UNIVERSIDADE DE SÃO PAULO
ESCOLA POLITÉCNICA

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**Computational study in fluid mechanics of bio-inspired geometries:
constricted channel and paediatric ventricular assist device**

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**Computational study in fluid mechanics of bio-inspired geometries:
constricted channel and paediatric ventricular assist device**

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To my mother

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This paragraph was the last I wrote in this thesis, because I did not know how to begin it. However, nothing of what is written here is more important to me than the gratitude and admiration I have for this person. I know that probably you will never read these words, but without your support my dreams would never come true. I dedicate this thesis to my mother.

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ABSTRACT

Numerical modelling and simulation are powerful tools for analysis and design, and with the improvement of computational power and numerical methods they are being applied on complex phenomena and systems. This work shows examples of the application of a very sophisticated numerical method, namely the Spectral/hp element method, in the study of the flow inside bio-inspired complex geometries. The two topics investigated are fluid dynamic instabilities in a constricted channel and flow inside a paediatric ventricular assist device were studied by means of computational fluid mechanics. The constricted channel is an idealized model of a nasal cavity, which is characterized by complex airway channels, and also bears some resemblance to a human artery in the presence of an atherosclerotic plaques. The paediatric ventricular assist device is an actual device, designed by the Bioengineering research group of the Heart Institute of the Medicine School of the University of São Paulo, which works as a pump that assists the left ventricle of patients waiting for transplantation. Therefore, the aim of this thesis is to contribute in the understanding of biological and bio-inspired geometries flows, using computational tools.

Linear and nonlinear stability were carried out for the constricted channel. Three different flow regimes were investigated: symmetric steady flow, which is stable for low Reynolds number, asymmetric steady flow, which rises as a result of the primary bifurcation of the symmetric flow and pulsatile flow. Direct stability analysis was carried out to determine the unstable regions and the critical values for each flow regime. The physical mechanisms behind the transition processes were studied by means of direct numerical simulations to characterize the bifurcations. Since the bifurcations had subcritical behaviour, the relevance of non-normal growth in these flows was assessed. Dependence on phase, Reynolds number and spanwise wavenumber of optimal modes were extensively investigated in stable regions of the three flow regimes. Convective instabilities were also studied in order to comprehend the physical mechanisms which led the optimal modes to their maxima growth, and different convective mechanisms were found.

The flow inside the paediatric ventricular assist device was analyzed by means of three-dimensional numerical simulations. A computational model based on special boundaries conditions was developed to model the pulsatile flow. In this model, the opening and closure of the mitral valve and diaphragm were represented with the use of specially devised boundary

conditions. The driving force and the flow direction of the diaphragm were defined by velocity distribution on the diaphragm wall, and the opening and closure of the mitral valve were performed by a velocity waveform which goes to zero in the systolic period. Flow patterns, velocity fields and time-average wall shear rate were analyzed to evaluate the performance of the device.

Keywords: *Paediatric ventricular assist device, bifurcation, instability, channel flow*

RESUMO

Modelagem e simulação numéricas são ferramentas poderosas para análise e design, e com a melhoria do poder computacional e dos métodos numéricos, eles estão sendo aplicados em fenômenos e sistemas complexos. Este trabalho mostra exemplos de aplicações de um método numérico sofisticado, o método dos elementos espectrais/*hp*, no estudo do escoamento dentro de geometrias complexas bio-inspiradas. Os dois tópicos investigados são: instabilidades em dinâmica de fluido em um canal constrito e o escoamento dentro de um dispositivo de assistência ventricular pediátrica. O canal constrito é um modelo idealizado de uma cavidade nasal, que é caracterizada por canais complexos da via aérea, e também tem semelhança com uma artéria humana na presença de placas ateroscleróticas. O dispositivo de assistência ventricular pediátrica é um dispositivo real, projetado pelo grupo de pesquisa de Bioengenharia do Instituto do Coração da Faculdade de Medicina da Universidade de São Paulo, que funciona como uma bomba que auxilia o ventrículo esquerdo dos pacientes à espera de transplante. Portanto, o objetivo desta tese é contribuir na compreensão de escoamentos em geometrias biológicas e bio-inspiradas, usando ferramentas computacionais.

Análises de estabilidade linear e não linear foram feitas para um canal constrito. Três diferentes regimes de escoamento foram empregados: escoamento estacionário simétrico, que é estável para baixo número de Reynolds, escoamento assimétrico, o qual é resultado da primeira bifurcação do escoamento simétrico e escoamento pulsátil. Análise de estabilidade direta foi executada para determinar as regiões instáveis em cada regime de escoamento. Os mecanismos físicos por trás do processo de transição foram estudados por meio de simulação numérica direta para caracterizar as bifurcações. Uma vez que, as bifurcações tiveram um comportamento subcrítico, a relevância do crescimento não normal nestes escoamentos foi avaliado. Assim, dependência com a fase, número de Reynolds e número de onda do modo tridimensional foram extensivamente investigados em regiões estáveis para os três regimes de escoamento. Instabilidades convectivas foram também estudadas a fim de compreender os mecanismos físicos que conduzem os modos ótimos para seus crescimentos máximos, e diferentes mecanismos convectivos foram encontrados.

O escoamento dentro do dispositivo de assistência ventricular pediátrico foi analisado por meios de simulações numéricas tridimensionais. Um modelo computacional baseado em

condições de contorno especiais foi desenvolvido para modelar o escoamento pulsátil. Neste modelo, a abertura e fechamento da válvula mitral e diafragma foram representados com o uso de condições de contorno especialmente elaboradas. A força motora e o direcionamento do fluxo do diafragma foram definidos por uma distribuição de velocidades na parede do diafragma, e a abertura e fechamento da válvula mitral foram executadas por uma função de onda de velocidade que vai a zero no período sistólico. Padrões do escoamento, campos de velocidade e tensão de cisalhamento no tempo foram analisadas para avaliar o desempenho do dispositivo.

Palavras-chave: *Dispositivo de assistência ventricular pediátrico, bifurcação, instabilidade, escoamento em canal*

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LIST OF ABBREVIATIONS

VAD	Ventricular assist device
ECMO	Extracorporeal membrane oxygenation
PVAD	Pediatric ventricular assist device
InCor	Heart Institute (<i>Instituto do Coração</i>)
CFD	Computational fluid dynamics
DNS	Direct numerical simulation
WSS	Wall shear stress
WSR	Wall shear rate
TAWSR	Time-average wall shear rate
ECG	Electrocardiogram
Penn State	Pennsylvania State University
LDV	Laser Doppler Velocimetry
PIV	Particle image velocimetry

LIST OF SYMBOLS

Ω	Domain
Ω^e	Element e
Ω^{st}	Standard element
$\mathbb{L}$	Differential problem
R	Residual
N_{dof}	Number of degrees of freedom
N_{el}	Number of elements
u	Continuos physical spance function
u^δ	Discretization of u
u_0	Solution selected to satisfy the initial and boundary condition
Φ	Trial or expansion function
$\hat{u}_j$	Unknown coefficients to Φ_j
v_i	Test or weight function
$\hat{\mathbf{u}}_j$	Vector with the coefficients $\hat{u}_j$
P	Polynomials order
ϕ_p	Local expansion modes
$\mathbf{x}$	Vector with the global cartesian coordinates
ξ	Local cartesian coordinate
$\alpha_q, \beta_q, \gamma_0$	Weights for mixed explicit-implicit integration
J_i, J_e	Orders of integration
Δt	Time step
$\mathbf{N}$	Advection operator
Re	Reynolds number
St	Strouhal number

$\mathbf{U}$	Base flow
p	Static pressure
t	Time
$\mathbf{u}$	Velocity vector
D	Channel width
s	Relative occlusion
L	Stenosis length
α	Womersley number
U_{red}	Reduced velocity
$\bar{u}_m$	time average flow velocity
$\bar{u}$	time-dependent inlet
T	Pulse period
U_∞	uniform inlet velocity
$u_{osc}(t)$	oscillatory velocity term
E_k	Kinetic energy in the spanwise Fourier mode k
σ	Complex growth rate
μ	Eigenvalue (Floquet multiplier)
τ	Time interval
G	Energy growth
β	Spanwise wavenumber
SV	Stroke volume
N	Beat rate
H	Ratio of the diastolic time to cycle time
$\mathbf{u}_{wall}$	Vector of the velocity distribution on the diaphragm wall
$u_{diaphragm}$	Diaphragm velocity
u_{inlet}	Inlet velocity imposed on the mitral port
R_d	Radius of the region of the diaphragm that is allowed to move

ν	Blood kinematic viscosity [cm ² /s]
ρ	Blood density [kg/m ³]
D_i	Diameter of the mitral port [cm]

1 INTRODUCTION

Numerical modelling and simulation are powerful tools for analysis and design. The main advantages of this approach, when compared to physical experiments, are: lower cost, greater flexibility and access to virtually all variables of the problem. Maybe the main challenge in computational modelling is to obtain a model that represents the physical system with enough accuracy and reasonable cost. Once an adequate model is obtained, many opportunities in analysis and design are open, such as sensitivity analysis, optimisation, control system design, and so on. One of the fields of the physical sciences that has seen a great development in computational modelling and simulation in the last decades is fluid mechanics, despite its inherent complexity. Nowadays, it is very common to see computational fluid dynamics being employed in design and analysis, both in industry and academia. With the current expansion of available computational power and development of new numerical methods and computational techniques, we expect to see numerical modelling being applied to systems of increasing complexity in the near future.

Fluid systems are ubiquitous in nature and engineering systems. In particular, all biological systems make great use of fluid flows in their physiology. Consequently, there are numerous examples of medical equipment that deal with fluid flow, e.g. respiratory and circulatory assistive devices. So there is an obvious opportunity of applying numerical simulation to understand biological systems or as a design tool for medical equipment, notwithstanding the complex interaction these flow systems have with other biological aspects, like cell behaviour, genetics, coupling with external systems, to cite a few. So the application of computational fluid dynamics in biological systems is an active field of research, and it has been contributing significantly to the advancement of life and medical sciences. This thesis intends to give a contribution towards this goal, applying computational techniques to analyze the stability of flows through stenotic geometries and investigate the flow behaviour inside a paediatric ventricular assist device.

Biological flow stability in stenotic geometries has extensively been studied in idealized models of human arterial flows due to its association with diseases in the arterial system

such as atherosclerosis. The distribution of atherosclerotic plaques in the arterial walls has been related to variation in blood flow characteristics (BERGER; JOU, 2000). The low and oscillatory wall shear stress theory are broadly accepted as explanations for the initiation and development of atherosclerosis (CARO; FITZ-GERALD; SCHROTER, 1971; KU, 1997). However, a systematic review by Peiffer, Sherwin & Weinberg (2013) indicated that the low/oscillatory shear theory are not supported by literature in some cases. Furthermore, recent studies show that multidirectional flow plays a key role for the understanding of atherogenesis (PEIFFER; SHERWIN; WEINBERG, 2013; MOHAMIED et al., 2014). Another interesting physiologic flow occurs in the nasal cavity, which is characterized by complex airway channels. The fluid mechanical properties in the human nasal airways are related to the physiological functions of the nasal breathing, being strongly influenced by the geometry of the flow passage. So the study of the fluid mechanical properties are fundamental to comprehend the physiologic and pathologic aspects (DOORLY; TAYLOR; SCHROTER, 2008; KIM et al., 2013).

Another important contribution of computational analysis in biological flow is the support in the development and evaluation of ventricular assist devices (VADs). VADs are mechanical circulatory support systems for treatment of end-stage heart failure. They can be used as a bridge to transplant, bridge to recovery or destination therapy (HETZER; STILLER, 2006; PAULIKS; UNDAR, 2008). Among the equipments and devices available for children, extracorporeal membrane oxygenation (ECMO) and centrifugal pump circuits have been the most widely used alternatives, particularly in small infants. These systems are preferred for support after cardiac operations and for use in patients who have concomitant respiratory failure, but are suitable for short-term application only and intensive care is obligatory. VADs qualify for long-term application and allow patients full mobilization, leading to a practically normal life. This device has a wide acceptance for temporary or long-term application, being used as a continuous support in adults for more than five years. These characteristics are extremely important for patients awaiting heart transplantation, especially in case of children, because of the difficulty of finding a compatible donor (HETZER; STILLER, 2006). However, patients who use VAD still suffer from an unacceptable rate of survival, although the treatment with VAD has obtained better results compared to medicines (BLUESTEIN; CHANDRAN; MANNING, 2010). Despite the wide acceptance of VADs in adults, their use in children still bring problems caused by the low pumping frequency that should be used to ensure adequate blood flow, resulting in high thromboembolic risk (ISHINO et al., 1997; FERRARA et al., 2010).

Bearing that in mind, computational studies are of extreme importance, because experiments are restricted to a few selected regions of interest in this kind of devices. Components such as the valves do not allow optical access around them, which is a great problem because

they play a major role in the flow field inside the VADs (HOCHAREON et al., 2004; DEUTSCH et al., 2006). The use of blood analog fluids also brings difficulties to optical access due to the need to adjust the refractive index of the analog fluid with the solid material of the chamber, which has surfaces that are normally curved, further hindering the optical access (LONG et al., 2005). In addition, important quantities like wall shear stress (WSS) become a great challenge to measure in vitro. So in vitro experiments are restricted to certain regions while in vivo data provide a minimal visualization of the flow field within the device. Thus, Computational Fluid Dynamics (CFD) is a powerful tool to visualize the three-dimensional flow field and WSS distribution on the VADs surface. Nevertheless, the development of a physical model that properly represent the flow nature with high fidelity is a process extremely delicate (AVRAHAMI; ROSENFELD; EINAV, 2006; AVRAHAMI et al., 2006; MEDVITZ et al., 2007; MEDVITZ et al., 2009). In VADs, modeling of the diaphragm, closure valves and flow transition is required. In addition, validated methodologies are essential to establish the accuracy of the model. Therefore, the development and improvement of a numerical method is of fundamental importance for optimizing a VAD.

1.1 Project aims

In this scenario, the motivation of the present thesis relies on the study of fluid mechanics in biological and bio-inspired geometries, employing computational modelling and simulation. The analyses presented in here can contribute to the understanding of the relationship between the fluid mechanics of such systems and the physiological behaviour observed in living systems.

In the recent decades, stability analysis has been emerged as an alternative way to investigate idealized models of biological flows, so that flow transition is one of the common themes studied at relevant Reynolds numbers for human physiologic flows as cited above. In addition, different stability methods have been used in an effort to understand the mechanisms of transition and turbulence in this systems. Amongst the methods applied, normal and non-normal stability analysis are the most common methods. In addition, DNS can be employed to fill the gap between hydrodynamic stabilities and a real flow and help to elucidate the convective mechanisms. Therefore, based on this idea steady and pulsatile flows were studied in a straight channel with a smooth constriction with 50% occlusion. Although in some parts an extensive theoretical approach is presented in the stability study, the geometry was thought as a idealized model of a nasal airway channel, and also bears some resemblance to a human artery in the presence of an atherosclerotic plaques.

As a direct application in biological flow, a computational study of the flow inside a

paediatric ventricular assist device (PVAD) was performed, in order to contribute to the development of the PVAD of the Heart Institute University of Sao Paulo Medical School Hospital (InCor) for patients under 25 kg of body weight. Thus, for a better comprehension of the blood flow within the device, a computational model was developed based on special boundary conditions, so that it was possible to analyze the flow field and draw hypothesis with respect to the relation between the fluid mechanics and thrombus formation and deposition on its surface and occurrence of hemolysis.

