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**Non-modal Linear Stability of the Interface
Between Aqueous Humor and Vitreous
Substitutes After Vitreoretinal Surgery**

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Abstract

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Non-modal linear stability of the interface between aqueous humor and vitreous substitutes after vitreoretinal surgery

by [Masoud Ghaderi Zefreh](#)

Vitreotomy is a common surgical treatment for retinal detachment. It consists in the removal of the natural vitreous and its replacement with so called tamponade fluids. These are immiscible with water and, therefore, an interface between the aqueous and the vitreous substitute forms into the vitreous chamber. Emulsification of the tamponade fluid is a possible complication of the procedure and is thought to occur as a result of mechanical instability of the aqueous/tamponade fluid interface. In this thesis work we consider, within an idealised framework, the stability of an interface between two immiscible fluids set in motion by movement of a rigid wall. The wall represents the retinal surface, the curvature of which is neglected. The stability analysis is done by using a linear non-modal approach to take into account the transient growth of the energy of the system at finite times.

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Chapter 1

Introduction

1.1 Eye Anatomy

When the five senses of the human beings are discussed the first thing that may come to mind is the sight. Using this power we can learn about the surrounding world more than using any other four senses. It gives us the ability to understand, differentiate and interpret the shape, color, distance and dimensions of objects in real world. We use this sense for different purposes everyday from watching TV, reading papers, driving, visiting people, etc.

The eye, as the primary member of this power, has a role which can be compared somewhat to a camera; both use the incoming light to produce an image, which can be easy to interpret. A camera produces the image on a film whereas the retina, a specialized layer of cells, carries this role in the eye.

The anatomy of the eye is shown on figure 1.1 and a few terms, which are used in the thesis, are discussed below.

Sclera The sclera, also known as the white of the eye, is the opaque, fibrous, protective, outer layer of the eye.

Cornea The cornea is a clear layer at the front and center of the eye. In fact, the cornea is so clear that you may not even realize it is there. It is located just in front of the iris, which is the colored part of the eye. The main purpose of the cornea is to help focus light as it enters the eye. If you wear contact lenses, the contact lens rests on your cornea.

Aqueous humor The aqueous humour is a transparent fluid similar to water, but containing low protein concentrations. It is located in the anterior and posterior chambers of the eye, the space between the lens and the cornea. It is not to be confused with

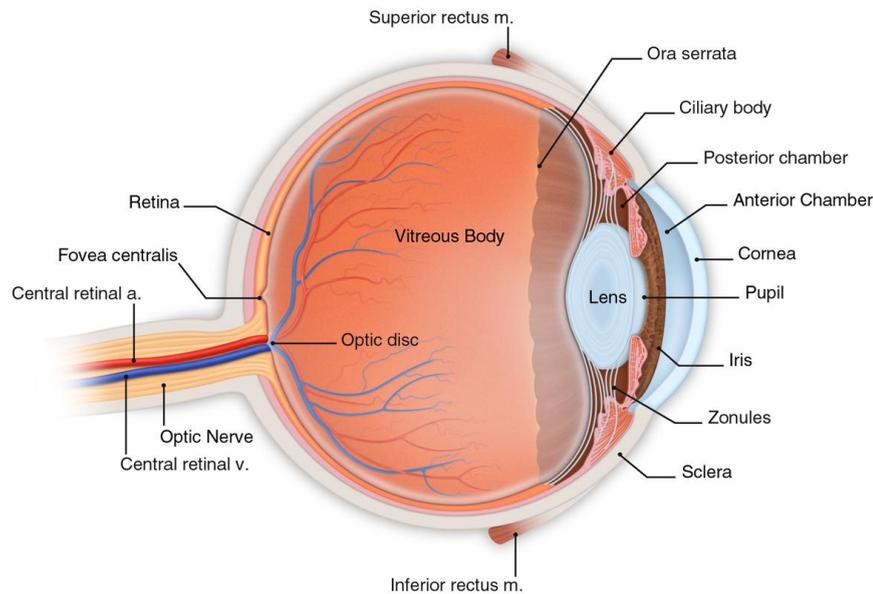


FIGURE 1.1: Anatomy of the human eye [1]

vitreous humour, which is contained within the larger cavity of the eye behind the lens. If the aqueous humor cannot properly drain out of the eye, optic nerve damage can occur which is known as *glaucoma* and can lead to the vision loss.

Vitreous humor The vitreous humor is the clear gel that fills the space between the lens and the retina in humans and other vertebrates. It is often referred to as the vitreous body or simply “the vitreous”.

Lens The crystalline lens is a transparent, biconvex structure in the eye that, along with the cornea, helps to refract light to be focused on the retina.

Retina The retina acts like the film in a camera to create an image. To do this, the retina, a specialized layer of cells, converts light signals to the optic nerve, which carries the signals to the brain. There, the brain processes the image. The retina is primarily made up of 2 distinct types of cells: rods and cones. Rods are more sensitive to light; therefore, they allow you to see in low light situations but do not allow color vision. Cones, on the other hand, allow you to see colors but require more light. The macula is located in the central part of the retina. It is the area of the retina that is responsible for giving you sharp central vision. The choroid is a layer of tissue that separates the retina and the sclera. It is mostly made up of blood vessels. The choroid helps nourish the retina.

1.2 Retinal Detachment

A retinal detachment is a separation of the retina from the underlying tissue within the eye (see figure 1.2). Most retinal detachments are a result of a retinal break, hole, or

tear. These retinal breaks may occur when the vitreous gel pulls loose or separates from the retina somewhere but keeps tight attachment points to it, where mechanical stresses concentrate. The vitreous is a clear gel that fills two-thirds of the inside of the eye and occupies the space in front of the retina. As the vitreous gel pulls loose, it will sometimes exert traction on the retina, and if the retina is weak, the retina will tear. Most retinal breaks are not a result of injury. Retinal tears are sometimes accompanied by bleeding if a retinal blood vessel is included in the tear. Many people develop separation of the vitreous from the retina as they get older. However, only a small percentage of these vitreous separations results in retinal tears.

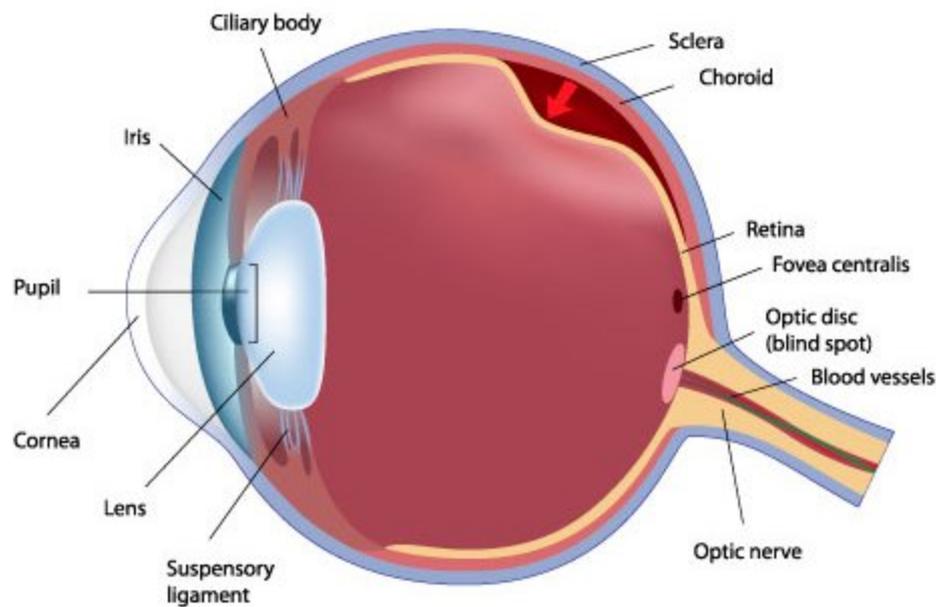


FIGURE 1.2: Retinal detachment [2]

Once the retina has torn, liquid from the vitreous gel can then pass through the tear and accumulate behind the retina. The buildup of fluid behind the retina is what separates (detaches) the retina from the back of the eye. As more of the liquid vitreous collects behind the retina, the extent of the retinal detachment can progress and involve the entire retina, leading to a total retinal detachment. A retinal detachment almost always affects only one eye at a time. The second eye, however, must be checked thoroughly for any signs of predisposing factors that may lead to detachment in the future. Detachment of the retina is a serious event, which may result in complete blindness.[5]

1.2.1 Symptoms, signs, causes and risk factors

Flashing lights and floaters may be the initial symptoms of a retinal detachment or of vitreoretinal fractions that precede the detachment itself. If the patient experiences a

shadow or curtain that affects any part of the vision, this can indicate that a retinal tear has progressed to a detached retina. In this situation, one should immediately consult an eye doctor since time can be critical. The goal for the ophthalmologist is to make the diagnosis and treat the retinal tear or detachment before the central macular area of the retina detaches.[5]

Studies have shown that the incidence of retinal detachments caused by tears in the retina is fairly low, affecting approximately one in 10,000 people each year. Many retinal tears do not progress to retinal detachment. Nevertheless, many risk factors for developing retinal detachments are recognized, including certain diseases of the eyes (discussed below), cataract surgery, and trauma to the eye. Retinal detachments can occur at any age but are most common in adults 40 years and older who are highly nearsighted (myopic) and in older people following cataract surgery.[5]

1.2.2 Treatments

If left untreated, retinal detachment can cause serious and permanent vision damage. Symptoms of retinal detachment should be considered an eye emergency, requiring immediate attention. The goal of treatment is to preserve or restore vision by reattaching the retina and eye surgeons use a variety of techniques. Holes in the retina through which fluid is seeping under the retina can be sealed with laser light treatment. *Pneumatic Retinopexy*, involves injection of a gas bubble into the eye to push the retina back into its position. *Scleral Buckling* makes use of a plastic band placed around the eye which pushes the wall of the eye back in contact with the detached retina. *Vitrectomy* removes the jelly-like material inside the eye, called vitreous, when it is aggravating a detachment by tugging on the retina. *Laser photocoagulation* prevents fluid from getting under the retina by scars that are result of the burns through the pass of an intense laser beam over the eye. *Cryopexy* is used to freeze and seal the retina so that the eye surgeon can treat the damaged retina.[5]

1.3 Vitrectomy and Vitreous substitutes

As it was said before, vitrectomy is a surgery that treats retinal breaks and retinal detachment. It consists in replacement of the whole vitreous humor, which is substituted with tamponade fluids. Vitreous substitutes can be classified into short-term tamponades and longer-term tamponades. The former are intended to remain in the vitreous chamber for a limited time, sufficient for retina reattachment to occur, and to be subsequently removed. The later are designed to be left in a vitreous chamber for much

longer time. Materials that form an interface with the aqueous environment of the eye can be effective in closing retinal breaks and holding the neural retina in place against the retinal pigment epithelium.[6]

1.3.1 Pros and Cons of Vitrectomy

Among all the other approaches for the treatment of retinal detachment, vitrectomy is the most common used. For most patients who undergo a vitrectomy, sight is restored or significantly improved. Bleeding, infection, progression of cataract and retinal detachment are potential problems, but these complications are relatively unusual. Generally vitrectomy has a high success rate. However, one of the problems that might occur in case silicon oil used as the vitreous substitute, is the emulsification which may happen between the aqueous humor and the silicon oil. The emulsified fluid can move from around the eye to the front of the eye and cover the lens. This means that the vision can be blurred.

1.4 Scope

Although the mechanics of emulsification is poorly understood, it is known that it occurs due to the mechanical instability of the system. Isakova et al in [7] have studied the stability of this system which is the two phase fluid consisting aqueous humor and silicon oil. Due to the fact that in linear stability theory, the critical Rayleigh number for a two-dimensional parallel flow is lowest for a two-dimensional perturbation, in their paper a two dimensional model is used. They reported the regions of parameters (viscosity ratio of the two fluids, surface tension, etc) applicable for the eye, for which the system is stable or unstable by using a linear modal stability analysis. A brief review of some of the previous works and their conclusion is discussed in the next chapter.

In this work, the same regions of parameters (for stable case) are studied by using a linear non-modal stability analysis approach. Unlike the modal analysis, where Squire's theorem can help to reduce the dimension and thus simplify the problem, there is no such theorem in non-modal analysis and so in our study we used a three dimensional model. In non-modal stability analysis the attention is put on the finite response of the system to see the effects of the non-normality of the system. Due to the non-normality of the system, the response to a small amplitude perturbation may go to a transient region before decaying in infinite time. This may be the source of the emulsification of silicon oil in the eye. At the end, the regions which have higher transient response are identified.

Chapter 2

Hydrodynamic Instability

2.1 Introduction

In hydrodynamic stability theory we study the response of laminar flow which is perturbed with a small amplitude. A flow is stable if it returns to its previous (laminar) state after some time and remains in that state and is defined unstable if it changes into a different state. The study of hydrodynamic stability can be performed with different methods:

1. *Natural phenomena and laboratory experiments.* Observations of nature and experiments are the primary means of study. All theoretical investigations need to be related, directly or indirectly, to understanding these observations.
2. *Numerical experiments.* Computational fluid dynamics has become increasingly important in hydrodynamic stability since 1980s. As numerical analysis has improved and computers have become faster and gained more memory, the Navier-Stokes equations may be integrated accurately for more complex flows. Indeed, computational fluid dynamics has now reached a stage where it can rival laboratory investigation of hydrodynamic stability by simulating controlled experiments.
3. *Linear and weakly nonlinear theory.* Linearization for small perturbations of a given basic flow is the primary method to be used in the theory of hydrodynamic stability, and it was the method used much more than any other until the 1960s. However, weakly nonlinear theory, which builds on the linear theory by treating the leading nonlinear effects of small perturbations, began in the nineteenth century, and has been intensively developed since the 1960s.

