = 15$, and (c) $Bn = 0.201$, $Ar = 5000$, $Bo = 30$. 
Figure 4.19 also demonstrates that the critical $Bn$ at which the bubble will stop moving is distinct for the three cases and depends mostly on the shape of the bubble. The higher the Bond number is, the more the bubble is deformed, becoming elongated in order to squeeze through the material as the critical condition approaches. This concurs with the conclusion of Dubash and Frigaard (2007) who, based on scaling arguments, mentioned that larger and more deformable bubbles are more difficult to immobilize. The variation of the distance between these two surfaces at the equatorial plane, $d_u$, is shown in figure 4.20. It decreases slowly with $Bn$ up to a critical point, after which it decreases exponentially and meets the x-axis at increasing values of $Bn$ as $Bo$ increases. We call the point of intersection with the x-axis critical Bingham number, $Bn_c$. Its values, shown in figure 4.21, are independent of the Archimedes number, when $Ar < 100$ and only slightly dependent on it at higher $Ar$ values. The Bond number does not affect $Bn_c$, if it is so small that surface tension does not allow the bubble to deform from its spherical shape, i.e. $Bo \leq 0.1$, or so large that the bubble deformation is restricted by the outer yield surface, the shape of which does not vary much with the surface tension of the bubble, i.e. $Bo \geq 50$.

![Figure 4.20](image-url)

**Figure 4.20** Variation of the distance between the two yield surfaces at the equatorial plane, $d_u$ vs. $Bn$ for various $Bo$. In an insert we show the definition of this distance.
Figure 4.21 Dependence of critical Bingham number on Bond and Archimedes numbers. The curves with $Bo = 0.01$ and $0.1$ are indistinguishable.

In these calculations of the critical conditions we used a mesh of the type given in figure 4.2b with $N = 10^4$. We repeated this calculation with a mesh of the type given in figure 4.2c with an even larger value $N = 5 \times 10^4$. The results are given in table 4.5 and demonstrate that neither the value of $N$ nor the structure of the mesh affect them. It is noteworthy that the Bingham number used so far in this work is related to the so-called yield stress parameter, $Y_g$, of BTAB by:

$$Y_g = \frac{3}{2} Bn$$

(4.32)

<table>
<thead>
<tr>
<th>Mesh, $N$</th>
<th>Bo</th>
<th>0.1</th>
<th>5</th>
<th>10</th>
<th>50</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M1$, $10^4$</td>
<td></td>
<td>0.143</td>
<td>0.175</td>
<td>0.192</td>
<td>0.212</td>
</tr>
<tr>
<td>$M2$, $5 \times 10^4$</td>
<td></td>
<td>0.142</td>
<td>0.174</td>
<td>0.192</td>
<td>0.214</td>
</tr>
</tbody>
</table>

Table 4.5 Critical $Bn$ values as a function of $Bo$ for two meshes (figures 4.2a and 4.2c) and values of $N$ $10^4$ and $5 \times 10^4$ at $Ar = 1$. 
The critical value for entrapment of a sphere in a Bingham fluid under creeping flow conditions was found in BTAB to be $Y_g = 0.143$, i.e. it is smaller by a factor of $2/3$ than that for a non-deformable bubble under the same conditions. This is the same ratio as the ratio of the terminal velocity of a solid sphere to that of a spherical bubble under the same buoyancy force. Clearly, the more retarding no-slip condition on the solid sphere requires a smaller yield stress to entrap it in a Bingham fluid than the shear free condition on a bubble surface.

![Figure 4.22](image)

**Figure 4.22** Dimensionless bubble rise velocity vs. $Bn$ for $Ar = 1$ and $Bo = 0.1$.

As the two yield surfaces tend to merge, the magnitudes of the velocity and rate of strain fields decrease everywhere in the domain that is still yielded. We stopped our computations at the value of $Bn$ for which they have just merged, because beyond that value the numerical error in computing such small variables becomes significant. In any case, it reasonable to monitor the bubble rise velocity as the Bingham number increases. This is shown in figure 4.22, for just the first case given in figure 4.20, where $Ar = 1$ and $Bo = 0.1$. We observe that as the Bingham number increases the logarithm of the terminal velocity decreases, but for $Bn > 0.13$ the slope of the curve decreases abruptly and then increases again. We attribute the sharp decrease in the slope to the approach of critical conditions, but the subsequent increase to the numerical error we described above. We have taken the slope of this curve at its inflection point and we can clearly see that it intersects the abscissa at
In other words, monitoring the terminal velocity results in the same critical number. The outcome similar is for all other cases we examined. This abrupt change in slope corresponds to the abrupt change in slope of the terminal velocity vs. bubble volume experimentally measured by Astarista and Apuzzo (1965). Unfortunately, these authors did not report the value of the material’s yield stress, so we cannot convert their bubble volumes to our Bingham numbers and directly compare our predictions to their measurements.