1.2 Overview of the study

The numerical simulations were performed using the Spectral/*hp* Element Method. High-order finite element method are sometimes seen as “dark arts” due to the difficulty of implementation, although there is loads of benefits associate to a very low numerical error and high geometric flexibility. However, Nektar++ spectral/*hp* element framework is a software designed to provide a modern development environment for these methods. Therefore, the choice of this method is justified because of the wide application in stability problems, in which a high accuracy of the base flow calculations is required. The method has been successfully used in modelling of biological flows (SHERWIN et al., 2000; VICENT et al., 2011; PEIFFER et al., 2012). For a summary of functionality one can see for example Cantwell et al. (2015), or for further details on the method itself, the reference book by Karniadakis & Sherwin (2005).

The main pre- and post-processing techniques employed for the CFD analysis were: the Gmsh (GEUZAINÉ; REMACLE, 2009) to generate the meshes in the pre-processing stage and the VisIt for the post-processing of the data. These two softwares for pre- and post-processing are open-source and were used to study stability analysis and the PVAD.

For the stability analysis, the linearized form of the Navier-Stokes equations were utilized in the methodology. The behaviour of infinitesimal perturbations were analyzed for different base flows, so that we could settle the global stability, or instability, of it. Direct numerical simulations were also performed in order to understand the physical mechanisms behind each flow regime investigated and then characterize their bifurcation. In addition, transient growth analyses were carried out so as to comprehend the convective mechanisms which lead the optimal modes to their maxima, as well as what is the effect of the optimal modes in a nonlinear analysis. A straight channel with a smooth constriction of %50 occlusion was chosen to be the geometry, in which the stability study was conducted, because this geometry produces a great separated flow after the constriction, which are normally associated with strong shear layers and

convective instabilities.

Concerning the computational simulations of the PVAD, we propose a model to simulate the diaphragm and mitral valve based on special boundary conditions. In other words, the driving force and the flow direction of the diaphragm are defined by velocity distribution on the diaphragm wall, and the opening and closure of the mitral valve are modelled by means of a velocity waveform.

1.3 Scope and structure of the thesis

The structure of the thesis is as follows. In chapter 2 the methodology used for the numerical simulations, linear and nonlinear stability analyses for the steady and time-periodic flows are presented. We then proceed with the fundamentals of the numerical method employed to perform the computational simulations in chapter 3. In chapter 4, the main works concerning the stability analysis on biological flows are delineated and the constricted channel geometry is described. Chapters 5 and 6 bring the results concerning the stability analyses for the constricted channel. A brief literature review regarding the main topics related to the InCor PVAD, as well as a discussion about the physiology and pathologies in the circulatory system which are indispensable for understanding the problems that reside in the development of the PVAD are presented in chapter 7. Chapter 8 shows the computational simulations carried out to study the flow inside a pneumatic PVAD under development, using a method developed which is based on special boundary conditions. Finally, in chapter 9, we draw the main conclusions of this thesis.

2 THEORETICAL FUNDAMENTALS

In this chapter, we present the equations that govern the fluid flow in the cases investigated in this thesis. We also present the mathematics of the stability and nonlinear analyses performed for the constricted channel.

The analysis is composed by four distinct parts, all of them based on the Spectral/hp discretization outlined in chapter 3. First, two-dimensional simulations of the incompressible Navier-Stokes equations are performed, in order to obtain the base flows for which the stability analyses are carried out. Afterwards, linear stability analysis of the two-dimensional base flows with respect to two- and three-dimensional perturbations are carried out. The results were used to determine the critical Reynolds number, as well as the parameter space for which the flow is linearly stable. The third part consists of computing the optimal growth for two- and three-dimensional perturbations in linearly stable conditions of the base flow. The maximum energy growth are obtained for different Reynolds numbers and spanwise wavenumbers. Beside this, the convective mechanisms which led to the local maximum growth are investigated. Finally, nonlinear numerical simulations are performed to characterize the bifurcation, in addition, nonlinear effects of optimal initial perturbations which have huge energy amplification are also investigated.

Below we delineate the basics of the stability and nonlinear theory to study hydrodynamic stability. Base flow calculations are delineated in §2.1. After that, in §2.2, the normal and non-normal stability theory is presented. Finally, in §2.3, the fully three-dimensional simulations is described, in order to evaluate the nonlinear effects and behaviour of small perturbations and transition mechanisms.

2.1 Two-dimensional base flow calculation

In this thesis, the fluid motion is governed by the incompressible Navier-Stokes equations, written in non-dimensional form using the channel width D as the reference length, the fluid density

ρ as the reference density and the mean velocity $\bar{u}_m$ as the reference speed:

$$\partial_t \mathbf{u} = -(\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla p + Re^{-1} \nabla^2 \mathbf{u}, \text{ with } \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, \quad (2.1)$$

where ∂_t denote a partial derivative with respect to time t , $\mathbf{u}(\mathbf{x}, t) = (u, v)(x, y, t)$ is the velocity vector, $p(\mathbf{x}, t)$ is the pressure field, Re is the Reynolds number and Ω is the flow domain. Note that the gravity was considered neglected, and fluid density was fixed at unity without any loss of generality.

In order to calculate the two-dimensional base flows, boundary conditions were imposed on (2.1) as follows. Dirichlet boundary conditions were imposed at the inflow boundary, at the solid walls we imposed no-slip condition and Neumann conditions were specified at the outflow boundary. The boundary conditions are summarized below

$$\mathbf{u}(\mathbf{x}, t) = \bar{u}(t) \hat{\mathbf{x}} \quad \text{for } \mathbf{x} \in \partial\Omega_i, \quad (2.2a)$$

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{0} \quad \text{for } \mathbf{x} \in \partial\Omega_w, \quad (2.2b)$$

$$\partial_x \mathbf{u}(\mathbf{x}, t) = \mathbf{0}, \quad p(\mathbf{x}, t) = 0 \quad \text{for } \mathbf{x} \in \partial\Omega_o, \quad (2.2c)$$

where Ω_i is the inflow boundary, Ω_w is the solid walls and Ω_o is the outflow boundary and $\bar{u}(t) = U_\infty + u_{osc}(t)$. The component U_∞ is a uniform inlet velocity, which was set to unity. The component $u_{osc}(t)$ is an oscillatory term, which is zero for the steady cases (symmetric and asymmetric flows), however this oscillatory term will only be discussed later in §6.1. Furthermore, for the symmetric flow, a free-slip condition was imposed at the centreline of the channel, in other words, the tangential velocity derivative normal to the centerline was set to zero, so as to ensure that the flow is symmetrically ejected from the throat. At the inflow and centreline boundaries and walls we imposed a high-order pressure boundary condition as described in Karniadakis, Israeli & Orszag (1991).

In the next subsection, an overview of the mathematical formulation and computational implementation of the normal and non-normal stability analyses are presented.

2.2 Normal and non-normal stability analysis

We considered two-dimensional base flows $\mathbf{U}(x, y, t)$ and investigated their stability with respect to an infinitesimal three-dimensional perturbations $\mathbf{u}'(x, y, z, t)$. The evolution of the infinitesimal perturbation in a spatial domain Ω is governed by the linearized Navier-Stokes

equations:

$$\partial_t \mathbf{u}' = -(\mathbf{U} \cdot \nabla) \mathbf{u}' - (\mathbf{u}' \cdot \nabla) \mathbf{U} - \nabla p' + Re^{-1} \nabla^2 \mathbf{u}', \text{ with } \nabla \cdot \mathbf{u}' = 0 \text{ in } \Omega, \quad (2.3)$$

where $p'(x, y, z, t)$ is the pressure perturbation.

If we consider a system that is homogeneous in the spanwise direction z , the perturbed velocity field can be decomposed into noninteracting modes, considering a Fourier modal expansion in z ,

$$\mathbf{u}'(x, y, z, t) = \hat{\mathbf{u}}(x, y, t) e^{i\beta z} + c.c. \quad (2.4)$$

and similarly for p' , where the spanwise wavenumber is $\beta = 2\pi/L_z$ (L_z is the spanwise wavelength of the instability). Since equation (2.3) is linear, modes with different β do not couple. Moreover, because the base flow z -velocity component is zero, perturbations are of the form

$$\mathbf{u}'(x, y, z, t) = (\hat{u} \cos \beta z, \hat{v} \cos \beta z, \hat{w} \sin \beta z), \quad (2.5)$$

$$p'(x, y, z, t) = \hat{p} \cos \beta z. \quad (2.6)$$

In addition, the linearized equations can be defined as an operator $\mathcal{A}(\tau)$ to describe the action of (2.3) on an initial perturbation $\mathbf{u}'(t=0)$ over a time interval τ such that $\mathbf{u}'(\tau) = \mathcal{A}(\tau) \mathbf{u}'(0)$.

2.2.1 Linear asymptotic stability analysis

To determine the asymptotic stability of the base flow $\mathbf{U}$, we need to solve the eigensystem of this forward evolution operator $\mathcal{A}(\tau)$. If $\mathbf{U}$ is steady, we can use any fixed arbitrary time T , however it must obey the Nyquist criterion. On the other hand, when U is T -periodic then we set $\tau = T$ and consider this as a temporal Floquet problem. The solution of the linear system (2.3) can be decomposed as a sum of eigenmodes $\mathbf{u}'(\mathbf{x}, t) = \sum_j \exp(\sigma_j t) \tilde{\mathbf{u}}_j + c.c.$, where σ_j is the complex growth rate of the eigenfunction $\tilde{\mathbf{u}}_j$. The stability is governed by the leading eigenmodes of the eigenproblem

$$\mathcal{A}(\tau) \tilde{\mathbf{u}}_j = \mu_j \tilde{\mathbf{u}}_j, \quad \mu_j \equiv \exp(\sigma_j \tau), \quad (2.7)$$

where μ_j is called a Floquet multiplier of the forward operator $\mathcal{A}(\tau)$ and σ_j the eigenvalues of largest real part of the system (2.3). A mode is linearly unstable if the real part of the growth rate, σ_j , is positive, which corresponds to $|\mu_j| > 1$. On the other hand, a mode is linearly stable when the real part of σ_j is negative, which corresponds to $|\mu_j| < 1$. In the steady case, the eigenmodes of $\mathcal{A}(\tau)$ and those of (2.3) are the same, however, for the T -periodic case, the

eigenmodes of $A(\tau)$ are the T -periodic Floquet modes $\mathbf{u}_j(\mathbf{x}, t + T) = \mathbf{u}_j(\mathbf{x}, t)$ evaluated at a specific temporal phase.

For normal stability analysis, the velocity boundary conditions that were imposed on this system are $\mathbf{u}' = \mathbf{0}$ on boundaries where Dirichlet conditions are specified for the base flow, and $\partial \mathbf{u}' / \partial \mathbf{n} = \mathbf{0}$ on boundaries where Neumann conditions are specified for the base flow. Further details on the algorithms for the stability calculations are given in Carmo et al. (2008).

2.2.2 Optimal transient growth

Transient growth analysis can predict the largest possible growth in energy for a specific system governed by a linear differential equation. Thus, the idea behind this method is to search for an initial condition, $\mathbf{u}'(0)$, which will give us the largest growth. The formalism is as follows. The transient growth is defined with respect to the energy norm of the perturbation. If the norm of the initial perturbation is $\|\mathbf{u}'(0)\| = \langle \mathbf{u}'(0), \mathbf{u}'(0) \rangle = 1$, where $\langle \cdot, \cdot \rangle$ denotes the standard L_2 inner product, then the energy of the perturbation after time τ , normalized with the initial energy is

$$\frac{E(\tau)}{E(0)} = \langle \mathbf{u}'(\tau), \mathbf{u}'(\tau) \rangle = \langle \mathcal{A}(\tau) \mathbf{u}'(0), \mathcal{A}(\tau) \mathbf{u}'(0) \rangle = \langle \mathbf{u}'(0), \mathcal{A}^*(\tau) \mathcal{A}(\tau) \mathbf{u}'(0) \rangle, \quad (2.8)$$

where E is the kinetic energy per unit mass of a perturbation and the operator $\mathcal{A}^*$ is the adjoint of the forward operator $\mathcal{A}$. The action of $\mathcal{A}^*$ is obtained by integrating the adjoint linearized Navier-Stokes equations

$$\partial_t \mathbf{u}^* = -(\mathbf{U} \cdot \nabla) \mathbf{u}^* - (\nabla \mathbf{U})^T \cdot \mathbf{u}^* - \nabla p^* + Re^{-1} \nabla^2 \mathbf{u}^*, \text{ with } \nabla \cdot \mathbf{u}^* = 0 \text{ in } \Omega, \quad (2.9)$$

backwards over the time interval τ . Thus, to compute the optimal growth of the perturbation, we need to act the symmetric operator $\mathcal{A}^*(\tau) \mathcal{A}(\tau)$ on $\mathbf{u}'$. Therefore, the optimal growth is obtained from the leading eigenmodes of

$$\mathcal{A}^* \mathcal{A}(\tau) \mathbf{v}_j = \lambda_j \mathbf{v}_j, \quad (2.10)$$

where λ_j and $\mathbf{v}_j$ are the eigenvalues and eigenmodes of $\mathcal{A}^*(\tau) \mathcal{A}(\tau)$, respectively, with $\|\mathbf{v}\| = 1$. The eigenvalues are non-negative and we assume ordering $\lambda_1 \geq \lambda_2 \geq \dots$. Thus, the optimal energy growth, $G(\tau)$, obtained at time τ is

$$G(\tau) = \max_{\|\mathbf{u}'(0)\|=1} \frac{E(\tau)}{E(0)} = \max_j \lambda_j = \lambda_1. \quad (2.11)$$

The boundary conditions for computing the eigenvalues of $\mathcal{A}^*(\tau) \mathcal{A}(\tau)$ were homogeneous Dirichlet, i.e., $\mathbf{u}' = \mathbf{0}$, on boundaries where Dirichlet and Neumann conditions are specified for

the base flow, for both the operator $\mathcal{A}(\tau)$ and $\mathcal{A}^*(\tau)$. Although, this kind of boundary condition is not rigorously correct for the outflow boundary, we have extended the channel long enough to ensure that the influence of that was negligible. Further details on the transient growth analysis can be seen in Blackburn, Barkley & Sherwin (2008), Cantwell, Barkley & Blackburn (2010).

In order to investigate the Re - and β -dependence on the maximum energy growth for two- and three-dimensional flows, two important quantities are defined as follows

$$G_{\beta}^{max}(Re) = \max_{\tau} G(\tau, Re, \beta) \quad (2.12)$$

and

$$\tau_{\beta}^{max}(Re) = \arg \max_{\tau} G(\tau, Re, \beta). \quad (2.13)$$

G_{β}^{max} is the maximum possible energy growth at a given Reynolds number and spanwise wavenumber over all time horizons and τ_{β}^{max} is the time in which it occurs.

A more detailed description of the time-stepper approach used here may be found in Tuckerman & Barkley (2000), Barkley, Blackburn & Sherwin (2008).

2.3 Nonlinear analysis

Knowing that the linear stability analysis can evaluate the onset of instabilities, variables such as the critical Reynolds number, wavelength and unstable mode topology can be determined. However, the understanding of instability mechanisms that play a key role after the onset of the transitions are beyond the scope of this theory. Thus, fully three-dimensional simulations are performed, in order to take the nonlinear effects into account, which can guide us to comprehend the instability mechanisms and classify the bifurcations. Besides that, optimal initial perturbations from transient growth, which have huge energy amplification in hysteretic regions can lead the initial disturbance to nonlinear saturation. If it happens, a bypass transition could occur for Reynolds numbers lower than the critical, so that the nonlinear three-dimensional calculations allowed us assess it. Therefore, the nonlinear analysis will highlight the main features of the bifurcations and nonlinear effects of steady flows in the constricted channel.