4. *Qualitative theory of bifurcation and chaos.* The qualitative theory of dynamical systems, as well as weakly nonlinear analysis, provides a useful conceptual framework to interpret laboratory and numerical experiments.
5. *Strongly nonlinear theory.* There are various mathematically rigorous methods, notably Serrins theorem and Liapounovs direct method, which give detailed results for arbitrarily large perturbations of specific flows. These results are usually bounds giving sufficient conditions for stability of a flow or bounds for flow quantities.[8]

2.2 Turbulence and Stability

Turbulent flow is inherently more energetic compared to its laminar counterpart and it is of engineering interest to reduce its effects. For example, in aircraft design where the turbulence in boundary-layer effects the drag force on the wings, or in the prototype fusion power plants where turbulent flow in the plasma causes difficulty in plasma containment. Trying to understand turbulence has been an important engineering problem as well as a mathematical one.[9]

The essential problems of hydrodynamic stability were recognized and formulated in nineteenth century, notably by Helmotz, Kelvin, Rayleigh and Reynolds[8]. In his experiment Reynolds brought out the main classification of the flows (laminar, transitional and turbulent). He injected a dye into a flow through a glass tube to observe the nature of the flow. If the velocities were sufficiently small the flow followed a straight line path apart a slight blurring due to the diffusion. When the velocities were increased the dye was blurred and seemed to fill the entire pipe. In this way the laminar, transitional and turbulent flows were observed. Reynolds has concluded that the smooth flow breaks down when the ration $\frac{V \cdot a}{\nu}$ exceeds a certain critical value, where

- V is the maximum velocity of the water in pipe;
- a is the radius of the pipe;
- ν is the kinematic viscosity of water.

This dimensionless number $\frac{V \cdot a}{\nu}$ is called the Reynolds number.

2.3 Linear Stability Analysis

In the linear stability analysis, as mentioned earlier, the nonlinear terms of a small amplitude perturbation are dropped so that the system is linearized. The stability of the system is determined by studying the linearized version. In the linear stability, we are interested in the minimum critical parameter above which a specific initial condition of infinitesimal amplitude grows exponentially. In linear modal stability analysis (LMSA), it is assumed that the solution behaves exponentially at infinite times. Therefore, the time derivative operator in Navier-Stokes equation can be replaced by the exponential growth. Therefore, an eigenvalue problem (IVP) needs to be solved to calculate the exponential growth and therefore to determine the stability of the system based on the eigenvalues.

Generally, the dimensionless Navier-Stokes equation for the perturbed flow in vector form can be written as

$$\frac{\partial \mathbf{u}}{\partial t} = -(\mathbf{U}\nabla\mathbf{u} + \mathbf{u}\nabla\mathbf{U}) - \nabla p + \frac{1}{Re}\nabla^2\mathbf{u}, \quad (2.1)$$

which can be considered as

$$\mathbf{A}\frac{\partial \mathbf{u}}{\partial t} = \mathbf{B}\mathbf{u}. \quad (2.2)$$

In the case of modal analysis, it is written as

$$\Omega\mathbf{A}\mathbf{u} = \mathbf{B}\mathbf{u} \quad (2.3)$$

which is a generalized eigenvalue problem in case \mathbf{A} is not the unit matrix.

In case the matrices \mathbf{A} and \mathbf{B} are non-normal a transient growth will appear in finite times before it grows or decays exponentially. This is due to the fact that the eigenvectors are not orthogonal and in short times their sum has more effect than the growth of eigenvalues. In figure 2.1, geometric representation is shown for a stable 2×2 system. The value of the maximum transient growth depends highly on the initial condition. It is interesting to find the initial condition that has maximum transient growth. This initial condition, which we refer to it as the optimum perturbation or optimal initial condition, shows the worst case where we have transient growth. In case the maximum of the optimal initial condition has a very high, then probably we need to change the parameters to put the system in a better situation.

Apart from the growth of the solution, it is also needed to define a measurement with which we can evaluate the growth. Although the norms in finite dimension are equivalent, in order to have the most realistic result we need to use a norm which has physical

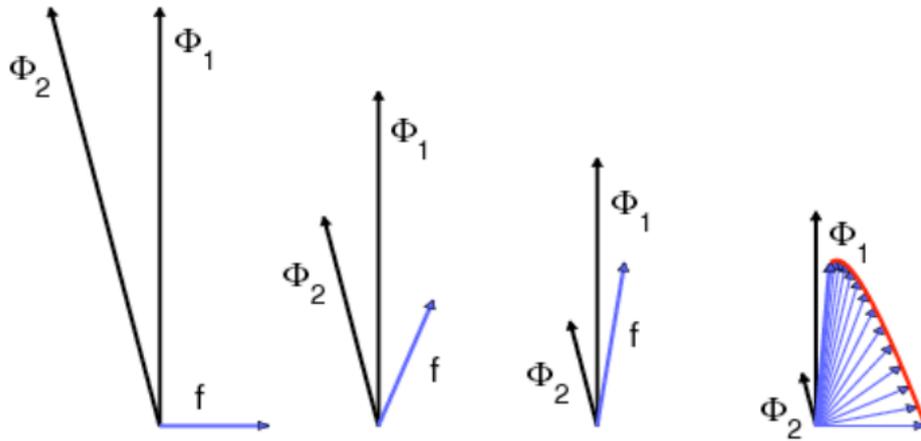


FIGURE 2.1: Transient growth of 2×2 stable system in finite time [3]

meaning. Therefore in our model, we use the norm which takes into account for the kinetic energy as well as surface tension and pressure.

In order to solve the optimization problem, we use a Lagrangian approach, which uses the definition of adjoint of the system to reduce the amount of equation needed for finding the optimal initial condition. In Lagrangian approach, the objective function as well as the constraints for the optimization form a function called the Lagrangian. To solve the optimization problem, one needs to find the stationary point of the Lagrangian.

2.4 Review of Related Previous Works

A lot of existing work on stability of unsteady flows is based on the assumption of quasi-steadiness, which means that the stability of the unsteady flow is determined by whether or not it is stable for all the velocity distributions if each of these distribution is assumed to persist. If the frequency of the primary flow is much less than the reference velocity divided by the reference length, it can be shown that the approach of quasi-steadiness can predict stability or instability over time intervals small compared with the period. If the instability was predicted, the slow variation of the primary flow with time may not affect the conclusion. But many flows predicted to be unstable by the approach of quasi-steadiness may turn out to be stable using Floquet analysis.[10]

Chia-Shun Yih has investigated in his paper [11] the stability of the layer of viscous fluid with the free surface which is set in motion by the lower boundary moving harmonically. He considered the stability of the primary flow which was completely unsteady. He studied the stability of the long waves by a perturbation method. This was the first time this approach had been applied to the problem of stability of the unsteady flows. Since the primary flow is the time-periodic the extension of the Floquet theorem was

applied together with the expansion in terms of the wave number due to the long-wave approach.

In 1970 Li has studied the stability of the two layers of liquid set in a motion by the lower boundary in his paper [12]. The investigation was made for the two superposed fluids with different viscosities and densities and with the free surface on top. The purpose was to see how an interface, which is a second surface of discontinuity in density and viscosity, will affect the stability of a single layer of fluid studied by Yih in [10][12]. In his paper Li also adopted the extended Floquet theorem in order to solve the Orr-Sommerfeld equation with the time-periodic coefficients. He concluded that it is the interfacial mode which governs the instability of the flow when the Froude number is less than 3. The interfacial mode reduces to a neutral mode with equal densities and viscosities. For the Froude number greater than 3 there would be a competition between the interfacial and free-surface modes in governing the stability or instability of the system.

Isakova et al [7], in 2004 studied the stability of two phase flow by adopting a simple model which represents the flow of the two phase fluid in the vitrectomized eye. In their paper, they assumed a quasi-steady model and defined regions of relative parameters for which the system is stable in a modal sense. For this, they used the Squire's theorem to exclude a large region of parameters as the unstable region by considering the eigenvalues of the eigenproblem associated to the system. They concluded that the increase of density ratio results in an unstable system for a fixed viscosity ratio while choosing a silicon oil with higher surface tension for the same viscosity ratio further stabilizes the system.

Chapter 3

Mathematical Formulation

In this chapter the background theory of the work and all the mathematical formulations and derivations are written.

The model and flow configuration is similar to that in [7]. We assume two immiscible fluid superposed over an oscillating flat surface. The lower fluid has lower density and is confined into small region while the upper fluid is semi-infinite. The frequency of the oscillating surface is given and it is assumed that the dynamics of the interface between the two fluids is much faster than the oscillation the plate (see figure 3.1).

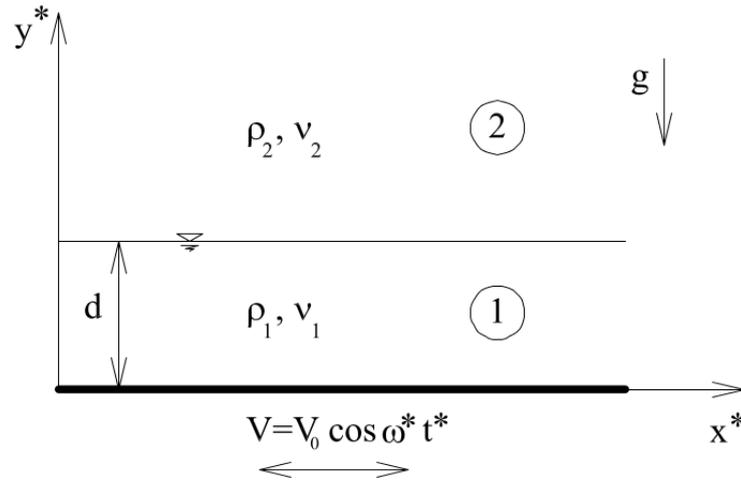


FIGURE 3.1: Schematic diagram of the problem [4]

It is assumed that the two fluids are immiscible and have viscosities μ_1^* , μ_2^* and densities ρ_1^* and ρ_2^* , respectively. We assume also, that the fluid 1 is occupying the region from $0 \leq y^* < d^*$ and the region $y^* > d^*$ is occupied by the second fluid and therefore the interface is at $y^* = d^*$. Thus the fluid 1 is closer to the rigid wall. There is a periodic motion at the rigid wall ($y^* = 0$) which induces the flow and this periodic motion is of

form

$$u_{\omega}^* = V_0^* \cos(\omega^* t^*) = \frac{V_0^*}{2} (e^{i\omega^* t^*} + c.c.), \quad (3.1)$$

where V_0^* is the amplitude of the oscillation, ω^* is the angular frequency of the oscillation, t^* is the time and *c.c.* stands for the complex conjugate. We denote the velocity vector and pressure corresponding to each fluid as $\bar{\mathbf{u}}_i$ and \bar{p}_i where $i = \{1, 2\}$. The V_0^* , ρ_1^* and d^* are used as the reference velocity, density and length, respectively, to make the governing equations dimensionless. Hence, the dimensionless variables are defined as

$$\mathbf{x} = \frac{\mathbf{x}^*}{d^*}, \quad \bar{\mathbf{u}}_i = \frac{\mathbf{u}_i^*}{V_0^*}, \quad \bar{p}_i = \frac{p_i^*}{\rho_1^* V_0^{*2}}, \quad t = \frac{V_0^*}{d^*} t^*, \quad \omega = \frac{d^*}{V_0^*} \omega^*, \quad (3.2)$$

where the vector $\mathbf{x} = (x, y, z)$ is a 3-tuple which represents the spatial coordinates of the system. x and z are the streamwise and spanwise coordinates while y is the wall-normal component. The stability analysis is studied by introducing a perturbation. The pressure and the components of the velocity corresponding to the perturbed flow can be written in the form of

$$\bar{p}_i = P_i + \hat{p}_i, \quad \bar{\mathbf{u}}_i = \mathbf{U}_i + \hat{\mathbf{u}}_i, \quad (3.3)$$

where \hat{p}_i and $\hat{\mathbf{u}}_i$ are the pressure and the components of the velocity of the perturbation and $\bar{\mathbf{p}}$ and $\bar{\mathbf{u}}$ are those of perturbed flow, respectively. Naming the components of the velocity for the perturbed flow and the perturbation as

$$\bar{\mathbf{u}} = (\bar{u}, \bar{v}, \bar{w}), \quad \hat{\mathbf{u}} = (\hat{u}, \hat{v}, \hat{w}), \quad (3.4)$$

allows us to write the governing equations in scalar form.

3.1 Basic Flow

The vectorial form of the dimensionless Navier-Stokes, using the dimensionless variables introduced in the beginning of this chapter, with the velocity vectors \mathbf{U}_i and pressures P_i can be written as

$$\frac{\mathcal{D}\mathbf{U}_1}{\mathcal{D}t} - \tilde{\mathbf{F}} = -\nabla P_1 + \frac{1}{Re} \nabla^2 \mathbf{U}_1, \quad (3.5)$$

for the first fluid and

$$\frac{\mathcal{D}\mathbf{U}_2}{\mathcal{D}t} - \tilde{\mathbf{F}} = -\frac{1}{\gamma} \nabla P_2 + \frac{m/\gamma}{Re} \nabla^2 \mathbf{U}_2, \quad (3.6)$$

for the second fluid, where $\frac{\mathcal{D}}{\mathcal{D}t}$ is the material derivative, $Re = \frac{V_0^* d^* \rho^*}{\mu_1^*}$ is the Reynolds number, $\gamma = \rho_2^*/\rho_1^*$ is the ratio between densities and $m = \mu_2^*/\mu_1^*$ is between the dynamic viscosities. The $\tilde{\mathbf{F}}$ is the vector $(0, \frac{1}{Fr^2}, 0)^{tr}$ with $Fr = \frac{V_0^*}{\sqrt{g^* d^*}}$ being the Froude number.