Dubash and Frigaard (2007) experimentally determined the critical Bingham number for bubble rise in a Bingham fluid and found that, depending on bubble aspect ratio, it varied between 0.01 and 0.15. Their upper limit falls within our predictions, although it should be recalled that the experimental bubble shapes resembled inverted teardrops and this should affect their mobility. On the contrary, the prediction of \( Bn_c \) using variational principles and a Newtonian flow field around a spherical bubble by the same authors (Dubash and Frigaard 2004) grossly overestimates it, since it places it in the range of 0.7-2. We examined the predictions of two inequalities resulting from these variational (Theorem 3) using the flow field and the bubble shape we have predicted in this work. Starting with very small \( Bn \) values the predicted \( Bn_c \) values are about 0.7 as reported by Dubash and Frigaard (2004). Increasing the \( Bn \) of the material affects not only the bubble shape but also the flow filed qualitatively as mentioned previously. This results in a continued decrease of the \( Bn_c \) value up to \( Bn \approx 0.12 \), for which \( Bn_c \approx 0.25 \). However, for larger values of \( Bn \), \( Bn_c \) started to increase. This is probably caused by the very small values of \( \dot{\gamma} \) that arise in the denominator of the inequality (35) in Dubash and Frigaard (2004). The situation did not change when inequality (51) was used.

Figure 4.23 shows the dependence of the bubble velocity (in mm/s) on the equivalent bubble radius (in mm) with the material’s yield stress as a parameter, keeping the other material properties close to those reported by Maxworthy et al. (1996) for the mixture of 80% glycerin in water. For small bubbles, their rise velocity is zero irrespective of the yield stress, but smoothly increases as the bubble size increases. This is understandable, given that an increase in bubble radius decreases \( Bn \). Bubble mobilization occurs earlier and higher velocities are attained for materials with a smaller yield stress. For easier comparison we have also included in the same figure the bubble terminal velocity in a Newtonian fluid.
Finally the drag coefficient is shown as a function of the Bingham number for a given value of $Ar$ (figure 4.24a) or for a given value of $Bo$ (figure 4.24b). In all cases, increasing $Bn$ from zero increases $C_d$ by several orders of magnitude and more abruptly as the critical conditions are approached, and for all practical cases the bubble is immobilized. The values of $C_d$ and its increase are larger for a less deformable bubble ($Bo = 0.01$) with less inertia ($Ar = 1$). As expected, given a value of $Ar$, increasing $Bo$ decreases the drag coefficient as the bubble deformability increases. Furthermore, given a value of $Bo$, increasing $Ar$ decreases the drag coefficient. This should be expected also, since according to (4.30) $C_d$ is inversely proportional to $Ar$. The same dependence is observed for a Newtonian fluid with $Bn = 0$, which concurs with the fact that here $C_d$ is inversely proportional to $Re$. However, instead of approaching a vertical asymptote, as in the case of a solid sphere (see BTAB), at some value of $Bn$, all curves attain a smaller slope. In the single case of a non-deformable bubble this is attributed to numerical error at these extreme values of $C_d \approx 10^6$, while in all other cases the change of slope is associated with a change in the shape of a deformable
bubble. Indeed, in figure 4.25 we plot the bubble height, $h$, and the axial distance of the outer yielded surface at the axis of symmetry, $S_u$, as a function of the Bingham number. We observe that for small values of $Bn$, $h$ does not change for $Bo = 0.1$ and slightly increases for $5 \leq Bo \leq 50$, whereas $S_u$ decreases as the outer yield surface approaches the bubble, more so at the axis of symmetry; see figure 4.9a. Above a characteristic value of $Bn$, $h$ increases significantly and almost linearly, whereas $S_u$ either decreases with a larger slope and tends to intersect the $h$ curve ($Bo = 0.1$), decreases with a smaller slope ($Bo = 5$) or increases for the remaining Bond numbers. In other words, at these characteristic $Bn$ values either (i) the outer yield surface approaches the bubble surface very rapidly and the bubble is entrapped ($Bo = 0.1$), or (ii) the bubble elongates forcing the outer yield surface to decrease its rate of approach to it, delaying bubble entrainment to higher $Bn$ values ($Bo = 5, 10$), or (iii) the bubble is slightly squeezed by the approaching yield surface and then elongates as in (ii) ($Bo = 50$). The values of $Bn$ at which the bubble starts to elongate correspond to the inflection points in the drag force in figure 4.24b.
Figure 4.24 The drag coefficient as function of the Bingham number, for various values of (a) $Ar$ and (b) $Bo$.