3 NUMERICAL METHODS

The fluid motion is governed by the continuity equation and Navier-Stokes equations, which can be reduced to equations (2.1), as previously mention in §1.2. However, to properly define the system, boundary conditions are necessary to establish the problem on $\partial\Omega$ and an initial condition at $t = 0$ must be given. Since in general no analytic solution is available, numerical techniques are normally employed to approximate the solution $(\mathbf{u}, p)$ in the computational domain Ω . Thus, in this chapter, the basics of the Spectral/*hp* Element Method is introduced, which is the numerical method used to solve the problems outlined in this thesis, so that the general concepts and the *hp* discretization will be discussed. Again, it is worth noting that the Spectral/*hp* Method was used to study hydrodynamic stability and the blood flow through the PVAD.

Further details about this method are given in the following sections. First, in §3.1, the main ideas on which the spectral/*hp* method is based are explained. Afterwards, in §3.2, a discussion about the weighted residuals method followed by a description of the Galerkin formulation are presented. In §3.3, the domain discretization and the different types of expansion bases are delineated. In §3.4, we will describe how to advance the discrete version of the equations that govern the flow in time. Finally, in §3.5, the kinetic energy calculations are described in the direct numerical simulations.

3.1 General concepts

The Spectral/*hp* Method is a discretization scheme whose basic ideas derive from the Finite Element Method and from the classic Spectral Method. The *h*-type discretization, where *h* represents the characteristic size of the elements, brings geometric flexibility, especially in complex flows with high dimensions, as generally is found in biological flows. In this method, the convergence is achieved by subdividing the computational domain into subdomains Ω^e (elements), in other words, reducing the size of the elements with a fixed-order polynomial. On the other hand, the *p*-type discretization, where *p* refers to the order of the expansion, is commonly

employed in a fixed mesh and the convergence is achieved by increasing the order of the polynomial, which results in an exponential convergence. The Spectra/hp method combines attributes from both the h -type and p -type extensions, which allows a combination of both approaches. Therefore, it is specially suitable for problems that involve complex geometry and require a high level of accuracy.

3.2 The weighted residuals framework and the Galerkin formulation

Considering a set of partial differential equations in a spatial domain Ω . This system is solved when an approximate solution satisfies a finite number of conditions, moreover the choice of the conditions that are to be satisfied will define the numerical method. This framework can be described considering a linear differential equation in a domain Ω denoted by

$$\mathbb{L}(u) = 0, \quad (3.1)$$

subject to appropriate initial and boundary conditions, where u represents a component of $\mathbf{u}$ or p . The spectral/hp element method looks for a solution of the form

$$u^\delta(\mathbf{x}, t) = u_0(\mathbf{x}, t) + \sum_{j=1}^{N_{\text{dof}}} \hat{u}_j(t) \Phi_j(\mathbf{x}), \quad (3.2)$$

where $\mathbf{x}$ denotes the spatial position, $\Phi_j(\mathbf{x})$ are analytic functions called the *expansion* (or *trial*) *functions*, $\hat{u}_j(t)$ are the N_{dof} unknown coefficients, and $u_0(\mathbf{x}, t)$ is selected to satisfy the initial and essential boundary conditions. The functions $\Phi_j(\mathbf{x})$ should satisfy homogeneous boundary conditions, i.e. they should be zero on Dirichlet boundaries, since essentially the boundary conditions of the problem are already satisfied by $u_0(\mathbf{x}, t)$. Substituting the approximation (3.2) into (3.1) produces a residual R :

$$\mathbb{L}(u^\delta) = R(u^\delta). \quad (3.3)$$

According to the method of weighted residuals, the following restriction is enforced on R in order to determine $\hat{u}_j(t)$, so (3.3) is reduced to a system of ordinary differential equations in $\hat{u}_j(t)$. If the original equation (3.1) is independent of time then the coefficients $\hat{u}_j$ can be determined directly from the solution of a system of algebraic equations.

$$\langle v(\mathbf{x}), R \rangle = 0 \quad \text{for } j = 1, 2, \dots, N_{\text{dof}}, \quad (3.4)$$

where the functions $v(\mathbf{x})$ are the *test* (or *weight*) *function* and the inner product $\langle f, g \rangle$ over a domain Ω is defined as

$$\langle f, g \rangle = \int_{\Omega} f(\mathbf{x})g(\mathbf{x})d\mathbf{x}. \quad (3.5)$$

Assuming that (3.4) is true for any $v(\mathbf{x})$, the approximation u^δ is exact. So it is possible to relax the requirement by choosing $v(\mathbf{x})$ to be expressed by an arbitrary linear combination of a finite set of known functions, that is,

$$v(\mathbf{x}) = \sum_{i=1}^{N_{\text{dof}}} a_i v_i(\mathbf{x}), \quad (3.6)$$

where $v_i(\mathbf{x})$ are known functions and the coefficients a_i are arbitrary. Substituting (3.6) and (3.3) into (3.4) and using the definition (3.5) leads to

$$\int_{\Omega} \sum_{i=1}^{N_{\text{dof}}} a_i v_i(\mathbf{x}) \mathbb{L}(u^\delta) d\mathbf{x} = 0. \quad (3.7)$$

Assuming that $\mathbb{L}$ is independent of time and substituting (3.2) into (3.7), we obtain

$$\begin{aligned} \int_{\Omega} \sum_{i=1}^{N_{\text{dof}}} a_i v_i(\mathbf{x}) \mathbb{L} \left[u_0(\mathbf{x}) + \sum_{j=1}^{N_{\text{dof}}} \hat{u}_j \Phi_j(\mathbf{x}) \right] d\mathbf{x} = \\ \sum_{i=1}^{N_{\text{dof}}} a_i \left\{ \int_{\Omega} v_i(\mathbf{x}) \mathbb{L}[u_0(\mathbf{x})] d\mathbf{x} + \int_{\Omega} v_i(\mathbf{x}) \mathbb{L} \left[\sum_{j=1}^{N_{\text{dof}}} \hat{u}_j \Phi_j(\mathbf{x}) \right] d\mathbf{x} \right\} = 0, \end{aligned}$$

so we are left with

$$\int_{\Omega} v_i(\mathbf{x}) \mathbb{L}[u_0(\mathbf{x})] d\mathbf{x} + \int_{\Omega} v_i(\mathbf{x}) \mathbb{L} \left[\sum_{j=1}^{N_{\text{dof}}} \hat{u}_j \Phi_j(\mathbf{x}) \right] d\mathbf{x} = 0 \quad \text{for } j = 1, 2, \dots, N_{\text{dof}}.$$

Once a_i is arbitrary, a set of algebraic equations is established which is sufficient to determine $\hat{u}_j$:

$$\sum_{j=1}^{N_{\text{dof}}} \left\{ \hat{u}_j \int_{\Omega} v_i(\mathbf{x}) \mathbb{L}[\Phi_j(\mathbf{x})] d\mathbf{x} \right\} = - \int_{\Omega} v_i(\mathbf{x}) \mathbb{L}[u_0(\mathbf{x})] d\mathbf{x}, \quad i = 1, 2, \dots, N_{\text{dof}}.$$

This set of equations can be written in matrix form

$$\mathbf{A} \hat{\mathbf{u}} = \mathbf{b}, \quad (3.8)$$

where $\hat{\mathbf{u}}$ is the vector with the coefficients $\hat{u}_j$, the components of the matrix $\mathbf{A}$ are given by

$$A_{ij} = \int_{\Omega} v_i(\mathbf{x}) \mathbb{L}[\Phi_j(\mathbf{x})] d\mathbf{x},$$

and the components of the vector $\mathbf{b}$ are

$$b_i = - \int_{\Omega} v_i(\mathbf{x}) \mathbb{L}[u_0(\mathbf{x})] d\mathbf{x}.$$

Within the framework of weighted residuals, as previously mentioned, the choice of the expansion functions $\Phi_i(\mathbf{x})$ and test functions $v_j(\mathbf{x})$ is what defines the numerical scheme. The Spectral/*hp* Element Method employs the Galerkin formulation, in which the set of test functions is the same as the set of expansion functions, i.e., $v_j(\mathbf{x}) = \Phi_j(\mathbf{x})$.

3.3 *hp* discretization

As mentioned previously, the computational domain of interest Ω is subdivided into N_{el} non-overlapping elements Ω^e for h-type discretization. Within these elements the solution is approximated using a polynomial expansion. In a one-dimensional discretization, the global expansion basis $\Phi_j(x)$ is constructed from a combination of local expansion modes $\phi_p^e(\xi)$ defined within each element, so that the equation (3.2) becomes

$$u^\delta(\mathbf{x}, t) = u_0(\mathbf{x}, t) + \sum_{j=1}^{N_{dof}} \hat{u}_j(t) \Phi_j(\mathbf{x}) = u_0(\mathbf{x}, t) + \sum_{e=1}^{N_{el}} \sum_{p=0}^P \hat{u}_p^e(t) \phi_p^e(\xi), \quad (3.9)$$

where P is the polynomial order of the expansion and ξ is the one-dimensional coordinate, which is defined in the standard region as follow $\Omega^{st} = \{-1 \leq \xi \leq 1\}$.

The local expansion bases can be classified as nodal and modal, however the choice of the local expansion is crucial for the efficiency and strongly influence the numerical implementation of the method. The modal bases, which were used in this thesis, are hierarchical in nature, so that a higher order modal basis can be constructed from lower basis modes. On the other hand, when nodal bases are employed, the approximate solution is evaluated at a fixed set of points. In addition, the continuous Galerkin method requires that the solution u^δ is C^0 continuous across the elements. For further details about the *hp* discretization the reader is referred to (KARNIADAKIS; SHERWIN, 2005).

3.4 Temporal discretization

The solution of the set of equations (2.1) in time can be obtained using a stiffly stable time splitting scheme (KARNIADAKIS; ISRAELI; ORSZAG, 1991), which each time-step is subdivided into three substeps, and the solution of the discretized Navier-Stokes equation is advanced from

Table 3.1: Stiffly-stable splitting scheme coefficients. Extracted from Karniadakis, Israeli & Orszag (1991).

Coefficient	1st order	2nd order	3rd order
γ_0	1	$3/2$	$11/6$
α_0	1	2	3
α_1	0	$-1/2$	$-3/2$
α_2	0	0	$1/3$
β_0	1	2	3
β_1	0	-1	-3
β_2	0	0	1

n to $n + 1$ as follows

$$\frac{\tilde{\mathbf{u}} - \sum_{q=0}^{J_i-1} \alpha_q \mathbf{u}^{n-q}}{\Delta t} = \sum_{q=0}^{J_e-1} \beta_q \mathbf{N}(\mathbf{u}^{n-q}) \quad \text{in } \Omega \quad (3.10)$$

$$\nabla^2 \bar{p}^{n+1} = \nabla \cdot \left(\frac{\tilde{\mathbf{u}}}{\Delta t} \right) \quad \text{in } \Omega \quad (3.11)$$

$$\frac{\gamma_0 \mathbf{u}^{n+1} - \tilde{\mathbf{u}}}{\Delta t} + \nabla \bar{p}^{n+1} = \frac{1}{Re} \nabla^2 \mathbf{u}^{n+1} \quad \text{in } \Omega, \quad (3.12)$$

where $\mathbf{N} = \mathbf{u} \cdot \nabla \mathbf{u}$ denotes the advection operator, which is treated explicitly due to its non-linear nature, J_i is the integration order for the implicit terms and J_e is the integration order for the explicit terms. Since the advection term is treated explicitly, Δt needs to satisfy a Courant–Friedrichs–Lewy (CFL) condition to guarantee the stability of the time scheme. The values of coefficients γ_0 , α_q and β_q for integration order up to three are given in table 3.1. This scheme requires that the boundary conditions are defined both for velocity and pressure, so that High-order Neumann boundary conditions for pressure are imposed on (3.11) as follows

$$\frac{\partial \bar{p}^{n+1}}{\partial n} = \mathbf{n} \cdot \left\{ \sum_{q=0}^{J_e-1} \beta_q \left[\mathbf{N}(\mathbf{u}^{n-q}) - \frac{1}{Re} (\nabla \times (\nabla \times \mathbf{u}^{n-q})) \right] \right\} \quad \text{on } \partial\Omega \quad (3.13)$$

For further details concerning the high-order pressure boundary condition the reader is referred to Karniadakis, Israeli & Orszag (1991) and for a matrix formulation of the problem to Karniadakis & Sherwin (2005).

3.5 Direct numerical simulation

For the nonlinear calculations we used the same approach as outlined in section 2.1. However, a Fourier expansion was applied in the discretization in the spanwise direction (KARNIADAKIS,

1990) of the two-dimensional base flow and the simulations were carried out with 4 or 8 Fourier modes (8 or 16 planes of data in the spanwise direction).

In order to evaluate the evolution of small perturbations of unstable modes or optimal initial perturbations as discussed above, the dimensionless amount of flow kinetic energy in each spanwise Fourier mode k is

$$E_k = \frac{1}{2A\bar{u}_m^2} \int_A \hat{\mathbf{u}}_{\mathbf{k}} \cdot \hat{\mathbf{u}}_{\mathbf{k}}^* dA, \quad (3.14)$$

where $\hat{\mathbf{u}}_{\mathbf{k}}^*$ is the complex conjugate of the velocity data in the k th Fourier mode and A is the two-dimensional cross-section of the domain being considered.

4 CONSTRICTED CHANNEL

Transition mechanisms have been extensively investigated in non-parallel flows with the goal of understanding fundamental concepts related to separated flow, absolute and convective instabilities (BARKLEY; GOMES; HENDERSON, 2002; BLACKBURN; BARKLEY; SHERWIN, 2008; CANTWELL; BARKLEY; BLACKBURN, 2010). Although a great effort has been made to comprehend instability mechanisms of some classical confined geometries, researchers still struggle to explain the origins of their instabilities (RANI; SHEU, 2006). Some of these confined geometries included contractions and expansions because they produce large shear layers with separated flow which are normally prone to strong instabilities (PITT; SHERWIN; THEOFILIS, 2004; SHERWIN; BLACKBURN, 2005; GRIFFITH et al., 2007; BLACKBURN; SHERWIN; BARKLEY, 2008). In addition, these simple geometries also have practical importance in biological flows as idealized models of human arterial flows in the presence of atherosclerotic plaque (PITT; SHERWIN; THEOFILIS, 2004; SHERWIN; BLACKBURN, 2005; MAO; SHERWIN; BLACKBURN, 2009) and in flow control (CHUN; SUNG, 1996). Bearing it in mind, a constricted channel was chosen as a bio-inspired geometry.

The chapter is organized as follow. In §4.1, a literature review is presented concerning stability studies on biological flows, then, in §4.2 the main parameters related to the constricted channel flow are presented.

4.1 Stability studies on biological flows

Important stability studies on biological flows can be found in the literature. Pitt, Sherwin & Theofilis (2004) performed biglobal stability analysis in a channel with a smooth constriction with 60% occlusion. Critical Reynolds numbers and spanwise wavenumbers of the unstable modes were presented for three different flow regimes, and showed that there is a symmetry breaking of the symmetric steady flow, so that a asymmetric steady flow took place after the primary instability. Barkley, Gomes & Henderson (2002) reported biglobal stability analysis in a backward-facing step with a 1:2 expansion. They found that the primary bifurcation of the two-dimensional steady flow gives rise to a three-dimensional flat roll localized in the first

recirculation region, adjacent to the step wall. A later publication employed nonlinear analysis to demonstrate that this transition occurs by a supercritical Hopf bifurcation (RANI; SHEU, 2006). Three-dimensional stability analysis and direct numerical simulation (DNS) were performed by Sherwin & Blackburn (2005) in an axisymmetric constricted tube with 75% occlusion. Firstly, for the steady flow, the critical Reynolds number was determined from linear stability analysis, being 722. The instability arises in the first azimuthal Fourier mode, so that it is consisted with the symmetry breaking of the jet, featuring a Coanda-type wall attachment due to the deflection of the centreline of the jet. The instability was found to be subcritical by DNS of the three-dimensional base flow for $Re = 750$ and hysteresis was observed as a result of the subcritical regime down to $Re = 688$. At four and ten diameters downstream of the throat there was a turbulent region, which was associated to the long-period oscillation of the jet between axial locations. Afterwards, following the same approach of the steady flow, the pulsatile flows were analyzed. So the pulsatile flows become unstable through a subcritical bifurcation and the primary instability was identified as a period-doubling vortex ring, in addition the vortex ring which were ejected from the throat presented alternating tilting with each pulse. However, the tilting vortex rings quickly breakdown, producing a localized turbulence at four diameters of the stenosis. Griffith et al. (2007) carried out stability analysis in a two-dimensional flow through a partially blocked channel and the mechanism behind the instability was presented. In addition, a numerical and experimental study in a circular tube with axisymmetric blockage of varying size using steady inlet flow was performed by Griffith et al. (2008). As an extension of their last work, Griffith et al. (2009) also undertaken a investigation concerning stability analysis but now for a pulsatile flow.