Considering the fact that with the assumption of laminar fully developed flow in the stream-wise direction, our solution is of form $\mathbf{U}_i = (U_i(y, t), 0, 0)^{tr}$, the governing equations can be simplified to

$$\frac{\partial U_1}{\partial t} = \frac{1}{Re} \frac{\partial^2 U_1}{\partial y^2}, \quad (3.7)$$

$$\frac{\partial P_1}{\partial y} = -Fr^{-2}, \quad (3.8)$$

$$\frac{\partial U_2}{\partial t} = \frac{m}{\gamma} \frac{1}{Re} \frac{\partial^2 U_2}{\partial y^2}, \quad (3.9)$$

$$\frac{\partial P_2}{\partial y} = -\gamma Fr^{-2}. \quad (3.10)$$

The boundary conditions are the same as for the perturbed flow and they will be discussed in following sections in details. They include no slip boundary condition at the wall, continuity of velocity and vorticity on the interface and vanishing of velocity and vorticity at distances far away from the interface. The equations 3.8 and 3.10 are linear first order ODEs and therefore it shows that the pressure has a hydrostatic distribution. For 3.7 and 3.9 we have to solve two parabolic equation with the prescribed boundary conditions. The solution as already discussed in [7] can be written in the form

$$U_1 = [c_1 e^{-ay} + c_2 e^{ay}] e^{i\omega t} + c.c., \quad (3.11)$$

$$U_2 = c_3 e^{-by} e^{i\omega t} + c.c., \quad (3.12)$$

where

$$a = \sqrt{i\omega Re}, \quad (3.13)$$

$$b = \sqrt{(\gamma/m)i\omega Re}, \quad (3.14)$$

$$c_1 = \frac{e^{a-b}}{2[e^{a-b}(a+mb) + e^{-a-b}(a-mb)]}, \quad (3.15)$$

$$c_2 = \frac{e^{-a-b}}{2[e^{a-b}(a+mb) + e^{-a-b}(a-mb)]}, \quad (3.16)$$

$$c_3 = \frac{a}{e^{a-b}(a+mb) + e^{-a-b}(a-mb)}. \quad (3.17)$$

3.2 Linear Stability Analysis

Using the dimensionless variables defined in the beginning chapter the dimensionless Navier-Stokes equation for the perturbed flow can be written as

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \bar{w} \frac{\partial \bar{u}}{\partial z} = -\frac{\partial \bar{p}}{\partial x} + \frac{1}{Re} \nabla^2 \bar{u}, \quad (3.18)$$

$$\frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} + \bar{w} \frac{\partial \bar{v}}{\partial z} + \frac{1}{Fr^2} = -\frac{\partial \bar{p}}{\partial y} + \frac{1}{Re} \nabla^2 \bar{v}, \quad (3.19)$$

$$\frac{\partial \bar{w}}{\partial t} + \bar{u} \frac{\partial \bar{w}}{\partial x} + \bar{v} \frac{\partial \bar{w}}{\partial y} + \bar{w} \frac{\partial \bar{w}}{\partial z} = -\frac{\partial \bar{p}}{\partial z} + \frac{1}{Re} \nabla^2 \bar{w}, \quad (3.20)$$

which after substituting 3.4 they simplify to 3.21-3.23

$$\frac{\partial \hat{u}}{\partial t} + U \frac{\partial \hat{u}}{\partial x} + \hat{v} U' = -\frac{\partial \hat{p}}{\partial x} + \frac{1}{Re} \nabla^2 \hat{u}, \quad (3.21)$$

$$\frac{\partial \hat{v}}{\partial t} + U \frac{\partial \hat{v}}{\partial x} = -\frac{\partial \hat{p}}{\partial y} + \frac{1}{Re} \nabla^2 \hat{v}, \quad (3.22)$$

$$\frac{\partial \hat{w}}{\partial t} + U \frac{\partial \hat{w}}{\partial x} = -\frac{\partial \hat{p}}{\partial z} + \frac{1}{Re} \nabla^2 \hat{w}. \quad (3.23)$$

Continuity equation for the perturbed flow is $\nabla \cdot \mathbf{u} = 0$ and using 3.3 and the continuity equation for the base flow can be written as

$$\frac{\partial \hat{u}}{\partial x} + \frac{\partial \hat{v}}{\partial y} + \frac{\partial \hat{w}}{\partial z} = 0. \quad (3.24)$$

For reducing the system, the change of variable

$$\hat{\eta} = \frac{\partial \hat{u}}{\partial z} - \frac{\partial \hat{w}}{\partial x}, \quad (3.25)$$

is used where $\hat{\eta}$ is the second component of vorticity and for simplicity we refer to it as the vorticity during the rest of this text. Differentiating 3.21 and 3.23 with respect to z and x , respectively, and subtracting them with the use of this definition we can write the ‘vorticity equation’ as

$$\left[\frac{\partial}{\partial t} + U \frac{\partial}{\partial x} - \frac{1}{Re} \nabla^2 \right] \hat{\eta} + \left[U' \frac{\partial}{\partial z} \right] \hat{v} = 0. \quad (3.26)$$

Taking the derivative of 3.21, 3.22 and 3.23 with respect to x , y and z respectively and summing them up we get

$$\nabla^2 \hat{p} = -2U' \frac{\partial \hat{v}}{\partial x}. \quad (3.27)$$

Finally using 3.27 and differentiating 3.22 with respect to y we have 3.28 which depends only on the vertical component of velocity and we refer to it as ‘velocity equation’.

$$\left[\left(\frac{\partial}{\partial t} + U \frac{\partial}{\partial x} \right) \nabla^2 - U'' \frac{\partial}{\partial x} - \frac{1}{Re} \nabla^4 \right] \hat{v} = 0. \quad (3.28)$$

All the equations in this section were derived for the first fluid and for simplicity the subscript was dropped. The governing equations for the second fluid can be derived similarly and with the same coefficients for pressure and Reynolds number as used in 3.1.

3.2.1 Quasi-Steady Approach

In this method, a Fourier mode for the solution is assumed in stream-wise directions, therefore one can express the solution in the following terms:

$$\hat{u} = u(\tau, y)e^{i(\alpha x + \beta z - \Omega t)} + c.c., \quad (3.29)$$

$$\hat{v} = v(\tau, y)e^{i(\alpha x + \beta z - \Omega t)} + c.c., \quad (3.30)$$

$$\hat{w} = w(\tau, y)e^{i(\alpha x + \beta z - \Omega t)} + c.c., \quad (3.31)$$

$$\hat{p} = p(\tau, y)e^{i(\alpha x + \beta z - \Omega t)} + c.c., \quad (3.32)$$

where $\alpha, \beta \in \mathbb{R}$, $\Omega \in \mathbb{C}$ and c.c. stands for complex conjugate. This allows us to simplify 3.28 and 3.26 into the following equations for the two phases of the fluids

$$\left[i\alpha(D^2 - k^2)U_1 - i\alpha U_1'' - \frac{1}{Re}(D^2 - k^2)^2 \right] v_1 = i\Omega(D^2 - k^2)v_1, \quad (3.33)$$

$$\left[i\alpha(D^2 - k^2)U_2 - i\alpha U_2'' - \frac{m/\gamma}{Re}(D^2 - k^2)^2 \right] v_2 = i\Omega(D^2 - k^2)v_2, \quad (3.34)$$

and

$$\left[i\alpha U_1 - \frac{1}{Re}(D^2 - k^2) \right] \eta_1 + i\beta U_1' v_1 = i\Omega \eta_1, \quad (3.35)$$

$$\left[i\alpha U_2 - \frac{m/\gamma}{Re}(D^2 - k^2) \right] \eta_2 + i\beta U_2' v_2 = i\Omega \eta_2, \quad (3.36)$$

where the subscript 1 and 2 refers to the bottom and top phase of the fluids, respectively. U' and U'' represent the first and the second derivative of the base flow with respect to vertical component and D is the differential operator with respect to y .

In addition, the continuity equation (3.25) may be simplified to:

$$i\alpha u + v' + i\beta w = 0. \quad (3.37)$$

The boundary conditions can be classified into three groups depending on the location

- on the wall,
- on the interface between the two fluids and
- at infinity or far away enough from the wall.

Generally speaking, the only boundary condition at the wall is the well-known no-slip:

$$v_1 = 0 \quad \text{at } y = 0. \quad (3.38)$$

However, by using the definition 3.25, we can write the corresponding boundary condition for vorticity at the wall:

$$\eta_1 = 0 \quad \text{at } y = 0 \quad (3.39)$$

Since we are assuming a quasi-steady approach, at each time instant corresponding to the perturbation, the wall is considered to be motionless. That is, the tangential components of the perturbation velocity are zero. This, together with the continuity equation, helps us to derive another independent condition for our problem. Recalling that 3.37 is valid at any point in the domain, we can use this and the no-slip boundary condition and derive another independent condition as

$$v'_1 = 0 \quad \text{at } y = 0. \quad (3.40)$$

The equation for the surface which represents the interface can be thought as:

$$F := 1 + \hat{\xi} - y = 0 \quad (3.41)$$

$$\text{with } \hat{\xi} = \xi(\tau) e^{i(\alpha x + \beta z - \Omega t)} + c.c. \quad (3.42)$$

The kinematic boundary condition can be derived from

$$\frac{\mathcal{D}F}{\mathcal{D}t} = 0, \quad (3.43)$$

where $\frac{\mathcal{D}}{\mathcal{D}t}$ is the material derivative and using a linearization on $y = 1$ we get

$$\frac{\partial \xi}{\partial t} + i\alpha \xi U - v = 0, \quad (3.44)$$

where U and v are evaluated at $y = 1$ and because of continuity of these components on the interface, those of any of the phases can be used.

Continuity of the components of the velocity as well as the tangential components of the stress are the conditions that need to be imposed for the continuity of the solution on the interface. However, we do not need to deal with all these components directly but rather some proper substitutions should be made in order to have everything in terms of vertical component of velocity and vorticity.

The normal vector for the surface equation 3.41 is:

$$\mathbf{n} = \begin{pmatrix} \frac{\partial \hat{\xi}}{\partial x} \\ -1 \\ \frac{\partial \hat{\xi}}{\partial z} \end{pmatrix}. \quad (3.45)$$

The two orthogonal vectors on the normal vector denoted as $\boldsymbol{\tau}_x$ and $\boldsymbol{\tau}_z$ can be found as

$$\boldsymbol{\tau}_x = \begin{pmatrix} 1 \\ \frac{\partial \xi}{\partial x} \\ 0 \end{pmatrix} \quad \boldsymbol{\tau}_z = \begin{pmatrix} 0 \\ \frac{\partial \xi}{\partial z} \\ 1 \end{pmatrix}. \quad (3.46)$$

The dimensionless Cauchy Stress tensor can be written as

$$\mathbf{T}_1 = \frac{1}{Re} \begin{pmatrix} 2i\alpha\hat{u}_1 & \frac{\partial\hat{u}_1}{\partial y} + U'_1 + i\alpha\hat{v}_1 & i\alpha\hat{w}_1 + i\beta\hat{u}_1 \\ \frac{\partial\hat{u}_1}{\partial y} + U'_1 + i\alpha\hat{v}_1 & 2\frac{\partial\hat{v}_1}{\partial y} & \frac{\partial\hat{w}_1}{\partial y} + i\beta\hat{v}_1 \\ i\alpha\hat{w}_1 + i\beta\hat{u}_1 & \frac{\partial\hat{w}_1}{\partial y} + i\beta\hat{v}_1 & 2i\beta\hat{w}_1 \end{pmatrix} - (P_1 + \hat{p}_1)\mathbf{I}_3, \quad (3.47)$$

for the first fluid and

$$\mathbf{T}_2 = \frac{m}{Re} \begin{pmatrix} 2i\alpha\hat{u}_2 & \frac{\partial\hat{u}_2}{\partial y} + U'_2 + i\alpha\hat{v}_2 & i\alpha\hat{w}_2 + i\beta\hat{u}_2 \\ \frac{\partial\hat{u}_2}{\partial y} + U'_2 + i\alpha\hat{v}_2 & 2\frac{\partial\hat{v}_2}{\partial y} & \frac{\partial\hat{w}_2}{\partial y} + i\beta\hat{v}_2 \\ i\alpha\hat{w}_2 + i\beta\hat{u}_2 & \frac{\partial\hat{w}_2}{\partial y} + i\beta\hat{v}_2 & 2i\beta\hat{w}_2 \end{pmatrix} - (P_2 + \hat{p}_2)\mathbf{I}_3. \quad (3.48)$$

For the continuity of velocity in the directions of normal to the surface and tangent to the surface, we can impose the boundary condition on the interface as

$$\boldsymbol{\tau}_x \cdot \bar{\mathbf{u}}_1 = \boldsymbol{\tau}_x \cdot \bar{\mathbf{u}}_2, \quad (3.49)$$

$$\boldsymbol{\tau}_z \cdot \bar{\mathbf{u}}_1 = \boldsymbol{\tau}_z \cdot \bar{\mathbf{u}}_2, \quad (3.50)$$

$$\mathbf{n} \cdot \bar{\mathbf{u}}_1 = \mathbf{n} \cdot \bar{\mathbf{u}}_2, \quad (3.51)$$

which after substitution and linearization around $y = 1$ is simplified to

$$u_1 + \xi U'_1 = u_2 + \xi U'_2 \quad (3.52)$$

$$w_1 = w_2 \quad (3.53)$$

$$v_1 = v_2 \quad (3.54)$$

Clearly, we should have everything in terms of v and η . Therefore, multiplying 3.52 by $i\beta$ and 3.53 by $i\alpha$ and subtracting we get:

$$\eta_1 + i\beta\xi U'_1 = \eta_2 + i\beta\xi U'_2 \quad \text{at } y = 1. \quad (3.55)$$

Conversely, if 3.52 is multiplied by $i\alpha$ and 3.53 by $i\beta$ and they are summed up, we can use the the continuity equation (3.37) to derive

$$v'_1 - i\alpha\xi U'_1 = v'_2 - i\alpha\xi U'_2 \quad \text{at } y = 1. \quad (3.56)$$