Figure 4.25 Bubble height, $h$, and axial distance of the outer yield surfaces, $S_u$, at the axis of symmetry vs. $Bn$. 

4.5 Conclusions

We simulated the rise of a bubble in a viscoplastic material for a wide range of material parameters. The simulation is based on the mixed finite element method for the discretization of the governing equations coupled with a quasi-elliptic mesh generation scheme in order to follow the large deformations of the physical domain. Our results allow us to determine the evolution of (a) the velocity and pressure fields in the fluid, (b) the shape of the liquid/air interface, (c) the domain of the unyielded material, (d) the critical Bingham number for bubble entrapment and (e) the dynamic parameters of the flow including the drag coefficient.

We examined the effect of the yield stress and the capillary, viscous and gravity forces. First, we verified the accuracy of our new code comparing our results with previous theoretical and experimental ones for a Newtonian fluid. Where possible, we extended earlier results to larger values of Reynolds and Weber numbers. In a viscoplastic fluid, the bubble rise velocity and, hence, both the Reynolds and Weber numbers decrease as the yield stress increases. Unyielded material exists at rear of the bubble at low Bingham numbers and large Bond and Archimedes numbers, when the bubble has a distorted oblate spheroidal shape. This unyielded area disappears at higher Bingham numbers as the shape of the bubble changes to a bullet-like shape allowing it to squeeze through the material. Unyielded material also arises around and far from the bubble and around the equatorial plane for $Bn \geq 0.1$. The size of these domains increases with the Bingham number and when they merge the bubble stops moving. As this critical Bingham number is approached the bubble tends to take a bullet-like shape owing to the higher effective viscosity at its equatorial plane and the lower viscosity at its poles. The critical Bingham number has strong dependence on the Bond number, an increase of which allows the bubble to deform more. Finally the drag coefficient decreases with the Bond and Archimedes number and increases with the Bingham number.

The predicted bubble shapes and the drag coefficient can be used to determine the material parameters, $\mu^*_0$ and $\tau^*_y$. The numerical approach presented here can be extended to calculate mass transfer coefficients from/to a bubble in a yield-stress fluid, which are unavailable today, despite being extremely important in determining optimal operating conditions for various chemical and physical processes.
Recommendations for future work

Bubble dynamics plays a central role in several practical applications and physical phenomena. During the last decade they have been used extensively in biomedicine and echocardiography. Thus it is important to study their mechanisms of formation, break up or even coalescence in 3D domains where the assumption of axial symmetry is not valid. These calculations apart from being time consuming, they are also memory demanding and parallel techniques must be implemented in order to get physical results in realistic times. The effect of viscosity must be also systematically examined, because it is crucial factor for the development or not of interfacial and hydrodynamic instabilities.

Recently bubbles have been used for the destruction of cancerous cells. In general their interaction with interstitial cells has attracted the interest of many researchers in medicine and biomedical engineering. So, the extension of the current algorithm to the study of such problems could offer us many answers about the lysis of cells when they interact with acoustic bubbles.

With regards to the motion of an isolated bubble in a Bingham fluid, we must complete the study of the effect of an oscillatory pressure field, in order to see under what values of the physical parameters, the bubble remains entrapped. Industrial applications and physical processes involve mass transfer from the gas to the liquid phase, affecting the motion of the bubble. Therefore, the introduction of such a mechanism in our algorithm could be significantly useful from a practical point of view.
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4. N. Chatzidai, J. Tsamopoulos, “Viscous effects on two interacting and deformable bubbles under an oscillatory pressure field”, to be submitted.
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