Transient energy growth is argued to play an important role in steady flows in complex confined geometries due to localized regions of convective instability as observed by Blackburn, Barkley & Sherwin (2008) in a backward-facing step and Cantwell, Barkley & Blackburn (2010) in an axisymmetric pipe with a sudden expansion. Non-normal growth in steady and pulsatile flows were also explored by Blackburn, Sherwin & Barkley (2008) in a stenotic tube, where it was shown that an optimal initial perturbation can produce huge energy amplification. Griffith et al. (2010) compared optimal transient growth with experimental observations for steady flow through an abrupt axisymmetric stenosis. Non-normal growth has also been extensively investigated with respect to the dependence on Reynolds number in the last years in confined (BLACKBURN; BARKLEY; SHERWIN, 2008; BLACKBURN; SHERWIN; BARKLEY, 2008; SMITH; BLACKBURN, 2010; CANTWELL; BARKLEY; BLACKBURN, 2010; SHEARD; BLACKBURN, 2010) and unconfined flows (CANTWELL; BARKLEY, 2010).

An example of a more realistic biological application was performed by Mao, Sherwin

Figure 4.1: Computational domain Ω and geometric parameters which define the constricted channel geometry (not to scale).

& Blackburn (2009), where they give a complete picture of a physiologic pulsatile flow in an stenotic tube. Firstly, modal stability was performed to determine the absolute unstable regions, afterward the non-modal stability was carried out in stable regions close to the primary bifurcation and an explosive optimal growth was found for the least stable mode. Finally, the optimal initial perturbation which gave the greatest optimal growth was introduced in as a initial condition in a DNS, so the non-normal growth mechanisms demonstrates that the flow exhibits bypass transition to turbulence, which could be common in human arterial flows. More recently, Griffith et al. (2013) performed a numerical study of the stenosis eccentricity for a steady flow through axisymmetric and eccentric sinuous stenoses.

4.2 Problem definition

The constricted channel geometry as well as the parameters that define the geometry are shown in figure 4.1. We consider a rigid straight channel with a smooth constriction with 50% occlusion. The channel has width D and throat spacing D_{min} . In our study, the width ratio is $D_{min}/D = 0.5$. The relative occlusion of the channel, which is defined by

$$s = 1 - \frac{D_{min}}{D}, \quad (4.1)$$

is therefore $s = 0.5$. Another important parameter is the stenosis length, L , which is equal to $2D$ in this work. The stenosis shape is based on the work of Sherwin & Blackburn (2005), so that the upper and lower stenosis walls are given by

$$y(x) = \pm 0.5D_{min} \pm 0.5(D - D_{min}) \sin^2\left(\frac{\pi x}{L}\right) \quad (-0.5 \leq (x/L) \leq 0.5), \quad (4.2)$$

where x is the streamwise coordinate measured from the narrowest point of the constriction and y is the perpendicular coordinate measured from the channel centreline.

In an ideal problem the channel domain is infinite, but in practice, the computational

domain Ω has finite inflow length L_i and outflow length L_o , upstream and downstream the throat, respectively. Hence, they were made sufficiently large to allow the results to be independent of these lengths; verification tests are shown in section 5.1. The constricted channel is assumed homogeneous (infinite) in the spanwise direction.

The fluid is considered to be Newtonian and the Reynolds number is defined as

$$Re = \frac{\bar{u}_m D}{\nu} \quad (4.3)$$

where $\bar{u}_m$ is the mean velocity of the fluid in an unconstricted cross section, D is the channel width and ν is fluid's kinematic viscosity.

5 BIFURCATIONS AND CONVECTIVE INSTABILITIES OF STEADY FLOWS

The goal of this chapter is to provide some new insights for the understanding of the bifurcations and convective mechanisms of steady flows in a constricted channel. Since Pitt, Sherwin & Theofilis (2004), there has been no discussion about the nature of the instabilities in constricted channel geometries, although several papers have focused in constricted axisymmetric geometries (GRIFFITH et al., 2008; GRIFFITH et al., 2010) and eccentric constrictions (SAMUELS-SON; TAMMISOLA; JUNIPER, 2015). However, one important difference between prismatic and axisymmetric is that the axisymmetric azimuthal periodicity has an upper limit length. It is noteworthy that Guevel, Boutyour & Cadou (2011) reported the bifurcation diagram of a fully three-dimensional sudden expansion channel flow, so that some similar results are here presented for a constricted channel. However, we extended the analysis to non-normal and nonlinear approaches.

This chapter is organized as follows. In §5.1, details of the parameters used in the simulations are given. After that, in §5.2 and §5.3, the results are presented for the symmetric and asymmetric flows, respectively.

5.1 Numerical approach

Figure 5.1 shows the close up of the computational mesh around the throat used for the present analysis. The refined discretization by quadrilateral elements around the throat was based on the mesh of the work of Sherwin & Blackburn (2005). The computational mesh was composed by 2974 spectral elements, being 2932 quadrilateral and 42 triangular. The inflow and outflow lengths were $30D$ and $75D$ from the throat of the stenosis. A domain this long is necessary to accommodate well the disturbance upstream and downstream during the transient growth and linear stability analysis.

To calculate the base flows, the equations (2.1) were solved in two-dimensions, using a stiffly stable splitting scheme (KARNIADAKIS; ISRAELI; ORSZAG, 1991). Time integration was

Figure 5.1: Close up of the computational mesh around the throat, the dimension is given in terms of channel height D . The mesh has 2974 spectral elements.

N	$G(16)$	% difference
9	2.3681×10^7	-
8	2.3666×10^7	0.06
7	2.3654×10^7	0.11
6	2.3650×10^7	0.13
5	2.3647×10^7	0.14
4	2.3644×10^7	0.16
3	3.2412×10^5	98.63

Table 5.1: Convergence of the two-dimensional optimal growth at $\tau = 16$ for $Re = 720$ with respect to the variation of the spectral element polynomial order N , computed with M_1

Mesh	L_i	L_o	$G(16)$	% difference
M_1	$30D$	$75D$	2.3650×10^7	—
M_2	$30D$	$85D$	2.3650×10^7	0.00
M_3	$35D$	$75D$	2.4095×10^7	-1.88

Table 5.2: Convergence of the two-dimensional optimal growth at $\tau = 16$ for $Re = 720$ with respect to the variation of the inflow and outflow lengths, computed with polynomial order $N = 6$.

carried out using second-order velocity-correction schemes with value of the non-dimensional time step of 0.001 and 0.0005 for the higher polynomial order. For all stability calculations, a Krylov subspace of dimension of 20 was used and in both methods the eigensolution convergence parameter was set to 10^{-5} .

The two-dimensional maximum energy growth for the highest Reynolds number evaluated in this paper occurs around $\tau = 16$ for $Re = 720$. Thus, we used these parameters to analyze the mesh convergence in the most challenging case simulated here. Table 5.1 shows the convergence of the two-dimensional optimal growth with respect to the polynomial order, using the mesh M_1 , which is the mesh adopted in this work (Table 5.2). It can be seen that, even for 4th order polynomials (i.e. 5th order accuracy in space) the convergence is reached with uncertainty less than 0.2%. Therefore, the base flows and the stability analyses for the symmetric and asymmetric flows were computed with $N = 6$. However, the fully three-dimensional simula-

tions of the nonlinear analysis were performed with $N = 5$. Table 5.2 depicts the convergence of the two-dimensional optimal growth with respect to the inflow and outflow lengths, using $N = 6$. It can be seen that there is no change in the optimal growth when the outflow length is varied. However, a longer inflow length is responsible for a small variation in the optimal growth, so that it produced a numerical error which is considered acceptable for the worst case.

5.2 Primary global instability

5.2.1 Base flow characteristics

The two-dimensional base flow features close to the primary instability are shown in figure 5.2, which illustrates vorticity contours, streamlines and velocity profiles for the symmetric flow at $Re = 270$. It can be seen, in figure 5.2(a), that the flow is symmetric when it goes through the throat with flow separation downstream of the narrowest section. After that, it expands and reattaches on the upper and lower walls of the channel. The flow ejected from the throat, which has strong vorticity, establishes two recirculating regions at each side of the channel, and shear layers that extend downstream to nearly $x/D = 2.82$. Figure 5.2(b) shows velocity profiles of the x -velocity along the channel height position for five different locations downstream of the throat. As expected by a constricted channel with 50% occlusion, the maximum x -velocity is higher than $2\bar{u}_m$ close to the throat, easily observed in the profile velocity at $x/D = 1$. The thicker solid line represents the velocity profile at $x/D = 30$ (inflow length) from the throat, so that at this point the flow is fully re-established, with the maximum velocity differing only 0.01% from its asymptotic value of $3/2U_\infty$. Hence, the inflow length is far acceptable for the development of the flow in the channel.

5.2.2 Normal stability analysis

In order to investigate the primary instability and to determine the unstable regions of the symmetric flow, the first step was to carry out a normal stability analysis. Figure 5.3(a) shows the leading eigenvalues, σ , as a function of spanwise wavenumber β for four different Reynolds number. All leading eigenvalues found were real and only one unstable mode was revealed in the Reynolds number range considered. The inset plot in figure 5.3(a) shows the leading eigenvalues, σ , as a function of Reynolds number for $\beta = 0$. The critical Reynolds number for two-dimensional disturbance is 281.2, determined by interpolation with uncertainty of less than 1%. Figure 5.3(b) shows the neutral stability curve for the primary instability in the constricted channel for Reynolds numbers up to 360. Everywhere to the right hand side of the

Figure 5.2: Two-dimensional base flow close to primary instability at $Re = 270$. (a) Vorticity contours and streamlines showing the recirculating regions. (b) Velocity profiles. Reattachment occurs at $x/D = 2.82$.

curve (dark region) the two-dimensional flow is linearly unstable to infinitesimal perturbations, so that the curve which separates the light and dark regions represents the parameter space for which the base flow is neutrally stable. The symmetric flow firstly becomes unstable for a three-dimensional perturbation and the unstable region quickly extends to a wide range of spanwise wavenumbers, however the Reynolds number for which the flow is unstable with respect to a two-dimensional perturbation is only slightly higher. The critical Reynolds number and corresponding spanwise wavenumber are $Re_c = 278.8 \pm 0.1$ and $\beta_c = 0.45 \pm 0.01$. The critical spanwise wavelength is $2\pi/\beta_c = 13.96$ channel widths. Pitt (2005) reported the onset of the primary instability at $Re = 278.5$ for $\beta = 0.45$, which agree with our value. Hence, the simulations parameters and mesh setup were considered to be properly chosen.

Pitt (2005) investigated the stability of the flow inside a 60% constricted channel with critical Reynolds number at $Re = 127.4$ and critical spanwise wavenumber of $\beta = 0.55$. This suggests that the narrower the constriction the lower the Reynolds number required for primary instability. On the other hand, the critical spanwise wavenumber is higher than in the case with 50% occlusion.

Figure 5.3: Linear stability analysis for the primary instability. (a) Plot of the leading eigenvalues, σ , against spanwise wavenumber β for different Reynolds numbers. Inset: the critical Reynolds number for $\beta = 0$ is $Re = 281.2$, determined by interpolation (b) Neutral stability curve for the symmetric steady flow in the constricted channel. In the region on the right hand side of the curve (dark region) the two-dimensional flow is linearly unstable to infinitesimal three-dimensional perturbation. The critical Reynolds number is $Re_c = 278.8$.

5.2.3 Nonlinear characterization of the bifurcation

Having established the critical values of the primary instability, the next step of our analysis consisted of understanding the mechanisms by which the bifurcation occurs, thus fully nonlinear three-dimensional simulations were performed around the primary instability. The simulations were initialized with the nonlinear saturation of the unstable base flow at $Re = 360$ with all Fourier modes saturated, however, when the Reynolds number was lower than 324 the three-dimensional ($\beta > 0$) Fourier modes went to zero, no matter if the base flow was seeded with the most unstable mode from linear stability analysis or with nonlinear saturation of a unstable base flow, although for the latter the three-dimensionalities held for longer times. The two-dimensional ($\beta = 0$) mode, however, presented growth and saturation, modifying the base flow and giving rise to an asymmetric flow field. Figure 5.4(a) shows a diagram that was built with the energy of the two-dimensional component of the Fourier modes ($k = 0$), the solid circles in the diagram mean the energy that was transferred from the base flow to the two-dimensional mode.

In order to investigate further this somewhat unexpected behaviour, additional calculations were carried out. For three-dimensional simulations any perturbation at Reynolds number in the hysteretic region, such as a white noise, no matter how small, was enough to lead the flow from symmetric to asymmetric, breaking the symmetry of the system (Figure 5.4(b)). In other words, any perturbation in the symmetric base flow for Reynolds number higher than 260 rose the initial energy up to the hysteretic curve in the three-dimensional nonlinear simulations.

Figure 5.4: (a) Bifurcation diagram of the symmetric steady flow for $\beta = 0.45$. The diagram was built with the energy of the two-dimensional component of the Fourier modes ($k = 0$). (b) Velocity contours perpendicular to x -direction of the three-dimensional flow at $Re = 270$, when it achieves nonlinear saturation of the two-dimension Fourier mode.

However, it is remarkable that the two-dimensional base flows calculated without the constraint in the centreline of the channel (slip condition) were perfectly symmetric even if they were calculated very close to the critical Reynolds number (approaching from lower Re).

As a final essay to evaluate the transition and verify if it had a fundamental three-dimensional character, although resulting in a two-dimensional flow, two-dimensional simulations at Reynolds numbers in the hysteretic region were initialized with the mode 0 (i.e., spanwise-averaged field) from the three-dimensional unstable base flow at $Re = 360$, which is an asymmetric flow field. It was observed that the asymmetric flow became symmetric with time until it was fully re-established. Seeing that, we concluded that the bifurcation is triggered by a three-dimensional mechanism, and the three-dimensional unstable mode transfers energy to two-dimensional (asymmetric) modes due to nonlinear interactions.

5.2.4 Non-normal stability analysis

From the linear stability analysis, we have established the critical Reynolds number, as well as the region where the flow is linearly unstable to infinitesimal two- and three-dimensional perturbations in the range of Reynolds number considered. Now we turn to the examination of the convective mechanisms and the largest transient energy growth for a given optimal initial perturbation as well as the behaviour of the maximum energy growth with spanwise wavenumber, Reynolds number and time.

An important aspect in this study is that, in most part, there is only a slight difference between the two- and three-dimensional analyses. The first aspect to notice is that the shape of the optimal initial conditions and their evolution in time are almost the same in both cases. In addition, there is a very small range of spanwise wavenumber for which the three-dimensional peak growth is slightly higher than in the two-dimensional case, as reported by Blackburn, Barkley & Sherwin (2008) in a backward-facing step as well. Thereby two distinct approaches were used. First, a two-dimensional study of Reynolds number dependence is described, in other words, time horizon and Reynolds number were allowed to vary, however the spanwise wavenumber is fixed ($\beta = 0$). After that, for the three-dimensional analysis, results are presented for fixed values of Reynolds number, allowing time horizon and spanwise wavenumber to vary.