Finally, the linearized version of the normal component is

$$v_1 = v_2 \quad \text{at } y = 1. \quad (3.57)$$

For vorticity, the continuity of the tangential components are enforced by using

$$\boldsymbol{\tau}_x^{tr} \mathbf{T}_1 \mathbf{n} = \boldsymbol{\tau}_x^{tr} \mathbf{T}_2 \mathbf{n}, \quad (3.58)$$

$$\boldsymbol{\tau}_z^{tr} \mathbf{T}_1 \mathbf{n} = \boldsymbol{\tau}_z^{tr} \mathbf{T}_2 \mathbf{n}, \quad (3.59)$$

which again after substituting for every term and simplifying we arrive to

$$u'_1 + i\alpha v_1 + U'_1 = m(u'_2 + i\alpha v_2 + U'_2), \quad (3.60)$$

$$w'_1 + i\beta v_1 = m(w'_2 + i\beta v_2). \quad (3.61)$$

Again, using the same trick, i.e, multiplying 3.60 by $i\beta$ and 3.2.1 by $i\alpha$ and subtracting we can obtain, by using the derivative for the definition 3.25

$$\eta'_1 + i\beta \xi U''_1 = m(\eta'_2 + i\beta \xi U''_2) \quad \text{at } y = 1, \quad (3.62)$$

which is now linearized for $y = 1$. As a remark, it should be noted that $U'_1 = mU'_2$. Similarly, we multiply 3.60 and 3.2.1 by $i\alpha$ and $i\beta$, respectively and sum the up. The only difference here is that we use the derivative of the continuity equation (3.37) to obtain the result. The linearized equation around $y = 1$ is

$$v''_1 + k^2 v_1 - i\alpha \xi U''_1 = m(v''_2 + k^2 v_2 - i\alpha \xi U''_2) \quad \text{at } y = 1. \quad (3.63)$$

For the normal component of vorticity, we use the fact that a jump in the normal component of the stress is admissible, which has to be balanced by the surface tension. That is,

$$\mathbf{n}^{tr} \mathbf{T}_1 \mathbf{n} - \mathbf{n}^{tr} \mathbf{T}_2 \mathbf{n} = S \left(\frac{1}{R_1} + \frac{1}{R_2} \right), \quad (3.64)$$

where S is the surface tension and $\frac{1}{R_1}$ and $\frac{1}{R_2}$ are the curvatures and therefore can be replaced by $\frac{\partial \xi}{\partial x} = i\alpha \xi$ and $\frac{\partial \xi}{\partial z} = i\beta \xi$. For the left side of the 3.64 we have the linearized form

$$\mathbf{n}^{tr} \mathbf{T}_1 \mathbf{n} - \mathbf{n}^{tr} \mathbf{T}_2 \mathbf{n} = 2(v'_1 - mv'_2) + \xi(P'_2 - P'_1) + (p_2 - p_1), \quad (3.65)$$

where by using the equation for base flow we can say

$$P'_2 - P'_1 = Fr^{-2}(1 - \gamma). \quad (3.66)$$

Moreover, by substituting 3.32 into 3.27 we obtain

$$k^2 p_1 = p_1'' + 2U_1' i \alpha v_1 \quad (3.67)$$

and on the other hand by taking the derivative of 3.22 with respect to y and using the 3.32 and 3.30 we get

$$p_1'' = i \Omega v_1' - i \alpha (U_1 v_1' + U_1' v_1) + \frac{1}{Re} (v_1''' - k^2 v_1') \quad (3.68)$$

Using 3.67 and 3.68 we can write an expression for pressure that depends only on the variables of our interest.

$$k^2 p_1 = i \Omega v_1' - i \alpha (U_1 v_1' - U_1' v_1) + \frac{1}{Re} (v_1''' - k^2 v_1') \quad (3.69)$$

Similar substitution is possible to be made for the second fluid with the difference that the last term on the right side of 3.67 for second fluid has additional coefficient γ and thus it is $2\gamma U_2' i \alpha v_2$. Therefore, the expression for the pressure is of the form

$$k^2 p_2 = \gamma \left[i \Omega v_2' - i \alpha (U_2 v_2' - U_2' v_2) \right] + \frac{m}{Re} (v_2''' - k^2 v_2') \quad (3.70)$$

The expressions 3.69 and 3.70 can be replaced for the term $p_1 - p_2$ on 3.65 to obtain the last boundary condition on the interface:

$$\begin{aligned} & \left[(v_1''' - 3k^2 v_1') + i \alpha Re (U_1' v_1 - U_1 v_1') \right] \\ & - \left[m (v_2''' - 3k^2 v_2') + i \alpha \gamma Re (U_2' v_2 - U_2 v_2') \right] \\ & - Sk^4 Re \xi + Fr^{-2} Re (\gamma - 1) k^2 \xi = i \Omega Re (\gamma v_2' - v_1') \quad \text{at } y = 1 \end{aligned} \quad (3.71)$$

The velocity and vorticity far away from the boundary decay. That is to say, as $y \rightarrow \infty$ the velocity and vorticity tend to zero.

$$v_2 \rightarrow 0 \quad \text{as } y \rightarrow \infty, \quad (3.72)$$

$$v_2' \rightarrow 0 \quad \text{as } y \rightarrow \infty, \quad (3.73)$$

$$\eta_2 \rightarrow 0 \quad \text{as } y \rightarrow \infty. \quad (3.74)$$

Another approach for dealing this condition would be to assume that at high elevations, the above components decay with an exponential rate. Therefore we can formulate this condition as

$$\begin{pmatrix} v_2(y) \\ v_2'(y) \\ \eta_2(y) \end{pmatrix} = \begin{pmatrix} \tilde{v}_2 \\ \tilde{v}_2' \\ \tilde{\eta}_2 \end{pmatrix} e^{-\lambda y}, \quad (3.75)$$

where \tilde{v}_2 , \tilde{v}'_2 and $\tilde{\eta}_2$ are constants and $\lambda = \sqrt{\alpha^2 + \beta^2}$. λ is found by replacing the assumed solution in the equations 3.34 and 3.36 and solving for λ .

3.3 Energy Calculation

In this section, we define an energy for the system which includes the disturbance kinetic energy of the two-fluid system together with the contribution of surface tension on the interface and potential energy caused by the movement of the interface.

First, for the disturbance kinetic energy for two fluids, we have

$$E_k^* = \int_{\mathcal{V}_1^*} \rho_1^* \frac{\mathbf{u}_1^* \cdot \mathbf{u}_1^*}{2} d\mathcal{V}^* + \int_{\mathcal{V}_2^*} \rho_2^* \frac{\mathbf{u}_2^* \cdot \mathbf{u}_2^*}{2} d\mathcal{V}^*. \quad (3.76)$$

The bound for the first integral, after scaling by $\rho_1^* V_0^{*2} d^{*3}$, i.e. making it dimensionless, can be considered as $\int_{\mathcal{V}_1} = \int_{\mathcal{X}} \int_{\mathcal{Z}} \int_0^{1+\xi}$. In specific, the bounds of the integral in y can be approximated as $\int_0^{1+\xi} = \int_0^1 + O[\xi^3]$. In a similar fashion, the bounds for the second integral can be approximated from 1 to ∞ . Finally, the dimensionless disturbance kinetic energy may be written as

$$E_k = \int_{\mathcal{V}_1} \frac{\hat{\mathbf{u}}_1 \cdot \hat{\mathbf{u}}_1}{2} d\mathcal{V} + \gamma \int_{\mathcal{V}_2} \frac{\hat{\mathbf{u}}_2 \cdot \hat{\mathbf{u}}_2}{2} d\mathcal{V}. \quad (3.77)$$

The other form of disturbance kinetic energy with respect to our variables of interest (v and η) is

$$E_k = \frac{1}{2k^2} \int_{\mathcal{V}_1} (k^2 |\hat{v}_1|^2 + |\mathbf{D}\hat{v}_1|^2 + |\hat{\eta}_1|^2) d\mathcal{V} + \frac{\gamma}{2k^2} \int_{\mathcal{V}_2} (k^2 |\hat{v}_2|^2 + |\mathbf{D}\hat{v}_2|^2 + |\hat{\eta}_2|^2) d\mathcal{V}. \quad (3.78)$$

If u , v are replaced by their Fourier mode, which were introduced before, the kinetic energy is simplified to

$$E_k = \frac{4\pi^2}{\alpha\beta k^2} \left[\int_0^1 (k^2 |v_1|^2 + |\mathbf{D}v_1|^2 + |\eta_1|^2) dy + \gamma \int_1^\infty (k^2 |v_2|^2 + |\mathbf{D}v_2|^2 + |\eta_2|^2) dy \right]. \quad (3.79)$$

Secondly, the potential energy due to gravity is considered. We define e_g^* , variable with respect to x and z , as

$$e_g^* = \int_{d^*}^{d^*+d^*\xi} \rho_1^* g y^* dy^* - \int_{d^*}^{d^*+d^*\xi} \rho_2^* g y^* dy^*, \quad (3.80)$$

where we introduce the scaling factor $\rho_1^* V_0^{*2} d^*$ for making dimensionless variable e_g and thus after the change of variable, the above integrals are solved and reduce to

$$e_g = \frac{1 - \gamma}{2Fr^2} (\xi^2 + 2\xi). \quad (3.81)$$

We need to integrate e_g for one period of x and z . Using the assumed form for ξ (3.42), it is observed that the terms which are periodic vanish and the only term that remains is the constant which is produced by ξ^2 . Therefore, the integral can be computed as

$$\begin{aligned} & \int_0^{\frac{2\pi}{\alpha}} \int_0^{\frac{2\pi}{\beta}} (\xi^2 + 2\xi) dz dx = \\ & \int_0^{\frac{2\pi}{\alpha}} \int_0^{\frac{2\pi}{\beta}} [\xi^2 e^{2i(\alpha x + \beta z)} + \bar{\xi}^2 e^{-2i(\alpha x + \beta z)} + 2|\xi|^2 + \xi e^{i(\alpha x + \beta z)} + \bar{\xi} e^{-i(\alpha x + \beta z)}] dz dx = \\ & \int_0^{\frac{2\pi}{\alpha}} \int_0^{\frac{2\pi}{\beta}} 2|\xi|^2 dz dx = 2|\xi|^2 \frac{4\pi^2}{\alpha\beta}. \end{aligned}$$

Integrating 3.81 and using the simplified integral we get the contribution of the gravity on the potential energy (at the interface) as follows:

$$E_g = \frac{4\pi^2}{\alpha\beta} \frac{1 - \gamma}{Fr^2} |\xi|^2. \quad (3.82)$$

Finally, we seek to express the energy due to the surface tension in terms of our variables. Therefore, we look for the area of the surface which is generated by interface between the two phases of fluids. Using the same principle, that the integral over a period of the periodic functions are zero, we simplify and integrate the following integral. Note that the dimensionless variables are used, thus the calculated area is already scaled by d^{*2} .

$$\begin{aligned} & \int_0^{\frac{2\pi}{\alpha}} \int_0^{\frac{2\pi}{\beta}} \sqrt{1 + \left(\frac{\partial \xi}{\partial x}\right)^2 + \left(\frac{\partial \xi}{\partial z}\right)^2} dz dx = \\ & \int_0^{\frac{2\pi}{\alpha}} \int_0^{\frac{2\pi}{\beta}} \sqrt{1 + 2\alpha^2 |\xi|^2 + 2\beta^2 |\xi|^2} dz dx \quad \Rightarrow \\ & \text{Area} = \sqrt{1 + 2k^2 |\xi|^2} \frac{4\pi^2}{\alpha\beta}. \end{aligned} \quad (3.83)$$

The total energy corresponding to the surface tension is therefore

$$\tilde{E}_{st} = S \frac{4\pi^2}{\alpha\beta} \sqrt{1 + 2k^2 |\xi|^2}. \quad (3.84)$$

The expression for the area can be expanded for $|\xi|$ to yield

$$\text{Area} = \frac{4\pi^2}{\alpha\beta} (1 + k^2 |\xi|^2 + O[|\xi|^4]), \quad (3.85)$$

which shows the increase of the area of the interface due to a perturbation. Therefore, the energy corresponding to the surface tension after a perturbation is

$$E_{st} = \frac{4\pi^2}{\alpha\beta} S k^2 |\xi|^2 \quad (3.86)$$

The total energy of the system is therefore, the summation of all the energy terms defined and calculated, i.e.,

$$E_{tot} = E_k + E_g + E_{st}, \quad (3.87)$$

which after substituting of the equivalent expressions, (3.79, 3.82 and 3.86) can be reordered as

$$E_{tot} = \frac{4\pi^2}{\alpha\beta} \left[\frac{1}{k^2} \int_0^1 (k^2 |v_1|^2 + |Dv_1|^2 + |\eta_1|^2) dy + \frac{\gamma}{k^2} \int_1^\infty (k^2 |v_2|^2 + |Dv_2|^2 + |\eta_2|^2) dy + \frac{1-\gamma}{Fr^2} |\xi|^2 + S k^2 |\xi|^2 \right] \quad (3.88)$$

3.4 Optimal Perturbation using Lagrange Multipliers

In this section, we seek to calculate the optimal initial condition which gives us the highest value of transient growth in short time. In this direction, first a short analysis is done on the integration of the system in time and thus defining a proper evolution operator. The constraints and the objective function are defined. First, an l_2 norm is chosen to obtain a optimal initial condition and to get a prototype of the solution to the problem. After that, the proper energy norm is defined and the optimization problem is solved with similar method. The method for solving the optimization problem includes using the adjoint problem as well as the direct problem, which results from a Lagrangian approach. Finally, for a recursive study, an estimation for the feasible initial condition is calculated.

3.4.1 System Formulation and Time Integration

The above governing equations and boundary conditions can be written in the form of

$$\mathbf{A} \frac{\partial \mathbf{q}}{\partial t} + \mathbf{B} \mathbf{q} = 0, \quad (3.89)$$

where

$$\mathbf{q} = (v_1, \eta_1, \xi, v_2, \eta_2)^{tr} \quad (3.90)$$

and \mathbf{A} and \mathbf{B} are linear and continuous spatial operators that include all the governing equation and boundary conditions discussed in previous section. In the discretized version of the problem, where all the derivatives are approximated by appropriate finite difference schemes depending on the location, the vector would be of form

$$\mathbf{q} = (v_1^{(0)}, \eta_1^{(0)}, \dots, v_1^{(int)}, \eta_1^{(int)}, \xi, v_2^{(int)}, \eta_2^{(int)}, \dots, v_2^{(\infty)}, \eta_2^{(\infty)})^{tr}, \quad (3.91)$$

where the superscripts represent the location (y-coordinate) at which the variable is evaluated. Introducing the Fourier form already used for these variables with a quasi-steady approach, $\frac{\partial}{\partial t}$ can be substituted with $-i\Omega$ and therefore we have a generalized eigenvalue problem to solve which can be written in the form of

$$\mathbf{B}\mathbf{q} = \Omega(i\mathbf{A})\mathbf{q}, \quad (3.92)$$

where Ω is the eigenvalue or the phase frequency and \mathbf{q} is the eigenvector. It is possible to scale the matrix \mathbf{A} or to divide the frequency by stream-wise number to obtain the phase velocity (c).