5.2.4.1 Dependence on Reynolds number

Figure 5.5 summarizes the optimal energy growth for two-dimensional perturbations before the primary instability. Figure 5.5(a) shows the optimal envelopes, $G(\tau)$, as a function of time horizon for Reynolds numbers from 45 up to 270. We recall, just to be clear, that each point in figure 5.5(a) corresponds to the energy growth of the optimal initial condition for a specific time τ . So, the maximum energy growth among all optimal initial perturbations is $G_0^{max}(270) = 2.01 \times 10^2$ at $\tau_0^{max} = 5.77$. It can be seen that all energy growth curves end up with an exponential decrease after the maximum growths, however, there is no growth at $Re = 45$ for any time interval. In addition, the dashed line represents the exponential decrease associated with the leading eigenmode, σ , of the normal analysis, which matches the transient growth exponential decrease at long times.

Optimal growth logarithmic contours in the (τ, Re) plane are shown in figure 5.5(b). The solid and dashed lines represent regions with $G \geq 1$ and $G < 1$, respectively. So, in the lighter regions above the line where $\log G = 0$ the optimal growth is larger than unity. In addi-

Figure 5.5: Dependence on Reynolds number of the two-dimensional transient energy growth before primary instability. (a) Energy growth envelopes, $G(\tau)$, as a function of τ for Reynolds number varying from 45 up to 270. The dashed line represents the exponential decrease associated with the leading eigenmode. (b) Logarithmic contours plot for two-dimensional optimal energy growth, $G(\tau, Re)$, as a function of τ and Re . The critical Reynolds number for the first growth is $Re_E = 49.5$. The dotted-line curve shows the local of maximum energy growth as a function of τ . Variation of maximum (c) growth and (d) time as a function of $Re^{5/4}$. The $\log G_0^{max}$ and τ_0^{max} increase linearly with $Re^{5/4}$. (e) Maximum energy growth as a function of time of maximum growth for the Reynolds number range from Re_E to Re_c . The $\log G_0^{max}$ grows linearly with τ_0^{max} .

tion, the dotted line, in figure 5.5(a,b), shows the local of maximum growth as a function of τ . From these data, an important observation can be made: the critical Reynolds number, Re_E , for which the energy growth first exceeds unity is obtained when $\partial G(\tau, Re_E)/\partial \tau|_{\tau=0} = 0$, in other words, this happens when the line $\log G = 0$ intercept the Re -axis as shown in figure 5.5(b). The critical value for the smallest growth is $Re_E = 49.5$ for two-dimensional perturbations, so that this value is lower than that found in a backward-facing step (BLACKBURN; BARKLEY; SHERWIN, 2008; CANTWELL; BARKLEY; BLACKBURN, 2010). It means that perturbations at Reynolds numbers below Re_E will decrease monotonically. It should be also noted that, in figure 5.5(a), the optimal growth curve at $Re = 90$ has a positive slope at $\tau = 0$; on the other hand, at $Re = 45$ the curve decreases monotonically.

Figure 5.5(c,d) shows the variation of maximum growth and time of maximum growth as a function of $Re^{5/4}$. The open circles represent the critical Reynolds numbers Re_E and Re_c for the two-dimensional analysis as indicated in figure 5.5(c). It is evident that the $\log G_0^{max}$ and τ_0^{max} increase linearly with $Re^{5/4}$. We found the expressions below

$$\log G_0^{max} \simeq 2.42 \times 10^{-3} Re^{5/4} \quad (5.1)$$

and

$$\tau_0^{max} \simeq 5.85 \times 10^{-3} Re^{5/4}. \quad (5.2)$$

These expressions are valid between Re_E and Re_c , in other words, they are acceptable from the Reynolds number for which there is the first smallest growth to the critical Reynolds number of the primary instability. Above Re_c , G_0^{max} diverges because the flow becomes linearly unstable. Notice that the critical values of G_0^{max} and τ_0^{max} were calculated by extrapolation of the equations (5.1) and (5.2), respectively. Thus, the critical maximum growth is $G_0^{max}(Re_c) \approx 2.71 \times 10^2$ and the corresponding critical time of maximum growth is $\tau_0^{max}(Re_c) \approx 6.10$. Similar exponential maximum growths were observed for other separated flows in confined and unconfined geometries, however, they do not obey the dependence with $Re^{5/4}$. A linear dependence with Reynolds number has been found in many studies, being them in a backward-facing step (BLACKBURN; BARKLEY; SHERWIN, 2008), steady flow in a stenotic pipe (BLACKBURN; SHERWIN; BARKLEY, 2008) and in an axisymmetric pipe with a sudden expansion (CANTWELL; BARKLEY; BLACKBURN, 2010). However, Cantwell & Barkley (2010) reported square dependence in a flow past a circular cylinder in the subcritical regime. Even more notable, Sheard & Blackburn (2010) found linear maximum growth for two regions with different power-law dependencies in a steady flow through an axisymmetric aneurysm model, so that the first region had a dependence of $Re^{9/5}$ and the second of $Re^{7/5}$. It is worth noting that the maximum energy growth for the confined flows cited above do not present the same Reynolds dependence

Figure 5.6: Plots of two-dimensional logarithmic contours of energy before primary instability, computed at $Re = 270$. (a) Optimal initial perturbation for $\tau = 6$. (b) Optimal perturbation growth outcome at $\tau = 6$. The vectors represent the velocity field.

as classical planar Couette flow (REDDY; HENNINGSON, 1993) and the Hagen-Poiseuille flow (SCHMID; HENNINGSON, 1994); they both reveal maximum growth dependence with Re^2 .

The $\log G_0^{max}$ is plotted in figure 5.5(e) as a function of τ_0^{max} . As expected from figure 5.5(c,d), $\log G_0^{max}$ grows linearly with τ_0^{max} . From (5.1) and (5.2) we obtain

$$\log G_0^{max} \simeq 0.414\tau_0^{max}. \quad (5.3)$$

We can draw two important conclusions. First, the energy growths for the Reynolds number range from the first smallest growth slightly above of Re_E to the critical value Re_c reach their maxima with the same growth rate. Secondly, it should be noted that, since they have the same growth rate, the optimal initial perturbations travel through the channel and reach the peak growth at different positions downstream from the throat, the farther from the throat the higher the Reynolds number.

In order to comprehend the structure of the perturbation for the most-amplified case at $Re = 270$, figure 5.6 shows the logarithmic contours of energy for $\beta = 0$. Optimal initial perturbation for $\tau = 6$ is shown in figure 5.6(a). Most of the initial disturbance is concentrated at the shear layer in the constriction and around the separated flow, however, there is also a mild energy upstream the constriction. In addition, the perturbation exhibits chevron-shaped contours upstream the constriction as well as in the shear layers, featuring a sinuous disturbance. This sinuous initial disturbance around the shear layer was also observed in others shear flows (BLACKBURN; BARKLEY; SHERWIN, 2008; BLACKBURN; SHERWIN; BARKLEY, 2008; CANTWELL; BARKLEY; BLACKBURN, 2010; GRIFFITH et al., 2010). Figure 5.6(b) shows the optimal perturbation at $\tau = 6$ corresponding to the initial condition shown in figure 5.6(a).

Figure 5.7: Two-dimensional optimal energy growth envelope and time evolution of optimal initial perturbations corresponding to $\tau = 6, 16$ and 40 for $Re = 270$. Solid circles denote the points where each curve of linear growth touches the envelope. The dashed line represents the exponential decrease associated with the leading eigenmode.

The evolution of the optimal perturbation is a wave packet, which becomes a series of spanwise counter-rotating rolls as emphasized by the velocity field vectors. Moreover, the minimal energy is located in the centre of the rollers, being advected downstream following the centre-line of the channel. The evolution of shear layers giving rise to spanwise counter-rotating rolls was also obtained in a backward-facing step (BLACKBURN; BARKLEY; SHERWIN, 2008) and in two-dimensional plane Couette and Poiseuille flows (FARRELL, 1988).

5.2.4.2 Time evolution of two-dimensional optimal initial perturbations

Figure 5.7 shows the two-dimensional optimal energy growth envelope along with three different optimal transient responses at $Re = 270$. It is evident that each curve accurately touches the optimal growth which corresponds to its τ value (solid circles). The transient evolution curves have similar shapes, indicating a similar dynamic development of the optimal initial perturbations, although there is a large difference in the time horizon τ considered. It should be also noted that the curves only have slightly differences compared to the optimal envelope, so that it suggests that the instability mechanism is the same for all these perturbations. Besides, it is noteworthy that in all cases the transient curves, after $t = 25$, decay with the same exponential rate corresponding to the leading eigenmode of the normal analysis, demonstrating that at long times the optimal mode achieves the asymptotic response.

Figure 5.8 shows the vorticity contours of the optimal initial perturbation for $\tau = 6$ and its evolution along the channel, together with the streamlines at $Re = 270$. The initial perturba-

Figure 5.8: Instantaneous vorticity contours for the linear evolution of the two-dimensional optimal initial perturbation corresponding to $\tau = 6$ together with streamlines of the base flow at $Re = 270$.

tion originates in the shear layers. Afterwards, the perturbation goes through the recirculating regions, ending up when both parts of the perturbation, from the upper and lower bubble, meet in a wave packet with the shape of a series of spanwise counter-rotating rolls around $t = 3$. Also, it can be clearly seen that the maximum energy growth occurs downstream of the recirculating zones ($t = 6$). At $t = 10$, this figure reveals that the disturbance is already quite stretched and acquiring a parabolic shape due to the mean strain field, which will continue to stretch the disturbance with the propagation of the wave packet.

5.2.4.3 Dependence on spanwise wavenumber

Now we turn our attention to three-dimensional transient growth analysis. So, at this stage, the perturbations are allowed to vary in the homogeneous direction with an additional parameter $\beta = 2\pi/L_z$, the spanwise wavenumber, for a fixed Reynolds number.

Figure 5.9 summarizes the optimal energy growth for three-dimensional perturbations before the primary instability. Figure 5.9(a) shows the transient growth, $G(\tau, \beta)$, as function of spanwise wavenumber β and time τ . The optimal growths increase in time to their maxima and afterwards the energy of all spanwise wavenumbers decrease monotonically. It can be seen that the energy growths have almost the same energy decrease rates for the spanwise wavenumbers from $\beta = 2$ to $\beta = 3.5$ between $\tau = 20$ and $\tau = 35$. Moreover, the growth envelope for $\beta = 1$ depicts the smaller energy decrease until $\tau = 40$. It should be noted that the growth envelopes have only slightly differences between them, suggesting similar dynamic evolution. The global maximum growth occurs for a spanwise wavenumber of $\beta = 2.116$, so that it gives a maximum energy growth of $G_{\beta}^{max}(270) = 3.14 \times 10^2$ at $\tau_{\beta}^{max} = 6.56$, which is a little bit

Figure 5.9: Dependence on spanwise wavenumber of the three-dimensional transient energy growth before primary instability. (a) Surface plot of energy growth envelopes, $G(\tau, \beta)$, as function of spanwise wavenumber β and time τ at $Re = 270$. (b) Cut of (a) for short times with β from 0 to 9 in steps of 1.

higher than the two-dimensional case. Figure 5.9(b) shows a cut of figure 5.9(a) for short time with β from 0 to 9 in steps of 1. At first glance, it is evident that optimal growth for higher spanwise wavenumbers are favored at short times, nevertheless they rapidly decrease and the smaller spanwise wavenumber are dominant. Blackburn, Sherwin & Barkley (2008), Cantwell, Barkley & Blackburn (2010) reported analogous behaviour for steady flow in a axisymmetric pipes and Abdessemed et al. (2009) also observed this behaviour for external flow.

From these data and similar analyses for $Re = 180$ and $Re = 90$, the maximum energy growth, G_{β}^{max} , and the corresponding time of maximum growth, τ_{β}^{max} , for spanwise wavenumbers from 0 to 9, were obtained and are shown in figure 5.10(a,b). The graph of $\log G_{\beta}^{max}$ against β is plotted in figure 5.10(a). For the three Reynolds numbers evaluated, the

Figure 5.10: Dependence on spanwise wavenumber of the three-dimensional transient energy growth for the symmetric steady flow. Variation of maximum growth (a) and time of maximum growth (b) as functions of β . (c) Maximum energy growth as a function of time of maximum growth. There is a constant growth rate for all β which relate $\log G_\beta^{max}$ and τ_β^{max} at $Re = 270$.

maximum growth increases with β up to a global maximum and afterwards there is a monotonic decrease for the higher spanwise wavenumbers. At $Re = 180$, the local maxima growth, after $\beta = 3.5$, decreases with a linear rate given by $\partial \log G_\beta^{max} / \partial \beta = -0.104$. More notable is that, after $\beta = 5$ all Reynolds numbers decrease with almost the same linear rate with β .

Regarding the figure 5.10(a,b), it is remarkable that there is a strong correlation between the maximum growth and the time of maximum growth. In other words, the larger the growth the longer it takes to reach the maximum growth. In order to understand this behavior, in figure 5.10(c), $\log G_\beta^{max}$ is plotted as a function of τ_β^{max} . It can be clearly seen that there is a constant growth rate for all β at $Re = 270$, so that it is possible to establish a linear relationship between $\log G_\beta^{max}$ and τ_β^{max} as follows

$$\log G_\beta^{max} \simeq 0.222 \tau_\beta^{max}, \quad (5.4)$$

Figure 5.11: Variation of maximum energy growth as a function of $Re^{1/9}$ for Reynolds number of 90, 180 and 270 and spanwise wavenumber of 3 up to 9 in steps of 1. The $\log G_\beta^{max}$ grows linearly with $Re^{1/9}$ for β from 5 to 9.

which is valid for spanwise wavenumbers from 0 up to 9, but based on the data we expected that this expression may be extended to higher spanwise wavenumbers. Therefore, varying the spanwise wavenumber, the optimal initial perturbations reach their maxima with a constant growth rate given by $\partial \log G_\beta^{max} / \partial \tau_\beta^{max} = 0.222$.

However, at lower Reynolds numbers the correlation between the maximum growth and time of maximum growth is weaker, so that the local maxima do not collapse in a line. For the range of spanwise wavenumber analyzed, this exponential growth effect only occurs at higher Reynolds number.

Figure 5.11 depicts the variation of the local maximum growth against $Re^{1/9}$. It is interesting that, for spanwise wavenumbers from 5 to 9, for which a exponential decrease in the local maximum growth is found with respect to β (Figure 5.10(c)), $\log G_\beta^{max}$ varies linearly with $Re^{1/9}$. However, for $\beta < 5$ there is a deviation from the linear growth. Hence, for $\beta \geq 5$ we can define the expression below

$$\log G_\beta^{max} \simeq 4.630 Re^{1/9}. \quad (5.5)$$

Now the local maxima growth can be associated with two different expressions after $\beta = 5$. The first of them, is the expression above. The second of them, is based on the relation $\partial \log G_\beta^{max} / \partial \beta = -0.104$ found in figure 5.10(c).

Having discussed the behaviour of the three-dimensional maximum energy growth

Figure 5.12: Plots of three-dimensional optimal perturbations before primary instability at $Re = 270$. Streamwise velocity iso-surfaces of the optimal initial perturbation (left-hand side). Vorticity iso-surfaces of the optimal perturbation growth outcomes (right-hand side). The pictures at the top show a side view and those at the bottom show a top view.

with Reynolds number, spanwise wavenumber and time, we now consider the structure of the three-dimensional optimal modes at $Re = 270$ as shown in figure 5.12. Streamwise velocity iso-surfaces for the optimal initial perturbations are shown at the left-hand side and vorticity iso-surfaces of the optimal perturbation growth outcomes corresponding to the initial conditions are shown at the right-hand side. The structure of the most-amplified mode for $\beta = 2.116$ and $\tau = 7$ is shown in figure 5.12(a). It is evident that the three-dimensional optimal initial condition is similar to the two-dimensional disturbance structure (figure 5.6(a)). As previously discussed in the two-dimensional case, most of the initial disturbance lies in the shear layers and the initial perturbation shows chevron-shaped contours, featuring a sinuous disturbance. The evolution of the optimal perturbation is also a wave packet. The vorticity iso-surfaces emphasizes the shape of the optimal mode as a series of spanwise counter-rotating rolls. Furthermore, the maximum energy growth occurs downstream the recirculating regions. However, at high β , the optimal initial perturbation has similar shape, however it is weaker, and the optimal mode present their optimal growth at the shear layers (Figure 5.12(b)).

Figure 5.13: Two-dimensional base flow close to secondary instability. Vorticity contours and streamlines, showing the recirculating regions at (a) $Re = 540$ and (b) $Re = 720$. (b) Velocity profiles at $Re = 540$. Reattachments occur at $x/D = 1.82$ and $x/D = 6.04$ for $Re = 540$.

5.3 Secondary global instability

5.3.1 Base flow characteristics

Now we turn our attention to the secondary global instability. The main characteristics of the two-dimensional base flow close to the secondary instability are shown in figure 5.13. In this figure we present the vorticity contours, streamlines and velocity profiles along the streamwise direction of the channel. It is remarkable that, as previously discussed, the base flow is asymmetric when the flow is ejected from the throat (Figure 5.13(a)). The two boundary layers in the constriction separate immediately after the narrowest section and turn upward. The streamlines clearly exhibit the upward deflection of the jet and the recirculating regions of different size in the flow, so that, at $Re = 540$, the reattachments on the channel walls occur at two different points. The first streamline on the top reattaches at $x/D = 1.82$ and the second on the bottom at $x/D = 6.04$. If we increase the Reynolds number a third recirculating region appears at the upper wall as shown in figure 5.13(b). Velocity profiles of the axial velocity as a function of the channel height from the central plane for $x/D = 1, 3, 5, 11$ and 30 at $Re = 540$ are shown in figure 5.13(c). Two aspects are noteworthy about these velocity profiles. The first is

that, when the asymmetric flow is deflected upwards, we can easily see the start of the deviation on y -direction at $x/D = 1$, afterwards it reaches its maximum y -position near $x/D = 3$. The second, which is not evident in the flow visualization, is that the flow deflects downwards, reaching its maximum deviation approximately at $x/D = 7$. After that the flow goes back to the central position and tends to the Poiseuille solution. At $x/D = 30$, as previously mentioned at $Re = 270$, the Poiseuille flow is re-established, however, with a difference of approximately of 1% from its asymptotic value.

5.3.2 Normal stability analysis

Following the same discussion for the primary instability, figure 5.14 shows the normal stability analysis of the two-dimensional base flow after the base flow symmetry breaking. Figure 5.14(a) shows leading eigenvalues against spanwise wavenumber for four different Reynolds numbers. It is possible to identify one unstable mode for this range of Reynolds number, however, a second mode is rising for smaller spanwise wavenumber, being evident at $Re = 720$. It suggests that, for higher Reynolds numbers it will become a second unstable mode. From this plot, we note that the spanwise wavenumber of the most unstable eigenvalues in each Reynolds number is around $\beta = 1.5$. In addition, all leading eigenvalues obtained are real, as previously observed for the primary instability, except for $\beta = 0.5$ at $Re = 720$, which appears to be a discontinuity in the curve. Figure 5.14(b) shows the neutral stability curve for the secondary instability in the constricted channel up to $Re = 720$. The asymmetric flow firstly becomes unstable for a three-dimensional perturbation. The critical Reynolds number and corresponding spanwise wavenumber are $Re_c = 562.0 \pm 0.1$ and $\beta_c = 1.47 \pm 0.01$. The critical spanwise wavelength is $2\pi/\beta_c = 4.27$ channel widths.

The critical Reynolds number and spanwise wavenumber for a 60% constricted channel are approximately 290 and 1.6 for the secondary instability (PITT; SHERWIN; THEOFILIS, 2004), respectively. As previously seen for the primary instability, the critical Reynolds number is lower and the critical spanwise wavenumber is higher than in a 50% constricted channel. These results were also found in a flow through a partially blocked channel (GRIFFITH et al., 2007). Therefore, it suggests that the narrower constriction the lower critical Reynolds number and the higher critical spanwise wavenumber for the transition of the primary and secondary instability.

Figure 5.14: Linear stability analysis for the secondary instability. (a) Plot of the leading eigenvalues, σ , against spanwise wavenumber β for different Reynolds numbers. (b) Neutral stability curve for the asymmetric steady flow in the constricted channel. In the region on the right hand side of the curve (dark region) the two-dimensional flow is unstable to infinitesimal three-dimensional perturbation. The critical Reynolds number is $Re_c = 562.0$.

5.3.3 Nonlinear characterization of the bifurcation

Once we found the neutral stability curve for the asymmetric flow, we proceeded with the nonlinear analysis, in order to classify the bifurcation observed. Figure 5.15 shows the bifurcation diagram of the asymmetric steady flow for $\beta = 1.47$, in which the energy was extracted from the first mode number ($k = 1$). The fully three-dimensional simulations were carried out with two different types of initial conditions. The first of them, the initial conditions were a linear combination of the base flow and the most unstable eigenmode taken from linear stability analysis, multiplied by a factor small enough to make the initial growth linear, being marked by hollow circles. The second of them, the solid circles, were the nonlinear saturation of the unstable base flow at $Re = 720$. It is evident from this diagram that the bifurcation exhibits a subcritical behaviour, but with some remarkable differences from what was observed for the primary bifurcation. The hysteresis in the vicinity of the critical point can easily be seen in figure 5.15, and extends far away from the critical point, achieving $Re = 495$. Afterwards, the kinetic energy of the spanwise Fourier modes have a sudden fall and goes to zero.

Another important finding related to subcritical bifurcation in confined flows was reported by Sherwin & Blackburn (2005), in which an axisymmetric stenotic tube with area reduction of 75% was analyzed. Using a fully three-dimensional simulation, they concluded that the instability was subcritical. Hysteresis was confirmed and the flow also exhibited instabilities quite far from the critical point in the nonlinear simulations. However, the analysis referred to the primary instability, rather than to the secondary instability as observed here.

Considering an asymmetric flow in a channel which has a closer relationship to our

Figure 5.15: Diagram of the subcritical bifurcation of the asymmetric steady flow for $\beta = 1.47$. The solid circles represent the DNS seeded with the nonlinear saturation of the unstable base flow at $Re = 720$ and the hollow circles with a linear combination of the base flow and the leading eigenmode.

system. The primary instability in a backward-facing step was determined by Barkley, Gomes & Henderson (2002), having a critical Reynolds number of 748, which is higher than in the constricted channel flow. Nevertheless, the nature of the bifurcation was defined by Rani & Sheu (2006), being a supercritical Hopf bifurcation. Therefore, even though the constricted channel and the backward-facing step are both flows confined by parallel walls the way how the flow bifurcates is strongly influenced by the shear layers when the flow separates.

5.3.4 Non-normal stability analysis

As previously done for the primary global instability, in this section transient growth analysis of the asymmetric base flow is presented.

5.3.4.1 Dependence on Reynolds number

Figure 5.16 summarizes the optimal energy growth for two-dimensional perturbations after the primary instability. Figure 5.16(a) shows the optimal envelopes, $G(\tau)$, versus time horizon for Reynolds numbers from 450 up to 720. The maximum energy growth among all initial perturbations is $G_0^{max}(720) = 2.24 \times 10^7$ at $\tau_0^{max} = 16.92$. The optimal energy curves go directly to their maxima and decrease monotonically afterwards. Figure 5.16(b) illustrates the optimal growth logarithmic contours in the (τ, Re) plane. Moreover, the dotted line in figure 5.16(a,b)

shows the local of maximum growth as a function of τ .

Variation of maximum growth and the time of maximum growth against Re are shown in figure 5.16(c,d). It can be clearly seen that the $\log G_0^{max}$ and τ_0^{max} increase with Re in a linear rate. Following the same analysis employed before we can write

$$\log G_0^{max} \simeq 1.13 \times 10^{-2} Re \quad (5.6)$$

and

$$\tau_0^{max} \simeq 2.27 \times 10^{-2} Re. \quad (5.7)$$

Although the expressions defined above are analyzed up to $Re = 720$, it is possible that, these relations may be valid for Reynolds numbers above $Re = 720$.

Blackburn, Barkley & Sherwin (2008) reported that the maximum growth increases exponentially with Re in a backward-facing step, such that $\partial \log G_0^{max} / \partial Re = 0.0118$, which is very close the results observed in this study for the asymmetric flow, thus the maximum growth, in both cases, increase with the same linear rate. However, the time of maximum growth increases with Re in a different linear rate, such that $\partial \tau_0^{max} / \partial Re = 0.14$. Therefore, it suggests that, the asymmetric channel flow, i.e. the flow regime and the channel geometry, may determine how the energy is transfered to the initial perturbation. Nevertheless, the way how the initial perturbation is created, such as in the shear layers, which determine its shape and its position will establish how long the initial perturbations will exchange energy with the flow and the distance that they will be convected before they die away.

In addition, although the primary instability in a backward-facing step (RANI; SHEU, 2006) and the secondary instability in a constricted channel occur by distinct mechanisms as discussed in the previous section, it does not influence how $\log G_0^{max}$ increases with Re , even though the Reynolds number is one of the main parameters together with the spanwise wavenumber to evaluate the transition. Hence, it can be concluded that, when the flow regime is established, asymmetric steady flow in this case, there is no effect from the previous bifurcation in the present regime flow, which was confirmed by the same exponential growth rate with Re .

Figure 5.16(e) plots $\log G_0^{max}$ as a function of τ_0^{max} . An important aspect to notice is the similar behaviour observed before the primary instability: $\log G_0^{max}$ grows linearly with τ_0^{max} . It suggests that this behaviour may be a pattern at any flow regime as also observed by (BLACKBURN; BARKLEY; SHERWIN, 2008; BLACKBURN; SHERWIN; BARKLEY, 2008). So using

Figure 5.16: Dependence on Reynolds number of the two-dimensional transient energy growth after primary instability. (a) Energy growth envelopes, $G(\tau)$, as a function of τ for Reynolds number varying from 450 up to 720. (b) Logarithmic contours plot for two-dimensional optimal energy growth, $G(\tau, Re)$, as a function of τ and Re . The dotted-line curve shows the local of maximum energy growth as a function of τ . Variation of maximum (c) growth and (d) time as a function of Re . The $\log G_0^{max}$ and τ_0^{max} increase linearly with Re . (e) Maximum energy growth as a function of time of maximum growth for the Reynolds number range from 450 to 720. The $\log G_0^{max}$ grows linearly with τ_0^{max} .

Figure 5.17: Two-dimensional optimal energy growth envelope and time evolution of optimal initial perturbations corresponding to $\tau = 1, 14$ and 50 for $Re = 540$. Solid circles denote the points where each curve of linear growth touches the envelope.

(5.6) and (5.7) we can find a linear expression as written below

$$\log G_0^{max} \simeq 0.498 \tau_0^{max}. \quad (5.8)$$

Therefore, even after the primary instability the linear expression above is plausible, so that, as previously noted, the energy of the optimal perturbations reach their maxima with the same growth rate, even after the transition. However, the slope of the curve is higher than before the transition, being $\partial \log G_0^{max} / \partial \tau_0^{max} = 0.498$ after and $\partial \log G_0^{max} / \partial \tau_0^{max} = 0.414$ before the transition, respectively.

5.3.4.2 Time evolution of two-dimensional optimal initial perturbations

Two-dimensional optimal energy growth envelope along with three different optimal transient responses at $Re = 540$ are shown in figure 5.17. The case $\tau = 1$, although it is a short time, exhibits a transient curve that has a huge increase in its energy before decay. On the other hand, the transient responses for $\tau = 14$ and $\tau = 50$ almost touch all the points, having only a slight difference from the optimal growth envelope. Nevertheless, they only touch their respective optimal growth. As previously observed, in the symmetric flow, the curves have similar shapes with slightly different amplitudes from the optimal envelope, indicating similar dynamic development of the initial condition and the same instability mechanism. It should be noted that, in this flow regime, even after $t = 50$ the energy growth do not achieve the asymptotic behavior dictated by the normal analysis, so that the non-normalities are still dominant.

Figure 5.18: Instantaneous vorticity contours for the linear evolution of the two-dimensional optimal initial perturbation corresponding to $\tau = 14$ together with streamlines of the base flow at $Re = 540$. Contours vary from $\omega_z D / \bar{u}_m = -8$ (dark contours) to $\omega_z D / \bar{u}_m = 8$ (light contours) for $0 \leq t \leq 4$ and from $\omega_z D / \bar{u}_m = -16$ (dark contours) to $\omega_z D / \bar{u}_m = 16$ (light contours) for $6 \leq t \leq 14$.

Figure 5.18 depicts instantaneous vorticity contours and streamlines of the optimal initial perturbation for $\tau = 14$ and its evolution along the channel at $Re = 540$. The initial perturbation which is created at the shear layers travels through the shear layers following the asymmetric flow. As also observed in figure 5.8, it is interesting to note that both parts of the disturbance which lie in the upper and lower bubble meet in a wave packet ($t = 6$). So that, even after primary instability, the way which the initial condition gives rise to a series of spanwise counter-rotating rolls is the same. At $t = 14$, the maximum energy growth occurs farther from the recirculating regions than the symmetric flow. It happens because at higher Reynolds number the perturbations are subject to smaller viscous diffusion as they travel through the channel. Furthermore, the wave packet is also slightly stretched in a parabolic shape by the mean strain field.

5.3.4.3 Dependence on spanwise wavenumber

Figure 5.19 summarizes the β -dependence of the three-dimensional transient energy growth for the asymmetric flow. Optimal energy growth, $G(\tau, \beta)$, is plotted against spanwise wavenumber β and time τ in figure 5.19(a). The spanwise wavenumber of the most-amplified perturbation is $\beta = 1.052$. Then, the global maximum energy growth is $G_\beta^{max}(540) = 2.41 \times 10^5$ at $\tau_\beta^{max} = 13.68$. As expected, the optimal transient curves for each β reach their maxima growth and after that they decrease monotonically without presenting any other local maximum. While in the symmetric flow the growth envelopes have only slight differences between them as shown in figure 5.9(a), the asymmetric flow has a notable change in the maximum growth and time of

Figure 5.19: Dependence on spanwise wavenumber of the three-dimensional transient energy growth after primary instability. (a) Surface plot of energy growth envelopes, $G(\tau, \beta)$, as a function of spanwise wavenumber β and time τ at $Re = 540$. (b) Enlargement of (a) for short times with β from 0 to 15 in steps of 1.

maximum growth for $\beta > 2.5$. Figure 5.19(b) shows a close-up of figure 5.19(a) for short times with β from 0 to 15 in steps of 1. Again, the higher β exhibit higher optimal growth at short times, however, afterwards the smaller β briskly exceed their energy.

Local maxima growth and its respective time of maxima growth were also calculated for $Re = 495$ and $Re = 450$. Figure 5.20 shows the variation of the maximum growth and time of maximum growth against β , highlighting three different branches of local maxima. For $\beta < 4$, there is only one branch, the *first branch*, which lies in the smaller spanwise wavenumber and exhibits the highest local maxima of this system. Increasing the spanwise wavenumber, at $\beta = 4$, there is a split up between the *first* and *second branches* for $Re = 450$, which is marked by a great decrease in the time of maximum growth. This is also observed for $Re = 495$ and

Figure 5.20: Variation of local maxima as a function of spanwise wavenumber for the asymmetric steady flow (after primary instability). There are three different branches of local maxima. (a) Maximum growth as a function of β . Inset: the *third branch*. (b) Maximum time as a function of β . The local maxima in the *second* and *third branch* decrease in a linear rate for the higher β .