In a more general case, where the dependency of \mathbf{q} with time is not known, one may integrate the 3.89 in time to find the vector \mathbf{q} at any time instance. Provided that the initial condition used for this integration satisfies the boundary condition at the wall, on the interface and at infinity, the final solution at any time must have the same property.

Considering the fact that the matrix \mathbf{A} in discretized version is singular (simply because not all the boundary conditions have time derivative), we have to implement a scheme that does not require inverting this matrix. Therefore, a collocation method or any other implicit method may be used. Here, a trapezoidal rule is applied to write the scheme as

$$\mathbf{A} \frac{\mathbf{q}^{i+1} - \mathbf{q}^i}{\delta t} + \mathbf{B} \frac{\mathbf{q}^{i+1} + \mathbf{q}^i}{2} = 0, \quad (3.93)$$

which can be reorganized to

$$\mathbf{q}^{i+1} = (\mathbf{A} + \mathbf{B} \frac{\delta t}{2})^{-1} (\mathbf{A} - \mathbf{B} \frac{\delta t}{2}) \mathbf{q}^i \quad (3.94)$$

Needless to say, the advantage of this method over backward (implicit) Euler, is that the rate of convergence is 2 whereas the latter is a first order approximation.

3.4.2 Adjoint Approach

Recall equation 3.89

$$\mathbf{A} \frac{\partial \mathbf{q}}{\partial t} + \mathbf{B}\mathbf{q} = 0, \quad (3.89)$$

we seek to derive the adjoint equation. We define

$$\mathcal{L}\mathbf{q} := \mathbf{A} \frac{\partial \mathbf{q}}{\partial t} + \mathbf{B}\mathbf{q} \quad (3.95)$$

$$\mathbf{a} \cdot \mathbf{q} = \langle \mathbf{a}, \mathbf{q} \rangle := \int_0^T \mathbf{a}^H \mathbf{q} dt, \quad (3.96)$$

with superscript H to be Hermitian. Also from the definition of the adjoint operator we have

$$\langle \mathbf{a}, \mathcal{L}\mathbf{q} \rangle = \langle \mathcal{L}^* \mathbf{a}, \mathbf{q} \rangle. \quad (3.97)$$

Since a quasi-steady approach is used it can be assumed that the matrices \mathbf{A} and \mathbf{B} are independent of time. Therefore, by using the definitions above and integration by part we have

$$\begin{aligned} 0 = \langle \mathbf{a}, \mathcal{L}\mathbf{q} \rangle &= \int_0^T (\mathbf{a}^H \mathbf{A} \frac{\partial \mathbf{q}}{\partial t} + \mathbf{a}^H \mathbf{B}\mathbf{q}) dt = \\ &= \int_0^T \left(- \left(\frac{\partial \mathbf{a}}{\partial t} \right)^H \mathbf{A}\mathbf{q} + \mathbf{a}^H \mathbf{B}\mathbf{q} \right) dt + [\mathbf{a}^H \mathbf{A}\mathbf{q}]_0^T = \\ &= \int_0^T \left(- \mathbf{A}^H \frac{\partial \mathbf{a}}{\partial t} + \mathbf{B}^H \mathbf{a} \right)^H \mathbf{q} dt + [\mathbf{a}(T)^H \mathbf{A}\mathbf{q}(T) - \mathbf{a}(0)^H \mathbf{A}\mathbf{q}(0)]. \end{aligned}$$

Using the identity 3.97, one can say

$$\mathcal{L}^* \mathbf{a} := -\mathbf{A}^H \frac{\partial \mathbf{a}}{\partial t} + \mathbf{B}^H \mathbf{a} = 0, \quad (3.98)$$

if it holds

$$\mathbf{a}(T)^H \mathbf{A}\mathbf{q}(T) - \mathbf{a}(0)^H \mathbf{A}\mathbf{q}(0) = 0. \quad (3.99)$$

Since 3.97 and 3.89 are continuous, so is 3.98 and therefore this approach of deriving the adjoint equation is called the continuous approach. It is also possible to formulate the adjoint equation in the discretized case. For the discretized version, one may rename the operator in 3.94

$$\mathbf{q}^{i+1} = \mathbf{C}\mathbf{q}^i \quad (3.100)$$

and do the same thing as for the continuous case to find the adjoint equation as

$$\mathbf{a}^i = \mathbf{C}^H \mathbf{a}^{i+1}. \quad (3.101)$$

Finally, the error defined as

$$error = |(\mathbf{a}^N)^H \mathbf{q}^N - (\mathbf{a}^0)^H \mathbf{q}^0| \quad (3.102)$$

shows how accurate the adjoint of the operator is.

3.4.3 Optimization of the Solution Vector

3.4.3.1 Continuous Approach

In this section we seek to formulate the maximization of some parameters in the output with respect to some other parameters in the input. In particular, it is sought to maximize the ratio between the norms of the solution at the final time and the initial condition. Clearly, the parameter of the optimization problem is all the feasible initial conditions that is, those which satisfy the boundary conditions. This can be formulated as

$$\max_{\mathbf{g}} \tilde{J}(\mathbf{q}, \mathbf{g}), \quad \text{where} \quad \tilde{J}(\mathbf{q}, \mathbf{g}) := \frac{\|\mathbf{q}(T)\|^2}{\|\mathbf{g}\|^2}, \quad (3.103)$$

with

$$\mathbf{g} := \mathbf{q}_0 = \mathbf{q}(0) \quad (3.104)$$

and $\mathbf{q}(T)$ being the solution of 3.89 at the final time. However, it is favorable to deal with the inverse and have a minimization problem instead. Therefore, the problem can be changed to

$$\min_{\mathbf{g}} J(\mathbf{q}, \mathbf{g}), \quad \text{where} \quad J(\mathbf{q}, \mathbf{g}) := \frac{\mathbf{g} \cdot \mathbf{g}}{\mathbf{q}(T) \cdot \mathbf{q}(T)}, \quad (3.105)$$

with the constraints 3.89 and 3.104. We use the standard notation for the constraints as

$$\mathbf{f} := \mathbf{A} \frac{\partial \mathbf{q}}{\partial t} + \mathbf{B} \mathbf{q}, \quad (3.106)$$

$$\mathbf{k} := \mathbf{q}(0) - \mathbf{g}, \quad (3.107)$$

to define the Lagrangian in the form of

$$\mathcal{L}(\mathbf{q}, \mathbf{g}, \mathbf{a}, \mathbf{b}) = J(\mathbf{q}, \mathbf{g}) - \mathbf{a} \cdot \mathbf{f} - \mathbf{b} \cdot \mathbf{k}. \quad (3.108)$$

Using the above definitions for J , f and k and inner production definition (3.96) for time evolutionary variables and l^2 product for other inner products, the Lagrangian is

$$\mathcal{L}(\mathbf{q}, \mathbf{g}, \mathbf{a}, \mathbf{b}) := \frac{\mathbf{g}^H \mathbf{g}}{\mathbf{q}(T)^H \mathbf{q}(T)} - \int_0^T \mathbf{a}^H \left(\mathbf{A} \frac{\partial \mathbf{q}(t)}{\partial t} + \mathbf{B} \mathbf{q}(t) \right) dt - \mathbf{b}^H (\mathbf{q}(0) - \mathbf{g}). \quad (3.109)$$

A necessary condition for the solution is that it is a stationary point for Lagrangian, i.e., where the first derivatives of \mathcal{L} with respect to all the four variables are zero. The state equations are found when these derivatives are with respect to the coefficients of the constraints, i.e., $\frac{\partial \mathcal{L}}{\partial \mathbf{b}}$ and $\frac{\partial \mathcal{L}}{\partial \mathbf{a}}$. The adjoint equation and optimality condition are when the derivative is with respect to the state vector and control vector, respectively. $\left(\frac{\partial \mathcal{L}}{\partial \mathbf{q}}, \right.$

$\frac{\partial \mathcal{L}}{\partial \mathbf{g}}$). In other word, we tend to solve

$$\delta \mathcal{L} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}} \cdot \delta \mathbf{a} + \frac{\partial \mathcal{L}}{\partial \mathbf{b}} \cdot \delta \mathbf{b} + \frac{\partial \mathcal{L}}{\partial \mathbf{q}} \cdot \delta \mathbf{q} + \frac{\partial \mathcal{L}}{\partial \mathbf{g}} \cdot \delta \mathbf{g}$$

For the first one we have:

$$\int_0^T \left(\mathbf{A} \frac{\partial \mathbf{q}(t)}{\partial t} + \mathbf{B} \mathbf{q}(t) \right)^H \delta \mathbf{a} dt = 0$$

or

$$\frac{\mathbf{A} \partial \mathbf{q}(t)}{\partial t} + \mathbf{B} \mathbf{q}(t) = 0, \quad (3.89)$$

Using the second term we get $(\mathbf{q}(0) - \mathbf{g})^H \delta \mathbf{b} = 0$ or

$$\mathbf{q}(0) = \mathbf{g}. \quad (3.104)$$

Equation 3.89 and 3.104 are **state equations**.

Taking the forth term and putting it equal to zero we get

$$\frac{2\mathbf{g}^H \delta \mathbf{g}}{\mathbf{q}(T)^H \mathbf{q}(T)} + \mathbf{b}^H \delta \mathbf{g} = 0$$

which after solving for \mathbf{g} simplifies to

$$\mathbf{g} = -\frac{1}{2} \mathbf{b} [\mathbf{q}(T)^H \mathbf{q}(T)], \quad (3.110)$$

Finally solving for the third term we have

$$\begin{aligned} & \frac{-2(\mathbf{g}^H \mathbf{g}) \mathbf{q}(T)^H \delta \mathbf{q}(T)}{(\mathbf{q}(T)^H \mathbf{q}(T))^2} - \int_0^T \mathbf{a}^H \left(\mathbf{A} \frac{\partial \delta \mathbf{q}(t)}{\partial t} + \mathbf{B} \delta \mathbf{q}(t) \right) dt - \mathbf{b}^H \delta \mathbf{q}(0) = \\ & \frac{-2(\mathbf{g}^H \mathbf{g}) \mathbf{q}(T)^H \delta \mathbf{q}(T)}{(\mathbf{q}(T)^H \mathbf{q}(T))^2} - [\mathbf{a}^H \mathbf{A} \delta \mathbf{q}]_0^T + \int_0^T \left(\frac{\partial \mathbf{a}(t)^H}{\partial t} \mathbf{A} - \mathbf{a}(t)^H \mathbf{B} \right) \delta \mathbf{q}(t) dt - \mathbf{b}^H \delta \mathbf{q}(0) = \\ & \left[\frac{-2(\mathbf{g}^H \mathbf{g}) \mathbf{q}(T)^H}{(\mathbf{q}(T)^H \mathbf{q}(T))^2} - \mathbf{a}(T)^H \mathbf{A} \right] \delta \mathbf{q}(T) + \int_0^T \left(\mathbf{A}^H \frac{\partial \mathbf{a}(t)}{\partial t} - \mathbf{B}^H \mathbf{a}(t) \right)^H \delta \mathbf{q}(t) dt \\ & \quad + (\mathbf{a}(0)^H \mathbf{A} - \mathbf{b}^H) \delta \mathbf{q}(0) \end{aligned}$$

where from the first to second line we do by integration by part. Collecting the terms for $\delta \mathbf{q}(T)$, $\delta \mathbf{q}(t)$ and $\delta \mathbf{q}(0)$ and putting each one equal to zero will result:

$$\mathbf{A}^H \mathbf{a}(T) = - \left[\frac{2\mathbf{g}^H \mathbf{g}}{(\mathbf{q}(T)^H \mathbf{q}(T))^2} \right] \mathbf{q}(T), \quad (3.111)$$

$$-\mathbf{A}^H \frac{\partial \mathbf{a}}{\partial t} + \mathbf{B}^H \mathbf{a} = 0, \quad (3.98)$$

$$\mathbf{b} = \mathbf{A}^H \mathbf{a}(0), \quad (3.112)$$

respectively. Equation 3.111 and 3.98 define the **adjoint equation** for $0 \leq t \leq T$. The expression for \mathbf{b} (3.112) can be replaced in 3.110 to find the **optimality condition**:

$$\mathbf{g} = -\frac{1}{2} \mathbf{A}^H \mathbf{a}(0) [\mathbf{q}(T)^H \mathbf{q}(T)]. \quad (3.113)$$

To solve the problem in the continuous approach one may use the algorithm 1 and the

Algorithm 1 Optimization, Continuous Approach

- | | | |
|----|--|--|
| 1: | $\mathbf{g} = \mathbf{g}_0$ | ▷ Initialization |
| 2: | do | |
| 3: | Solve state equation 3.89 with initial condition 3.104 | ▷ time forward |
| 4: | Solve adjoint equation 3.98 with initial condition 3.111 | ▷ time backward |
| 5: | Update \mathbf{g} by optimality condition 3.113 | |
| 6: | while not converged | ▷ Convergence of J (3.105) may be considered |
| 7: | return J using 3.105 | |
-

direct and adjoint solver already discussed. However, on the step 4 of the algorithm, it is needed to solve 3.111 to have $\mathbf{a}(T)$ explicitly. This requires to solve an under-determined system, because \mathbf{A} is singular. In order to avoid this, we need to solve the optimization problem in a discretized approach which is described in the following section.

3.4.3.2 Discrete Approach

In this approach, we use the discretized version of the system and do the same calculation as in the previous, to derive the procedure to solve the optimization problem 3.105.