$Re = 540$, but at $\beta = 4.5$. Finally, at $\beta = 7$, a second branch of local maxima appears in the system, which we call *third branch*. So that, for $\beta \geq 7$, the system has two branches of local maxima. These three branches are classified according to the optimal modes, related to each maximum growth. Therefore, there are three different optimal modes in this system.

Figure 5.20(a) illustrates the variation of local maximum growth as a function of β . The inset plot, in figure 5.20(a), shows the *third branch*. The *second* and *third branches* have

Figure 5.21: (a) Maximum energy growth as a function of time of maximum growth at $Re = 540$; (b) close-up of (a) for short times of the local time of maximum growth. There is constant growth rates which relate maximum growth and time of maximum growth for the higher β in the *second* and *third* branch.

almost the same maxima growth for the range of spanwise wavenumber analyzed, and also the maximum growth logarithm decreases monotonically with a linear rate for the higher β . The *second branch* decreases with a linear rate given by $\partial \log G_\beta^{max} / \partial \beta = -0.071$ and the *third branch* by $\partial \log G_\beta^{max} / \partial \beta = -0.105$. It is noteworthy that the linear rate found in the *third branch* is the same observed before the primary instability (Figure 5.10(c)), however, the *second branch* decreases with a different linear rate.

Figure 5.21 plots $\log G_\beta^{max}$ as a function of τ_β^{max} . As we can see, the three branches defined above are shown as clusters of points in figure 5.21(a), and there is no global correlation between the local maxima for all β . It is evident that, unlike what was observed for the symmetric steady flow when all β collapsed in almost a straight line close to the critical Reynolds

number, it only occurs for the higher β for the asymmetric steady flow. So that, once again, there are notables constant growth rates which relate maximum growth and time of maximum growth. However, in this case it collapsed for two different branches (*second* and *third branch*) of local maxima as shown in figure 5.21(b). So we obtain the two expressions below

$$\log G_{\beta}^{max} \simeq 0.755\tau_{\beta}^{max} \quad (5.9)$$

and

$$\log G_{\beta}^{max} \simeq 0.329\tau_{\beta}^{max}, \quad (5.10)$$

for the *second* and *third branches*, respectively. It should be noted that neither of the linear empirical functions match that found in equation (5.4), although the *third branch*, in figure 5.20(a), has the same exponential decrease rate observed for the symmetric steady flow. Therefore, this may be associated with the convective scales. The asymmetric steady flow has a shorter and a longer recirculating regions which have different scales (see §5.3.1), hence the energy growth mechanisms associated with the shear layers have different scales for the *second* and *third branches*. However, the fact that the symmetric steady flow and the *third branch* of the asymmetric flow have the same exponential decrease rate with β suggests that the way which the optimal modes exchange energy with the base flow is preserved in the symmetric and asymmetric flows, at least in one mechanism, being a feature of the constricted channel flow but not of the flow regimes. In addition, after $\beta = 15$ the *third branch* vanished, consequently only the *second branch* remains. The linearity is maintained until $\beta = 30$, only at $\beta = 40$ the maximum growth begins to move away from the linear approximation, tending to the origin.

In order to illustrate the physical mechanism in each branch, the optimal initial perturbations and their respective optimal growth outcomes at $Re = 540$ are plotted figure 5.22. Streamwise velocity iso-surfaces for the optimal initial perturbations are shown at the left-hand side and vorticity iso-surfaces of the optimal perturbation growth outcomes corresponding to the initial condition are shown at the right-hand side. Firstly, the structure of the most-amplified perturbation for the first branch is considered, which occurs for $\beta = 1.052$ and $\tau = 14$ and is shown in figure 5.22(a). It can be seen that the optimal initial condition also lies around the throat, being stronger at the shear layers and upstream the throat with chevron-shaped pattern, like occurred before the transition, however, spreading more widely upstream and downstream the throat. As expected, both shear layers play the major role to trigger the optimal growth. In addition, the optimal perturbation is asymmetric with respect to the channel centreline because of the upward deflection of the shear layers in the asymmetric base flow. The evolution of the initial condition also becomes a wave packet and the optimal growth occurs after the recirculating regions, however, this wave packet is longer in the streamwise direction compared to before

Figure 5.22: Plots of three-dimensional optimal perturbation after primary instability at $Re = 540$ for the three different branches. Streamwise velocity iso-surfaces of the optimal initial perturbation (left-hand side). Vorticity iso-surfaces of the optimal perturbation growth outcomes (right-hand side). The pictures at the top show a side view and those at the bottom show a top view.

the transition.

As previously highlighted, when the spanwise wavenumber is increased along the *first branch* of the asymmetric steady flow, as previously highlighted, it drops to the *second branch* around $\beta = 4.5$ and afterwards the *third branch* appears, so that two other distinct modes arise. In addition, they are quite different from the modes which are normally found in channels. Figure 5.22(b) shows the mode that lies in the *second branch* at $\beta = 9$ and $\tau = 2$. As we can see, in this case, the optimal initial perturbation is concentrated close to the throat and mostly within the large recirculating region at the lower channel part. Nevertheless, a chevron-shape

pattern is revealed in the optimal initial perturbation, consequently a sinuous disturbance is also the trigger for the optimal growth in the *second branch*. The optimal perturbation growth outcome occurs in the shear layers, the perturbation has a chevron-shaped pattern opposite to the initial condition and it is deflected upward by the asymmetric flow. It is noteworthy that this initial condition does not give rise to the wave packet formed by the series of spanwise counter-rotating rolls in the peak growth. In addition, even if it takes place for higher time horizons, it is not the dominant mechanism anymore. The mode which lies in the *third branch* at $\beta = 9$ and $\tau = 5$ is shown in figure 5.22(c). It is singular that the optimal initial perturbation is stretched upstream and downstream from the throat at the upper channel part. Moreover, a modest quantity is also within the short recirculating region as well as in the shear layers. It should be noted that, this is the first time that the optimal mode is not based on mainly in a sinuous disturbance. More interesting is that the optimal perturbation growth outcome travels over the lower bubble. Hence, the large recirculating region weakly contributes to the optimal growth in the *third branch*.

5.3.5 Nonlinear effects triggered by optimal perturbations

We have shown that the asymmetric flow has a subcritical bifurcation and the non-normal stability analysis demonstrated that three-dimensional optimal initial perturbations can achieve energy growth of the order of 10^5 for Reynolds numbers close to the critical values. In this section, we are interested in knowing what is the behaviour of those initial conditions in a nonlinear study, taking the relative energy level between the base flow and the optimal initial perturbation into account and, more important, if it is possible to raise the energy of a finite perturbation up to the top hysteretic curve by non-normal growth and nonlinear saturation.

A two-dimensional asymmetric base flow at $Re = 558$ was seeded with three-dimensional optimal initial perturbations for $\beta_c = 1.47$ (critical spanwise wavenumber) with four different energy levels. Two different analyses were performed, being the first with 4 Fourier modes and the second with 8 Fourier modes. From the non-normal stability analysis, time horizon was chosen to be $\tau = 15$, so that the optimal growth in this condition is $G(15, 1.47) = 3.57 \times 10^5$.

5.3.5.1 Bypass transition

Figure 5.23 shows three-dimensional DNS at $Re = 558$ and $\beta = 1.47$ seeded with optimal initial perturbations for $\tau = 15$. The evolution of the energy was analyzed for four different energy levels for the first mode number. It can be verified that the most amplified initial condition occurred when the relative amount of energy between the base flow and the initial condition

Figure 5.23: Three-dimensional DNS at $Re = 558$ and $\beta = 1.47$ seeded with optimal initial perturbations for $\tau = 15$. Nonlinear effect on energy growth for the first mode number for (a) 4 Fourier modes and (b) 8 Fourier modes. The dashed line represents the exponential decrease associated with the leading eigenmode.

is 10^{-12} . Besides this, at this relative energy level, the maximum energy growth found was 3.72×10^5 at $t = 14.84$ for the case with 8 Fourier modes, which is close to the optimal growth calculated with non-normal analysis. It should also be noted that the initial conditions with the lower relative energy levels match the exponential decrease associated with the leading eigenvalue of the normal analysis after long times.

However, the initial condition with 10^{-5} of relative energy level did not decay monotonically after the peak growth in both cases, achieving nonlinear saturation. This is an example of a bypass transition, once it was found that this flow is linearly stable at $Re = 558$. Note that the curves which saturate were marked with different line styles, and they are also highlighted in figure 5.24 to make it clearer. When the perturbations reach a certain energy level, there is a redistribution of energy to the higher Fourier modes, such that the three-dimensional structures of the flow hold until the transition. More surprisingly, depending on the quantity of spanwise Fourier modes used, the flow achieved nonlinear asymptotic saturation (4 Fourier modes) or an oscillatory regime (8 Fourier modes) as shown in figure 5.24.

Looking at the case with 4 Fourier modes, after the peak growth all modes started to decay, but after some time there was a redistribution of energy and all modes grew to nonlinear saturation, and when the flow saturated it reached another steady state. On the other hand, for 8 Fourier modes the flow achieved nonlinear saturation faster than with 4 modes, although they exhibited similar behaviour. However, when the energies got close to the transition, the three-dimensional modes were pushed up and afterwards started to decay again. This pattern repeated with time, such that the system presented an oscillatory behaviour. It is worth mentioning that a three-dimensional simulation was also carried out with only 2 Fourier modes, however the

Figure 5.24: Time series of energies E_k in spanwise Fourier modes of the optimal initial perturbations with relative energy levels of 10^{-5} at $Re = 558$ and $\beta = 1.47$ for (a) 4 Fourier modes and (b) 8 Fourier modes.

energy of the first Fourier modes went to zero, and it did not achieve a saturated state. Therefore, the instability depends on the higher Fourier modes to achieve the transition.

The energy of the two-dimensional base flow was subtracted from the two-dimensional Fourier mode ($k = 0$) in both cases. Looking at the two-dimensional modes more closely, in the graphs at the bottom of figure 5.24, it is possible to see that, when the energy of the two-dimensional modes achieved a local minimum, the energies of the three-dimensional modes were going to the saturated state, so that they took energy out from the two-dimensional modes. However, the system does not stay in the saturated state and afterwards the three-dimensional modes started to give the energy back to the two-dimensional mode until it reestablished its energy, reaching a local maximum at the end of the process. This oscillatory behaviour goes indefinitely for the case with 8 Fourier modes, but, using 4 modes the flow stays stable in the saturated state after the first oscillation. Hence, we can conclude that the physical mechanism behind this remarkable behaviour occurs by energy exchange between the two- and three-dimensional modes.

It is noteworthy that this oscillatory behaviour is similar to bursts observed in channel Couette and Poiseuille flows (WALEFFE, 1997; ZAMMERT; ECKHARDT, 2014; BRETHOUWER, 2016). The physical mechanism of this burst occurs by energy exchange between the mean flow ($k = 0$) and the smaller scales, so that it agrees with our results, once the physical mechanism

Figure 5.25: Three-dimensional DNS at $Re = 558$ and $\beta = 1.47$, using 8 Fourier modes. (a,c) Vorticity contours of the plane 0 in Fourier space subtracted from the two-dimensional base flow. (b,d) Vorticity contours of a slice from the constricted channel centreline. Contours vary from $\omega_z D / \bar{u}_m = -3.5$ (dark contours) to $\omega_z D / \bar{u}_m = 3.5$ (light contours) for (a,b) and from $\omega_z D / \bar{u}_m = -0.5$ (dark contours) to $\omega_z D / \bar{u}_m = 0.5$ (light contours) for (c,d).

of energy exchange is analogous. In addition, it only happened when the nonlinear analysis was performed with 8 Fourier modes, proving that it was necessary higher spanwise discretization to achieve the smaller scales to trigger the bursts. Therefore, a minimum range of scales must be resolved to develop this cyclic burst behavior.

5.3.5.2 Modes interaction

Now we are going to explore the physical mechanism behind this oscillatory behaviour by flow visualization. The shaded region in figure 5.24(b) highlights the time interval in which there is an energy exchange between the two- and three-dimensional modes. The present analysis is focused in this particular region, in order to understand what is happening in the flow field.

Figure 5.25 shows results from three-dimensional DNS at $Re = 558$ and $\beta = 1.47$, using 8 Fourier modes. Vorticity contours of the Fourier mode 0 (two-dimensional) subtracted

from the two-dimensional base flow is illustrated in figure 5.25(a,c). It can be seen that, at $t = 480$ (local minimum energy of the two-dimensional mode), there is a intense vorticity fluctuation after the recirculating regions, demonstrating that the two-dimensional mode is strongly affected by the three-dimensional modes. On the other hand, when the two-dimensional mode achieves its local maximum at $t = 525$, all the three-dimensional disturbed flow went away downstream the throat and afterwards the flow becomes well-behaved with a weak vorticity in the shear layers. Inspecting the three-dimensional flow in figure 5.25(b,d), as expected, at $t = 480$ the flow is highly three-dimensional when it reaches the saturated state, so that there is a great interaction between the three-dimensional modes, not only with the two-dimensional mode as previously mentioned from figure 5.24. At the end of the process at $t = 525$, the three-dimensional structures almost disappear. This makes clear that the three-dimensional effects are really fed with energy from the two-dimensional mode, bearing in mind that when the two-dimensional mode takes the energy back the three-dimensional structures vanish.

6 BIFURCATION AND CONVECTIVE INSTABILITIES OF A PULSATILE FLOW

The intent of this study is to extend the discussion of the last chapter, where symmetric and asymmetric steady flows, being the last a result of the primary bifurcation, were investigated in a constricted channel in order to comprehend the transition mechanisms in these two flow regimes. The aim of this chapter is to understand the physical mechanism behind the primary bifurcation of another flow (pulsatile flow) in the same geometry. Floquet stability analysis was carried out to find the flow parameters for which the flow is linearly unstable and its critical values were obtained. Afterwards, direct numerical simulations were performed to characterize the transition. In addition, non-normal analysis was performed to map the transient growth behaviour through different parameters.

In §6.1, the dimensionless parameters which define the pulsatile flow are given. Afterwards, in §6.2, convergence tests and computational simulations set up are described. Results are presented, in §6.3, concerning the transition mechanism and convective instabilities behind the primary bifurcation.

6.1 Dimensionless parameters

The base flow is created by a time periodic inflow. The time-dependent inlet, $\bar{u}(t)$, has a uniform cross-sectional velocity, which implies that it does not depend on space coordinates. Thus, the temporal averaged flow velocity is

$$\bar{u}_m = \frac{1}{T} \int_0^T \bar{u}(t) dt, \quad (6.1)$$

where T is the pulse period. The channel width D and the average velocity $\bar{u}_m$ are used as length and velocity scales, respectively, so the time scale is $D/\bar{u}_m$. We can now define the dimensionless parameters of the flow that are the time-averaged Reynolds number $Re = \bar{u}_m D/\nu$ and the reduced velocity $U_{red} = \bar{u}_m T/D$, where ν is the kinematic viscosity of the fluid. The reduced velocity gives the number of channel widths the mean flow travels in a period. An-

Figure 6.1: The inlet velocity waveform, $\bar{u}(t)$, as a function time for the pulsatile flow.

other dimensionless parameter commonly employed in pulsatile flows is the Womersley number $\alpha = (\pi Re / 2U_{red})^{1/2}$. In our study we fixed the reduced velocity, and so the effect of viscosity is parameterized only by the Reynolds number.