Using the same technique, we can derive the initial condition for the adjoint equation as

$$\mathbf{a}^N = - \left[\frac{2\mathbf{g}^H \mathbf{g}}{((\mathbf{q}^N)^H \mathbf{q}^N)^2} \right] \mathbf{q}^N \quad (3.114)$$

and the optimality condition as

$$\mathbf{g} = -\frac{1}{2} \mathbf{a}^0 [(\mathbf{q}^N)^H \mathbf{q}^N]. \quad (3.115)$$

Therefore, we can use algorithm 2 to find the maximum for the energy function. Clearly,

Algorithm 2 Optimization, Discrete Approach

- 1: $\mathbf{g} = \mathbf{g}_0$ ▷ Initialization
 - 2: **do**
 - 3: Solve state equation 3.100 with initial condition 3.104 ▷ time forward
 - 4: Solve adjoint equation 3.101 with initial condition 3.114 ▷ time backward
 - 5: Update \mathbf{g} by optimality condition 3.115
 - 6: **while** not converged ▷ Convergence of J (3.105) may be considered
 - 7: **return** J using 3.105
-

in this case for the evaluation of J , $\mathbf{q}(T)$ should be replaced by \mathbf{q}^N .

3.4.4 Optimization of Energy

In order to write the energy as a function of the solution vector \mathbf{q} we use the below matrices to extract the variables and insert them in 3.88. Using the definition for discretized solution vector 3.91 we can define with \mathbf{q} from 4.1

$$\mathbf{q}_1 = \mathbf{I}_{q_1} \mathbf{q}, \quad \mathbf{q}_2 = \mathbf{I}_{q_2} \mathbf{q}, \quad \xi = \mathbb{1}_\xi^H \mathbf{q}, \quad (3.116)$$

where

$$\mathbf{I}_{q_1} = \begin{pmatrix} 1 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & \cdots & 0 \end{pmatrix}, \quad \mathbf{I}_{q_2} = \begin{pmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & 0 & \cdots & 1 \end{pmatrix}, \quad (3.117)$$

$$\mathbb{1}_\xi = \begin{pmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{pmatrix}^H, \quad (3.118)$$

$$\mathbf{q}_1 = (v^{(0)}, \eta^{(0)}, \dots, v^{(ny1)}, \eta^{(ny1)})^{tr} \quad \text{and} \quad (3.119)$$

$$\mathbf{q}_2 = (v^{(ny1+1)}, \eta^{(ny1+1)}, \dots, v^{(ny+1)}, \eta^{(ny+1)})^{tr}. \quad (3.120)$$

As discussed in [13] we can rewrite the expression for E_k as

$$E_k = \frac{4\pi^2}{\alpha\beta} \left[\frac{1}{k^2} \int_0^1 \mathbf{q}_1^H \mathbf{M}_1 \mathbf{q}_1 dy + \frac{1}{k^2} \int_1^\infty \mathbf{q}_2^H \mathbf{M}_2 \mathbf{q}_2 dy \right]. \quad (3.121)$$

where \mathbf{M}_1 and \mathbf{M}_2 are the discretized matrices corresponding to the continuous operators

$$\mathbf{M}_{1c} = \begin{pmatrix} -D^2 + k^2 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{M}_{2c} = \gamma \begin{pmatrix} -D^2 + k^2 & 0 \\ 0 & 1 \end{pmatrix}. \quad (3.122)$$

Substituting for the definitions, we can now write the energy in terms of \mathbf{q} as

$$E_{tot} = \frac{4\pi^2}{\alpha\beta} \left[\frac{1}{k^2} \int_0^1 \mathbf{q}^H \mathbf{M}_{q_1} \mathbf{q} dy + \frac{1}{k^2} \int_1^\infty \mathbf{q}^H \mathbf{M}_{q_2} \mathbf{q} dy + \frac{1-\gamma}{Fr^2} |\mathbb{1}_\xi^H \mathbf{q}|^2 + Sk^2 |\mathbb{1}_\xi^H \mathbf{q}|^2 \right], \quad (3.123)$$

where

$$\mathbf{M}_{q_1} = \mathbf{I}_{q_1}^H \mathbf{M}_1 \mathbf{I}_{q_1} \quad \text{and} \quad \mathbf{M}_{q_2} = \mathbf{I}_{q_2}^H \mathbf{M}_2 \mathbf{I}_{q_2} \quad (3.124)$$

We define $\tilde{J} = \frac{E_{tot}(T)}{E_{tot}(0)}$ as defined in 3.103 and we seek to maximize this ratio over all the initial conditions. As discussed in 3.4.3, we can minimize the inverse of \tilde{J} and this would result the same state equation 3.89 with the initial condition 3.104. In addition, the adjoint equation remains the same (3.98). However, to find the optimality condition and the initial condition for the adjoint equation, we need to solve

$$\frac{\partial \mathcal{L}}{\partial \mathbf{q}} \cdot \delta \mathbf{q} + \frac{\partial \mathcal{L}}{\partial \mathbf{g}} \cdot \delta \mathbf{g} = 0. \quad (3.125)$$

The expression for the first term is

$$- \frac{E(\mathbf{g}) E'(\mathbf{q}(T)) \delta \mathbf{q}(T)}{(E(q(T)))^2} - \mathbf{a}(T)^H \mathbf{A} \delta \mathbf{q}(T) + Adj. + (\mathbf{a}(0)^H \mathbf{A} - \mathbf{b}^H) \delta \mathbf{q}(0) = 0, \quad (3.126)$$

where E' is defined by 3.133, and for the second would be

$$\frac{E'(\mathbf{g}) \delta \mathbf{g}}{E(q(T))} + \mathbf{b}^H \delta \mathbf{g} = 0. \quad (3.127)$$

From the first two terms in 3.126 we get the initial condition for the adjoint equation:

$$- \frac{E(\mathbf{g})}{(E(\mathbf{q}(T)))^2} E'(\mathbf{q}(T)) = \mathbf{A}^H \mathbf{a}(T). \quad (3.128)$$

In addition, from 3.126 we can derive 3.112

$$\mathbf{b} = \mathbf{A}^H \mathbf{a}(0) \quad (3.112)$$

which can be replaced into 3.127 to yield the optimality condition

$$E'(\mathbf{g})^H = -\mathbf{A}^H \mathbf{a}(0) (E(q(T))). \quad (3.129)$$

Both 3.128 and 3.129 require the expression for the derivative of energy. The energy is a scalar valued function, however, the derivative with respect to a vector will be a vector

valued function which can be calculated as

$$\begin{aligned} \frac{\alpha\beta}{4\pi^2} E'(\mathbf{q}) &= \frac{1}{k^2} \int_0^1 \mathbf{q}^H (\mathbf{M}_{q_1} + \mathbf{M}_{q_1}^H) dy \\ &\quad + \frac{1}{k^2} \int_1^\infty \mathbf{q}^H (\mathbf{M}_{q_2} + \mathbf{M}_{q_2}^H) dy + \frac{2(1-\gamma)}{Fr^2} \mathbf{q}^H \mathbf{I}_\xi + 2Sk^2 \mathbf{q}^H \mathbf{I}_\xi, \end{aligned} \quad (3.130)$$

where $\mathbf{I}_\xi = \mathbb{1}_\xi \mathbb{1}_\xi^H$ and the last two terms are derived because

$$|\xi|^2 = |\mathbb{1}_\xi^H \mathbf{q}|^2 = (\mathbb{1}_\xi^H \mathbf{q})^H (\mathbb{1}_\xi^H \mathbf{q}) = \mathbf{q}^H \mathbb{1}_\xi \mathbb{1}_\xi^H \mathbf{q} = \mathbf{q}^H \mathbf{I}_\xi \mathbf{q}, \quad (3.131)$$

and therefore

$$\frac{\partial |\xi|^2}{\partial \mathbf{q}} = \mathbf{q}^H (\mathbf{I}_\xi + \mathbf{I}_\xi^H) = 2\mathbf{q}^H \mathbf{I}_\xi. \quad (3.132)$$

Finally, we need to get rid of the integrals in 3.130 in order to have the derivative directly depending on \mathbf{q} . In other words, we need the derivative to be in the form of $E' = \mathbf{C}\mathbf{q}$ so that we can solve 3.129. Considering the fact that \mathbf{q} is a vector, we can approximate the integrals to value of the integrand in discrete form multiplied by the grid size. Therefore, 3.130 is simplified to

$$\frac{\alpha\beta}{4\pi^2} E'(\mathbf{q})^H = \left[\frac{\Delta}{k^2} (\mathbf{M}_{q_1} + \mathbf{M}_{q_1}^H + \mathbf{M}_{q_2} + \mathbf{M}_{q_2}^H) + \frac{2(1-\gamma)}{Fr^2} \mathbf{I}_\xi + 2Sk^2 \mathbf{I}_\xi \right] \mathbf{q}. \quad (3.133)$$

Using the discretized version for the direct and adjoint solver (3.100, 3.101) we can modify the initial condition for the adjoint equation and the optimality condition to cancel out the singular matrix \mathbf{A} , i.e

$$\mathbf{a}^N = -\frac{E(\mathbf{g})}{(E(\mathbf{q}^N))^2} E'(\mathbf{q}^N), \quad (3.134)$$

$$\mathbf{g} = -\mathbf{M}^{-1} \mathbf{a}^0 (E(\mathbf{q}^N)), \quad (3.135)$$

respectively and

$$\mathbf{M} = \frac{\Delta}{k^2} (\mathbf{M}_{q_1} + \mathbf{M}_{q_1}^H + \mathbf{M}_{q_2} + \mathbf{M}_{q_2}^H) + \frac{2(1-\gamma)}{Fr^2} \mathbf{I}_\xi + 2Sk^2 \mathbf{I}_\xi. \quad (3.136)$$

Introducing the above equations allows us to use algorithm 3 for finding the optimal perturbation.

3.4.5 Polynomial Fitting for Initial Condition

For the case when we change the parameters of the fluids such as viscosity ratio, etc. in order to find the optimal perturbation, we need to solve the optimization problem

Algorithm 3 Optimum perturbation

-
- 1: $\mathbf{g} = \mathbf{g}_0$ ▷ Initialization
 - 2: **do**
 - 3: Solve state equation 3.100 with initial condition 3.104 ▷ time forward
 - 4: Solve adjoint equation 3.101 with initial condition 3.134 ▷ time backward
 - 5: Update \mathbf{g} by optimality condition 3.135
 - 6: **while** not converged ▷ Convergence of $\frac{E(T)}{E(0)}$ may be considered
 - 7: **return** $E(T)$
-

starting with an initial guess which satisfies the boundary condition. One option, which is not very fast though accurate, is to take an eigenvector of the system, preferably the one associated with the eigenvalue that has the highest imaginary part. Another method would be to use a combination of continuous functions to construct an initial condition such that this initial vector satisfies all the boundary condition. For this problem, a basis of polynomials and exponential functions are used to take into account all the 12 boundary conditions.

We need polynomial for v such that $v(y) = \begin{cases} v_1(y) & \text{if } 0 \leq y \leq 1 \\ v_2(y) & \text{if } 1 \leq y < \infty \end{cases}$ and the following conditions are satisfied:

$$v_1 = 0 \quad \text{at } y = 0, \quad (3.38)$$

$$v_1' = 0 \quad \text{at } y = 0, \quad (3.40)$$

$$v_1' - i\alpha\xi U_1' = v_2' - i\alpha\xi U_2' \quad \text{at } y = 1, \quad (3.56)$$

$$v_1 = v_2 \quad \text{at } y = 1, \quad (3.57)$$

$$v_1'' + k^2 v_1 - i\alpha\xi U_1'' = m(v_2'' + k^2 v_2 - i\alpha\xi U_2'') \quad \text{at } y = 1, \quad (3.63)$$

$$\begin{aligned} & \left[(v_1''' - 3k^2 v_1') + i\alpha Re(U_1' v_1 - U_1 v_1') \right] \\ & - \left[m(v_2''' - 3k^2 v_2') + i\alpha\gamma Re(U_2' v_2 - U_2 v_2') \right] \\ & - Sk^4 Re\xi + Fr^{-2} Re(\gamma - 1)k^2\xi = i\Omega Re(\gamma v_2' - v_1') \quad \text{at } y = 1, \end{aligned} \quad (3.71)$$

$$v_2 \rightarrow 0 \quad \text{as } y \rightarrow \infty \quad (3.72)$$

$$v_2' \rightarrow 0 \quad \text{as } y \rightarrow \infty. \quad (3.73)$$

The right hand side of 3.71 should be taken zero. Taking v as

$$v(y) = \begin{cases} v_1(y) = c_6 \frac{e^{-1}}{2} y^2 + c_1 (1-y)y^2 & \text{if } 0 \leq y \leq 1 \\ v_2(y) = \frac{c_6}{2} y^3 e^{-y} + c_7 (y-1)^2 e^{-\lambda y} & \text{if } 1 \leq y < \infty \end{cases} \quad (3.137)$$

satisfies all the conditions with

$$c_1 = -i\alpha\xi(U_1' - U_2'), \quad c_2 = -i\alpha\xi(U_1'' - mU_2''), \quad c_3 = i\alpha Re, \quad (3.138)$$

$$c_4 = i\alpha\gamma Re, \quad c_5 = Sk^4 Re\xi - Fr^{-2} Re(\gamma - 1)k^2\xi \quad (3.139)$$

c_6, c_7 can be calculated from solving the 2×2 linear system made by 3.63 and 3.62:

$$\frac{2e(-6c_1 - c_5 + 3c_1k^2 + c_1c_3U_1 - 12c_1\lambda + 3c_2\lambda)}{3k^2(m-1)(\lambda-2) - 4m + 2c_3U_1(1-\gamma) - c_3U_1' + c_4U_2' - 6\lambda + 3m\lambda} \quad (3.140)$$

$$c_7 = \frac{(c_2 - 4c_1)e^\lambda}{2m} + \frac{e^{\lambda-1}(1 + k^2/2 - m/2 - k^2m/2)}{2m}c_6 \quad (3.141)$$

For the vorticity we need a function such that $\eta(y) = \begin{cases} \eta_1(y) & \text{if } 0 \leq y \leq 1 \\ \eta_2(y) & \text{if } 1 \leq y < \infty \end{cases}$ and the following conditions are satisfied:

$$\eta_1 = 0 \quad \text{at } y = 0, \quad (3.39)$$

$$\eta_1 + i\beta\xi U_1' = \eta_2 + i\beta\xi U_2' \quad \text{at } y = 1, \quad (3.55)$$

$$\eta_1' + i\beta\xi U_1'' = m(\eta_2' + i\beta\xi U_2'') \quad \text{at } y = 1, \quad (3.62)$$

$$\eta_2 \rightarrow 0 \quad \text{as } y \rightarrow \infty. \quad (3.74)$$

Taking η as

$$\eta(y) = \begin{cases} \eta_1(y) = \frac{e^{-1}}{2}y^2 + c_8(1-y)y^2 & \text{if } 0 \leq y \leq 1 \\ \eta_2(y) = \frac{y^3}{2}e^{-\lambda y} + c_9e^{1-y} + c_{10}(y-1)e^{-y} & \text{if } 1 \leq y < \infty \end{cases} \quad (3.142)$$

with the coefficients

$$c_8 = i\beta\xi(U_1'' - mU_2''), \quad c_9 = i\beta\xi(U_1' - U_2'), \quad c_{10} = e^{1-\lambda}\left(\frac{1}{m} - \frac{3}{2} + c_9e^\lambda + \frac{\lambda}{2}\right) \quad (3.143)$$

satisfies all the equations.

3.5 Non-modal Growth Using Eigenvalue Decomposition (Diagonalized Approach)

Another method to see the transient gain of a solution is to convert the energy norm into an L_2 norm. In this approach, a gain is calculated which is the envelope of all the perturbations optimized for all times. This method is much faster because no optimization solver is needed to calculate the gain.

As before the aim is to calculate $\max_{\forall \mathbf{q}_0} \frac{\|\mathbf{q}(t)\|}{\|\mathbf{q}_0\|}$, but this time we want to have this as a function for all times. Therefore we use the definition of the norm and the solution operator $\exp(\mathcal{S}t)$.

$$\max_{\forall \mathbf{q}_0} \frac{\|\mathbf{q}(t)\|}{\|\mathbf{q}_0\|} = \max_{\forall \mathbf{q}_0} \frac{\|\exp(\mathcal{S}t)\mathbf{q}_0\|}{\|\mathbf{q}_0\|} = \|\exp(\mathcal{S}t)\| := G(t) \quad (3.144)$$

We need to convert the latter norm to l_2 norm. This is done by decomposing the solution operator. To do this, the eigenvalues of the system are sorted according to the imaginary part from the highest to the lowest. Then the eigenvectors corresponding to the first few (Ne) sorted eigenvalues are selected to construct the matrix \mathcal{M} . It should be noted that in principle this number of eigenvectors can be much smaller than the dimension of the system but it should also be considered that very few eigenvectors cannot capture the non orthogonality of the system and they will show a modal behavior at finite time. The entries of the matrix \mathcal{M} are calculated as follows

$$\mathcal{M}_{mn} = \int_{\Omega} \mathbf{q}_n^H \mathbf{M} \mathbf{q}_m \, d\Omega, \quad (3.145)$$

where the matrix M is the one calculated by 3.136 and \mathbf{q}_n and \mathbf{q}_m are the eigenvectors associated with the n th and m th sorted eigenvalues, respectively. Since \mathbf{M} is real, positive definite and symmetric, \mathcal{M} will be a Hermitian matrix which is also positive definite. It can be decomposed using an SVD decomposition. In addition, since for the diagonal entries we have real values, it can also be decomposed using Cholesky factorization. Therefore, \mathcal{M} is decomposed into $\mathbf{F}^H \mathbf{F}$ where either \mathbf{F} is the result of the Cholesky decomposition or Schur decomposition or it is

$$\mathbf{F} = \Sigma^{1/2} \mathbf{U}^H \quad (3.146)$$

where

$$\mathcal{M} = \mathbf{U} \Sigma \mathbf{U}^H \quad (3.147)$$

is the SVD decomposition of \mathcal{M} . Finally, $G(t)$ can be evaluated as

$$G(t) = \|\mathbf{F} \exp(t\mathbf{\Lambda}) \mathbf{F}^{-1}\|_2^2 \quad (3.148)$$

where

$$\exp(-i\mathbf{\Lambda}t) = \begin{pmatrix} \exp(t\lambda_1) & & \\ & \ddots & \\ & & \exp(-i\lambda_{N_e}t) \end{pmatrix} \quad (3.149)$$

and λ 's are sorted as discussed before.

Chapter 4

Numerical Approach

In this chapter, the numerical approaches for solving eigenvalue problems, integration and other approximations are described.

4.1 Discretization Setup

Since the the spatial dimensions are scaled by d^* , the dimensionless wall normal coordinate equals 1 at the interface. A uniform mesh in the spatial coordinates is used for the problem. In other words, the step size in the wall normal direction (y) is constant in both regions.

The domain for the first fluid (close to the wall) is from index 0 to $ny1$ and for the the second fluid is from $ny1 + 1$ to $ny + 1$. Clearly, the index $ny1$ and $ny1 + 1$ should have the same altitude.

The vector of solution is defined to contain the values of velocity and vorticity for different values of y from 0 to the interface, the interface component and finally from interface to $y = y_{max}$, i.e,

$$\mathbf{q} = (v^{(0)}, \eta^{(0)}, \dots, v^{(ny1)}, \eta^{(ny1)}, \xi, v^{(ny1+1)}, \eta^{(ny1+1)}, \dots, v^{(ny+1)}, \eta^{(ny+1)})^{tr} \quad (4.1)$$

The matrices \mathbf{A} and \mathbf{B} therefore contain the governing equations 3.33-3.35 for all the rows except for those corresponding to $v^{(0)}, \eta^{(0)}, v^{(1)}, v^{(ny1)}, \eta^{(ny1)}, v^{(ny1+1)}, \eta^{(ny1+1)}, v^{(ny)}, v^{(ny+1)}, \eta^{(ny+1)}$ and ξ . The latter contains the kinematic boundary condition 3.44 and the rest include the 12 boundary conditions discussed in chapter 3.

Thus we can say $\mathbf{q} \in \mathbb{C}^N$ and $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{N \times N}$ where \mathbf{q} any solution vector and $N = 2 * ny + 5$.

Concerning the fact that for the discretization of 3.74 a second order backward approximation needs a 5-point stencil, we need to have at least 5 points available for velocity before the interface. This means the minimum number possible for $ny1$ is 4.

Also, we need to have a domain which is large enough so that the assumption of asymptotic convergence is valid. In order to achieve this, we took a domain which the region for the second fluid is at least 100 times bigger than that of the fluid close to the wall.

4.2 Finite difference schemes

In order to solve the eigenvalue problem 3.92 or to integrate the equation 3.89 with a given initial condition, we need to discretize the differential operators. In this work all the approximations are of second order, which means terms with third order or higher have been neglected.

For the case where the first derivative or third derivative of a quantity has to be taken, which happens close to wall or interface only, a backward or forward difference scheme is used depending on the situation. In order to get an approximation of second order for these derivatives we use the identities

$$f'_i = \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h}, \quad (4.2)$$

$$f'_i = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}, \quad (4.3)$$

for backward and forward first derivative, respectively, and

$$f'''_i = \frac{5f_i - 18f_{i-1} + 24f_{i-2} - 14f_{i-3} + 3f_{i-4}}{2h^3}, \quad (4.4)$$

$$f'''_i = \frac{-3f_{i+4} + 14f_{i+3} - 24f_{i+2} + 18f_{i+1} - 5f_i}{2h^3}, \quad (4.5)$$

for the third derivative backward and forward, respectively.

We use the second derivative of quantities both on walls and in the interior of our domain. Therefore, we need backward, forward and center schemes for the second derivative which are

$$f''_i = \frac{2f_i - 5f_{i-1} + 4f_{i-2} - f_{i-3}}{h^2}, \quad (4.6)$$

$$f''_i = \frac{-f_{i+3} + 4f_{i+2} - 5f_{i+1} + 2f_i}{h^2}, \quad (4.7)$$

$$f''_i = \frac{f_{i+1} - f_i + f_{i-1}}{h^2}. \quad (4.8)$$

Finally, we need the approximation for the fourth derivative which is used in the interior of the domain, i.e, we need a center difference scheme to approximate the fourth derivative which is

$$f_i^{(IV)} = \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{h^4}. \quad (4.9)$$

When we integrate over the time, a center difference scheme is used to maintain the second order accuracy for time as well. This scheme is around $j + \frac{1}{2}$ and clearly all the terms should be expanded and approximated accordingly.

$$\dot{f}_j = \frac{f_{j+1} - f_j}{2(\frac{k}{2})} \quad (4.10)$$

4.3 Eigenvalue Problem

A generalized eigenvalue problem (GEP) for a pair of matrices (\mathbf{B}, \mathbf{A}) is a scalar lambda or a ratio $\beta/\alpha = \lambda$, such that $\mathbf{B} - \lambda * \mathbf{A}$ is singular. It is usually represented as the pair (β, α) , as there is a reasonable interpretation for $\alpha = 0$, and even for both being zero.

The right generalized eigenvector $\mathbf{v}(j)$ corresponding to the generalized eigenvalue $\lambda(j)$ of (\mathbf{B}, \mathbf{A}) satisfies

$$\mathbf{B}\mathbf{v}(j) = \lambda(j)\mathbf{A}\mathbf{v}(j). \quad (4.11)$$

The left generalized eigenvector $\mathbf{u}(j)$ corresponding to the generalized eigenvalues $\lambda(j)$ of (\mathbf{B}, \mathbf{A}) satisfies

$$\mathbf{u}(j)^H \mathbf{B} = \lambda(j)\mathbf{u}(j)^H \mathbf{A}. \quad (4.12)$$

In our problem, in order to find the spectrum of the GEP and thus determine the stability of the system based on the eigenvalues, we use the built-in function “zggeev” from the linear algebra package (LAPACK [14]). The mentioned function returns the set of α 's and β 's and in case commanded, it will return the right and left eigenvectors for non-symmetric matrices \mathbf{A} and \mathbf{B} .

4.4 Reduction of the System

Using the boundary conditions on the wall, interface and infinity one can exclude a few points to reduce the degree of the freedom as well to remove the zeros of the eigenvalues of the system. These equalities which can be driven using the identities for boundary

conditions, are as follows:

$$v_0 = 0, \quad (4.13)$$

$$\eta_0 = 0, \quad (4.14)$$

$$v_1 = v_2/4, \quad (4.15)$$

$$\eta_{ny1+1} = \frac{1}{3+3m} [m(4\eta_{ny1+2} - \eta_{ny1+3}) + 4\eta_{ny1-1} - \eta_{ny1-2} + 3c_9 - 2hc_8], \quad (4.16)$$

$$\eta_{ny1} = \frac{1}{3+3m} [m(4\eta_{ny1+2} - \eta_{ny1+3}) + 4\eta_{ny1-1} - \eta_{ny1-2} + 3c_9 - 2hc_8] - c_9, \quad (4.17)$$

$$v_{ny} = \frac{1}{4}v_{ny-1} [1 + 4e^{-\lambda h}] - \frac{1}{4}v_{ny-2}e^{-\lambda h}, \quad (4.18)$$

$$v_{ny+1} = \frac{1}{4}v_{ny-1}e^{-\lambda h} [1 + 4e^{-\lambda h}] - \frac{1}{4}e^{-2\lambda h}v_{ny-2}, \quad (4.19)$$

$$\eta_{ny+1} = e^{-\lambda h}\eta_{ny}. \quad (4.20)$$

4.5 Decompositions

There are two possibilities to decompose the matrix \mathcal{M} into \mathbf{F} and \mathbf{F}^H as discussed in the previous chapter. The first method is to use SVD decomposition for which an eigendecomposition of the matrix $\mathcal{M}\mathcal{M}^H$ is used. The product is a Hermitian positive definite matrix and therefore has real positive eigenvalues. The eigenvalues and eigenvectors were computed using the subroutine “zgeev” from [14]. Once the matrix of eigenvectors are formed they can be considered as the left matrix for SVD and conjugate transposed of the same matrix is the right matrix. The singular values are the square roots of the eigenvalues of $\mathcal{M}\mathcal{M}^H$.

Another method, which gives practically the same result in our case, is to use the subroutine “zpotrf” from [14] to directly decompose \mathcal{M} into its Cholesky factors. Both of the methods discussed have an error of order 10^{-16} or less when the order of matrices are up to 100.

Chapter 5

Results

5.1 Comparison to Previous Studies

When the spectrum of the (\mathbf{A}, \mathbf{B}) is calculated, the stability of the system is determined by the sign of the imaginary part of the eigenvalue with maximum imaginary part. If a system is stable, then all the imaginary parts are negative, otherwise in our problem, there is only one eigenvalue that has an imaginary part above zero and the rest are negative. It should be noted that due to the nature of our problem and singularity of matrix \mathbf{A} there are eigenvalues that are $\frac{\beta}{\alpha}$ where $\alpha = 0$. We do not consider these eigenvalues in our study.

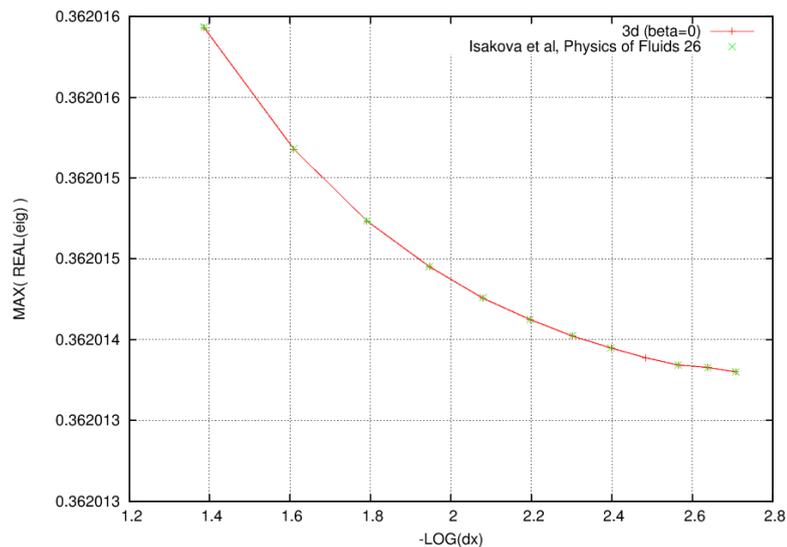


FIGURE 5.1: Convergence of the real part of the dominant eigenvalue

Isakova et. al ([7], [4]) have studied the stability of such a system with a 2-D approach. In our problem, although the equations are derived for 3-D case, putting the

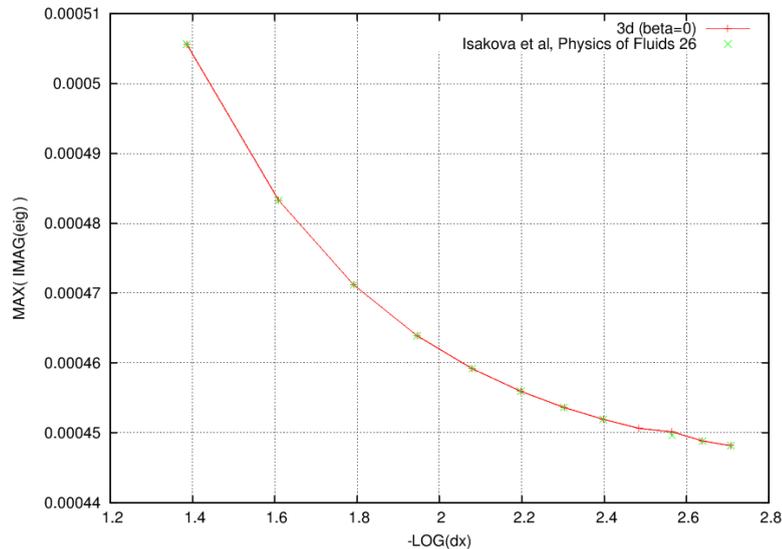


FIGURE 5.2: Convergence of the imaginary part of the dominant eigenvalue

spanwise wave number $\beta = 0$, the physical problem will be the same as the one considered as in [7]. Therefore, one may expect to get the same stability status provided that all the physical parameters and the discretization setup are the same. Figures 5.1 and 5.2 show these results by comparing the real part and the imaginary part of the dominant eigenvalue, respectively. The dominant eigenvalue or the least stable eigenvalue or the most unstable eigenvalue is referred to the one which has the highest imaginary part. The mentioned figures also show the convergence of this eigenvalue under the increase of the resolution of the space. As seen from the figures, the real part change is less than 0.001% and the change of imaginary part after when the $-\log(dx)$ goes above 1.8 is less than 4%. Therefore, it seems that a resolution of this order (equivalent to 600 nodes) is enough for the rest of the calculations.

5.2 Integration in Time and Convergence

Given an initial condition we need to have a solver for system 3.89, i.e., to integrate 3.89 in time. Due to the fact that \mathbf{A} is singular, a forward scheme cannot be used for integration. Therefore a backward and a trapezoidal scheme is used. The result of the convergence of the growth rate with respect to time resolution for a stable base flow is provided in figure 5.3.

It is also interesting to see the convergence of the norm of the solution when the energy norm is used. Figure 5.4 shows such convergence for a specific unstable case when the initial condition is a perturbed eigenvector.

Transient growth of a solution can go to an order of 10^3 . Figure 5.5 shows an example of transient growth in log scale for the given values. As shown in the figure, the system

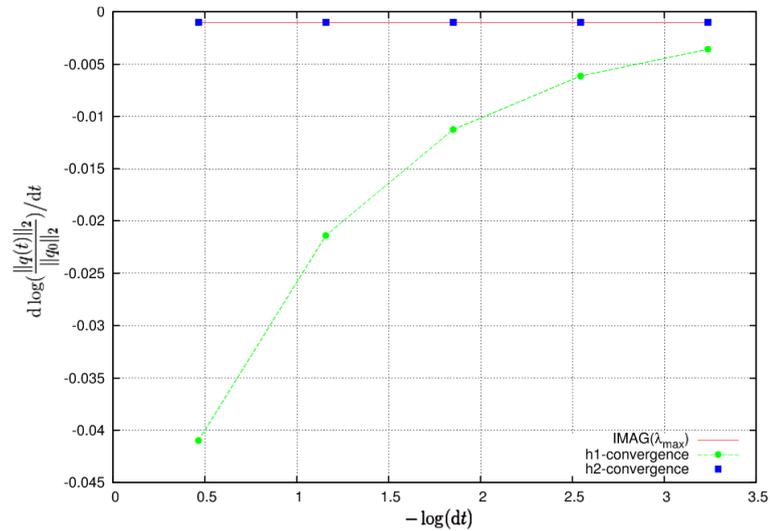


FIGURE 5.3: Convergence of (the l_2 norm of) the solution towards the dominant eigenvalue using Euler (h1) and Crank-Nicholson (h2) scheme (stable base flow)

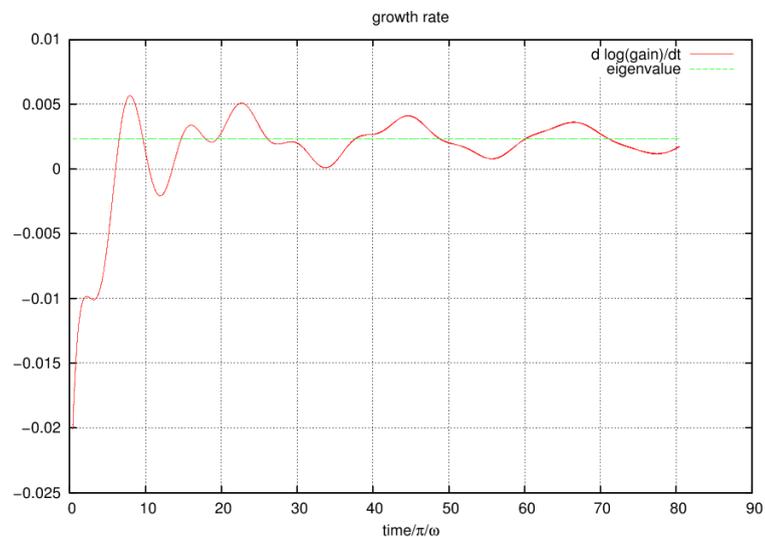


FIGURE 5.4: Convergence of (the energy norm of) the solution towards the dominant eigenvalue using Crank-Nicholson scheme (unstable base flow)

is linearly stable and given enough time it will decay but the interesting thing is that before starting to decrease the solution has a peak which is much larger than that of the initial condition.

Given the hypothesis that emulsion is triggered in an unstable system due to growth of perturbations, one can say that for an stable system that is non-normal enough the same phenomena can be valid.

Finally, figure 5.6 shows how the increase of the viscosity ratio can damp the system and so reduce the transient energy. This, in fact, complements the result from the linear modal stability analysis. The modal analysis performed on the same problem ([7]) tells

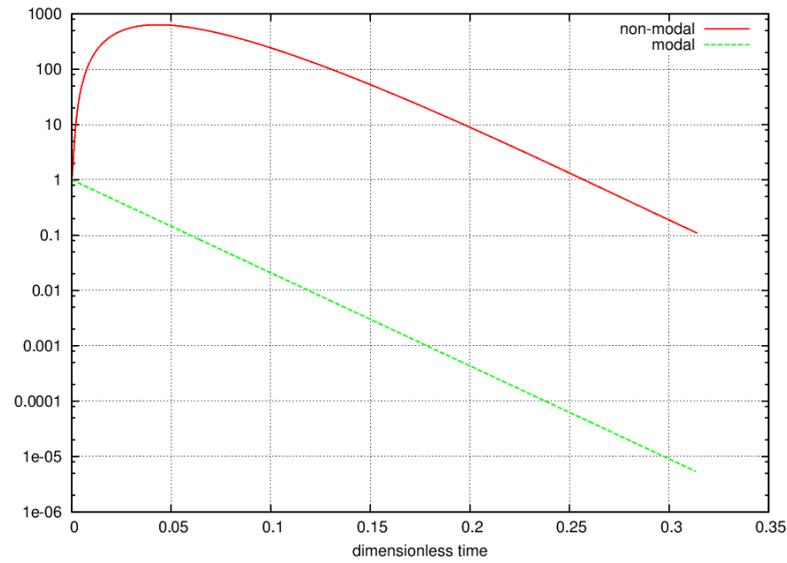


FIGURE 5.5: Growth rate of a solution in time for modal and non-modal approaches for values of $m = 1$, $Re = 7$, $S = 14$, $\gamma = 1$, $\alpha = 70$, $L_\beta = 60$

us that the increase of the viscosity ratio increases the minimum unstable wave-length and therefore we can say the system is going toward stability. Our result, on the other hand, shows that the non-normality decreases for the increase of this parameter and given a viscosity ratio high enough we get a completely damped system.

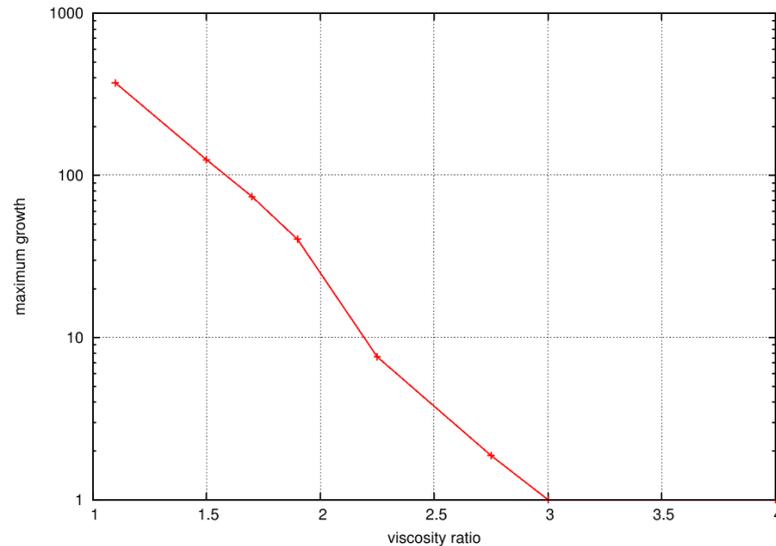


FIGURE 5.6: Maximum growth rate with for the increase of viscosity ratio for values of $Re = 7$, $S = 14$, $\gamma = 1$, $\alpha = 70$, $L_\beta = 60$

Chapter 6

Conclusions and Future Works

In this work the stability of two immiscible fluids set in motion by a flat wall oscillation has been studied. As the continuation of [7], this model can be considered as another step in studying problems related to the employment of silicone oils in order to treat retinal detachments, since the instability of the oil-aqueous interface might lead to the generation of oil bubbles and, eventually, to emulsion.

The quasi-steady approach was used due to the fact that the scaled frequency of oscillation is sufficiently small. Together with this approach the non-modal linear stability theory was applied. With this technique, we studied the evolution in time of small perturbations of the interface. It is observed that for stable systems, although they have exponential decay for long times, they can be amplified up to an order of 1000 before actually they start decaying. This can be a complement to the result from the modal linear stability analysis of the same problem from [7].

For values of the controlling parameters that are realistic for the physical problem and are reported in [7] for stable systems, we found that the maximum growth decays as the viscosity ratio increases. This means that the non-normality of the systems tends to have less effect for larger values of viscosity ratio. Whether instability will actually manifest itself in the real case of the human eye depends on a number of factors that need to be considered in future work. However, this work demonstrates that formation of oil droplets in the eye potentially can be caused by an instability process or by the transient growth of the stable system induced by eye rotations and can be explained on purely mechanical grounds.

It is possible to see the effect of wave length both in the span-wise and stream-wise direction to have a more realistic conclusion of the effect of surface tension and viscosity

ratio on the stability and orthogonality of the system. Also there are several other possibilities to extend this work to make it closer to the real case:

- More realistic geometry, which can be studied including effect of wall curvature and gravity;
- Inclusion of the effect of wall roughness. If the layer of the fluid is very thin then the presence of ripples on the wall might affect greatly stability conditions;
- Use of the Floquet theory. This analysis might be applied to study the stability of periodic solutions when the quasi-steady approach is not valid;
- Numerical simulations of the fully non-linear equations.

Appendix A

Codes

In this appendix a brief outlook of the code is provided.

Main Program

```
! Written by Masoud Ghaderi Zefreh
! #####
! #####

! calling the required libraries from CPL language

! Definition of variables

! find the index of interface
Find_Interface()

! define dimensionless wall coordinates
Spatial_Coordinates()

! define time distribution
Time_Distribution()

! Calculate the coefficients for finite difference approximation
SetDerivatives

! Calculation of the base flow
BaseFlow(tin,Re,mval,omega,gamma)

! Constructing (the matrices of) the system
System(A,B)

! Constructing the matrices for calculation of the energy
EnergyMats(M1,M2,M_q1,M_q2,G)

! reducing the matrices
```

```
Trim(A,A_TRIM)
Trim(B,B_TRIM)

! calculation of the spectrum of the system
rt=Glob()

! performing a non_modal stability analysis including:
! optimizing over all initial conditions
! and
! calculation of the growth rate with the norms:
! L2
! and
! energy norm
NonModal_L2()
NonModal_Energy()

! sort the eigenvalues with respect to the imaginary part
SORT(imgLambda,indices)

! constructing the matrix Mmn (based on eigenvectors)
MakeMmn()

! performing an SVD decomposition on matrix Mmn
SVD(Mmn,lMat,sMat)

! Calculation of the matrix F
MakeF()

! Calculating the gain of the matrix
Gain()

! Calculation of the errors e.g. SVD decomposition, etc.
Errors()
```

Some of the subroutines (e.g. calculation of spectrum of the system) are taken from [4]. The subroutines for calculation of the SVD and Cholesky decomposition are taken from [14].

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