The velocity waveform is shown in figure 6.1. The pulse oscillates around the temporal averaged flow velocity with a sinusoidal shape, so that the velocity waveform applied in the pulsatile flow is a single-harmonic pulse given by

$$\bar{u}(t) = \bar{u}_m \{1 + 0.75 \sin[2\pi(t + t_0)/T]\}, \quad (6.2)$$

where t_0 is a parameter to change the phase of the pulse, as discussed in section 6.3.4.1. Note that the maximum velocity of the pulsatile waveform is $\bar{u}_{max} = 1.75\bar{u}_m$.

In the present paper, the reduced velocity employed is $U_{red} = 10$ and we explored a range of Re up to 315, covering the primary global instability.

6.2 Computational simulations

A close up of the mesh around the throat is shown in figure 6.2. The quadrilateral mesh approach around the throat applied in the steady case was used here with almost the same level of refinement. The two-dimensional computational mesh was composed by 2136 spectral elements, being 1994 quadrilateral and 42 triangular. The inflow and outflow lengths were $30D$ and $40D$ relative to the throat of the stenosis. The extensive inflow length was used to let the flow develop properly, once we have a uniform time-dependent inlet, as well as accommodate the disturbance upstream during the Floquet stability and transient growth analyses.

Figure 6.2: Close up of the computational mesh around the throat, the dimension is given in terms of channel height D . The mesh has 2136 spectral elements.

N	σ	% difference
9	0.044379	-
8	0.044379	0.00
7	0.044371	0.02
6	0.044373	0.01
5	0.044537	-0.36
4	0.044543	-0.37
3	0.023681	46.64

Table 6.1: Convergence of the three-dimensional leading eigenvalues at $Re = 315$ for $\beta = 1$ with respect the variation of the spectral element polynomial order N , computed with M_1 .

Mesh	L_i	L_o	σ	% difference
M_1	$30D$	$40D$	0.044373	—
M_2	$30D$	$50D$	0.044373	0.000
M_3	$35D$	$40D$	0.044372	0.002

Table 6.2: Convergence of the three-dimensional leading eigenvalues at $Re = 315$ for $\beta = 1$ with respect the variation of the inflow and outflow lengths, computed with polynomial order $N = 6$.

Although transient growth analysis can experience huge energy amplification from a particular optimal initial perturbation, it was only applied in lower Reynolds numbers, which is less challenging numerically. Thus, in order to study the worst case for convergence, Floquet stability analysis was chosen as the method to perform the convergence testes, since this method was carried out at the highest Reynolds number in the present study. Table 6.1 shows the convergence of the three-dimensional leading eigenvalues with respect to the polynomial order, using the mesh M_1 , which is the mesh adopted in this work (Table 6.2). Polynomials of degree 4 (i.e. 5^{th} order accuracy in space) achieved excellent convergence results, then, just to be rigorous with our calculations, polynomials of degree 6 were used in the discretization of the mesh for two-dimensional base flows and the most part of the stability calculations. However, the second pulse period during the transient growth calculations and the fully three-dimensional simulations were carried out with polynomials of degree 5, due to the high computational cost.

Table 6.2 depicts the convergence of the three-dimensional leading eigenvalues with respect to the inflow and outflow lengths, using $N = 6$. It is easy to notice that, for the cases tested, there is no influence of the mesh length in the stability calculations, i.e. if we increase the upstream or the downstream lengths of the mesh M_1 the percentage difference of the leading eigenvalues are negligible. Therefore, we consider that the convergence was reached with uncertainty less than 1%.

Equation (2.1) was used to solve the two-dimensional pulsatile base flows, employing the stiffly stable splitting scheme presented by Karniadakis, Israeli & Orszag (1991). Time integration was carried out using a second-order velocity-correction schemes with value of the non-dimensional time step of 0.001 for the two-dimensional base flows and stability analyses and 0.002 for the three-dimensional simulations. For normal and non-normal stability analyses, the pulsatile base flows were pre-computed and stored as data: 192 time-slices were stored (BLACKBURN; SHERWIN; BARKLEY, 2008) and the base flows were reconstructed from these data, using Fourier interpolation. Krylov subspace of size 24 was used in the stability calculations and the criterion for convergence of the eigensolution was that the residual should be lower than 10^5 .

6.3 Results

6.3.1 Base flow characteristics

The two-dimensional pulsatile base flow features through four stages of the pulse are shown in figure 6.3, which illustrates x -velocity and vorticity contours at $Re = 225$ and $U_{red} = 10$. The Womersley number in this system is $\alpha = 5.9$. It can be seen that, at the peak velocity, there is a strong jet through the throat, so that the shear layers are symmetrically formed at the constriction. Afterwards the leading pulse front is developed in the flow separation until it detaches and propagates downstream. It should be noted that the pulsatile flow only ejects one weak pulse per cycle period, which does not propagate so long, quickly vanishing in the base flow. It agrees with the results of (PITT, 2005) for a pulsatile flow in a constricted channel with 60% occlusion, considering a reduced velocity and Womersley number close to our study. (BLACKBURN; SHERWIN, 2007) also reported similar behaviour for a pulsatile flow in a stenotic tube, which always ejects only one pulse front, in this case a vortex ring, per pulse cycle for a single harmonic waveform.

Figure 6.4 shows the x -velocity profiles at the throat by channel height position for four phase points during the pulse period for the same conditions as those in figure 6.3. In this

Figure 6.3: Contours of x -velocity and vorticity for the two-dimensional base flow at $Re = 225$ with $U_{red} = 10$ ($\alpha = 5.9$) through four stages of the pulse. In each phase of the pulse, the figure at the top is the x -velocity and at the bottom the vorticity. Contours of streamwise velocity are between $u/\bar{u}_m = 0$ (dark contours) and 2.5 (light contours). Contours of vorticity vary from $\omega_z D/\bar{u}_m = -10$ (dark contours) to $\omega_z D/\bar{u}_m = 10$ (light countours).

figure, it is evident that the flow is ejected symmetrically through the throat, as also seen in figure 6.3. At peak velocity, $t = 0.25T$, the flow reaches its maximum of $u(t) \approx 4\bar{u}_m$, which is expected for a constricted channel with 50% occlusion. As expected, at $t = 0.75T$, when the waveform achieves the minimum velocity, there is a drastic fall of x -velocity, clearly verified by the velocity profiles in figure 6.4. The abrupt deceleration is responsible for the detachment of the pulse front from the throat. An important aspect to notice is that, as previously mentioned, pulsatile flows in stenotic tubes eject vortex rings when the flow separation is detached from the throat (SHERWIN; BLACKBURN, 2005; BLACKBURN; SHERWIN, 2007; GRIFFITH et al., 2009). Griffith et al. (2009) reported that, in these cases, the axial velocity has a local maximum near the inside walls for part of the pulse cycle, however, in constricted channels the maximum velocity occurs at the centreline of the flow throughout the whole cycle.

Figure 6.4: Streamwise velocity profiles at the throat at four phase points during the pulse period for $Re = 225$ and $U_{red} = 10$ ($\alpha = 5.9$).

6.3.2 Floquet stability calculations

Now we turn our attention to the primary instability. Normal stability analysis was performed to evaluate the critical values of the pulsatile flow in a constricted channel. Figure 6.5(a) shows the leading eigenvalues, σ , as functions of spanwise wavenumber β for five different Reynolds numbers. It can be seen that there is only one unstable mode for this Reynolds number range, in addition all leading eigenvalues found were real and corresponding Floquet multipliers positive. Figure 6.5(b) depicts the neutral stability curve for the primary instability for Reynolds numbers up to $Re = 315$. Everywhere to the right hand side of the curve (dark region) the two-dimensional flow is linearly unstable to infinitesimal perturbations, so that the curve which separates the light and dark regions represents the parameter space for which the base flow is neutrally stable. The critical Reynolds number and corresponding spanwise wavenumber are $Re_c = 247.8 \pm 0.1$ and $\beta_c = 0.78 \pm 0.01$, respectively, for $U_{red} = 10$, such that $\alpha = 6.2$. The critical spanwise wavelength is $2\pi/\beta_c = 8.06$ channel widths.

Taking a narrower constricted channel for comparison, Pitt (2005) reported critical values for a constricted channel with 60% occlusion for three different fixed Womersley numbers from 4 to 8. The critical Reynolds numbers is lower and the critical spanwise wavenumber is higher than in our study. This same behaviour was observed by (GRIFFITH et al., 2009) for pulsatile flows through stenotic circular pipes. Thus, the narrower the constriction the lower the critical Reynolds number and the higher the critical spawise wavenumber required for the primary instability, considering similar Womersley numbers. It is noteworthy that it also happens

Figure 6.5: Floquet stability analysis for pulsatile flow in a constricted channel. (a) Plot of the leading eigenvalues, σ , against spanwise wavenumber for five different Reynolds number. (b) Neutral stability curve for primary instability. In the region on the right hand side of the curve (dark region) the two-dimensional flow is linearly unstable to infinitesimal three-dimensional perturbation. The critical Reynolds number is $Re_c = 247.8$.

in steady flows for the primary and secondary instabilities in constricted channels as discussed in the chapter 5. In addition, in pulsatile flows in constricted channels, when the Womersley number increases the critical Reynolds number and spanwise wavenumber increase (PITT, 2005), so that it is possible to have a higher or lower critical Reynolds number and spanwise wavenumber for a narrower constriction, depending on the Womersley number.

Considering a stenotic tube with 75% occlusion, Blackburn & Sherwin (2007) performed biglobal stability analysis with the same reduced velocity of this work ($U_{red} = 10$) and found a critical Reynolds number of $Re_c \approx 590$. Hence, it suggests that the primary instability first happens in constricted channels than in stenotic tubes, using equivalent parameters. In addition, it is also true for symmetric steady flows, being the critical Reynolds number for the constricted channel 278.8 (see §5.2.2) and for the stenotic tube 722 (SHERWIN; BLACKBURN, 2005).

Figure 6.6 illustrates the most unstable mode at $Re = 270$ for $\beta = 0.78$. The mode lies downstream the throat with most part within the shear layers, where the leading pulse front is formed, and it is symmetric with respect to the channel centerline. However, the streamwise velocity at the top of the channel is negative and at the bottom is positive, which induces a symmetry breaking. In addition, looking at the spanwise velocity component in figure 6.6(c,d), it can be seen that the mode lead the system to a three-dimensional flow. It should also be noted that there is a weak non zero region of the mode located in the previous pulse which has already detached from the throat, however the sign of the streamwise velocity alternated from the first to the second pulse (figure 6.6(b)). It should be noted that it is not an effect of the

Figure 6.6: Streamwise velocity iso-surfaces of the three-dimensional unstable mode at $Re = 270$ for $\beta = 0.78$. (a) side view, (b) top view. Spanwise velocity iso-surfaces for (c) side view and (d) top view.

period-doubling bifurcation because the eigenvalues found in the Floquet analysis are real and the corresponding Floquet multipliers positive. On the other hand, Blackburn & Sherwin (2007) studying a pulsatile flow with $U_{red} = 10$ in a stenotic tube demonstrated that the system has a period-doubling nature.

An important aspect to notice is that the real part of the leading eigenvalues (growth rate) for $\beta = 0$ are not zero (figure 6.5(a)), in other words, the Floquet multipliers are different from unity ($|\mu| \neq 1$). The Floquet stability theory says that any autonomous time-periodic system has a neutrally stable Floquet mode, such that $|\mu| = 1$ (see e.g. Guckenheimer & Holmes (1983)). The pulsatile flow presented here is a system with a time-periodic forcing, due to the fact that the periodicity of the flow is imposed in the inflow boundary condition, so the periodic flow is not autonomous. (GIORIA et al., 2009) found similar behaviour for the flow around a circular cylinder forced to oscillate, which also had a time-periodic forcing imposed on the boundary condition.

6.3.3 Nonlinear characterization of the bifurcation

Once we found the regions for which the pulsatile flow is absolutely unstable, the next step of our study was the characterization of the bifurcation and understanding of the mechanisms behind the transition. Thus, fully three-dimensional simulations were carried out to evaluate the

Figure 6.7: Three-dimensional DNS at $Re = 270$ for $\beta = 0.78$ seeded with the most unstable mode. Time series of energies E_k in spanwise Fourier modes. (b) Vorticity contours of the three-dimensional flow, when it achieves nonlinear saturation of the two-dimensional Fourier mode.

primary instability of the pulsatile flow (Figure 6.7). Results from the three-dimensional direct numerical simulation of the pulsatile base flow seeded with the most unstable mode taken from the Floquet stability analysis at $Re = 270$ and $\beta = 0.78$ are shown in figure 6.7(a). It can be seen that, although the flow is linearly unstable in this region and the Floquet mode induces the flow to three-dimensions (Figure 6.6), the three-dimensional modes went to zero, however their energies were transferred to the two-dimensional mode ($k = 0$), which slightly increased its energy and then achieved the nonlinear saturated state, demonstrating an unexpected transition mechanism.

It is noteworthy that a similar behaviour was observed for the symmetric steady flow (see §5.2.3). Although, in both flows, the jets which go through the constriction are symmetrically ejected from the throat, we expected they would have a similar physical mechanism, however this energy transfer to the two-dimensional mode produced different effects in the symmetric and pulsatile flows. The former tended to an asymmetric steady flow while the latter reestablished a symmetric pulsatile flow, which is close to the flow before the transition, however the pulse front detached from the throat is a bit stronger (figure 6.7(b)).

Additionally, Pitt (2005) reported a different transition mechanism for the primary bifurcation of a pulsatile flow with $U_{red} = 15.7$ in a constricted channel with a higher stenotic degree, so that, through the transition process, the three-dimensional modes achieve the nonlinear saturated state, being a supercritical bifurcation. Hence, we can conclude that any changes in the stenotic degree or velocity reduced could lead to different transition process even if the constriction shape is similar.

6.3.4 Non-normal calculations

Given the unusual character of the bifurcation shown above and the possibility of having subcritical transition, we decided to investigate the non-normal stability characteristics of this flow. Transient growth was calculated considering different Reynolds numbers, spanwise wavenumbers, phases and times. For this analysis, we evaluated the largest transient energy growth for a given optimal initial perturbation, and investigated convective mechanisms as well as the maximum energy growth behaviour. This approach is applied at absolutely stable regions since we have already established the linearly unstable regions of the system.

Before starting our analysis, it is noteworthy that the two-dimensional transient growth investigation for steady flows have just a slight difference from the three-dimensional cases, considering smaller spanwise wavenumber, in channels as reported by Blackburn, Barkley & Sherwin (2008). However, it is also valid for pulsatile flow as will be discussed in section 6.3.4.4. Thus, three different approaches will be used. Firstly, a two-dimensional study is carried out to understand what is the influence on the optimal growth introducing disturbances at distinct instants of the pulse cycle. Afterward, still a two-dimensional investigation, Re -dependence is performed, in other words, time horizon and Reynolds number are allowed to vary, however the spanwise wavenumber is fixed ($\beta = 0$). In addition, for the Re -dependence two distinct starting phases are chosen to be analyzed. Finally, for the three-dimensional case, results are presented for a fixed value of Reynolds number, allowing time horizon and spanwise wavenumber to vary for a single starting phase.

6.3.4.1 Dependence on phase

As previously discussed, in this section, we will add a new parameter in our study, the phase t_0 at which the disturbance is introduced in the pulsatile base flow. Note that for $t_0/T = 0.25$ the disturbance is initiated at the peak velocity and for $t_0/T = 0.75$ at the lower velocity of the pulse. Figure 6.8 summarizes the dependence on phase of the optimal energy growth for two-dimensional perturbations before primary instability. Figure 6.8(a) shows the energy

Figure 6.8: Dependence on phase of the two-dimensional transient energy growth of the pulsatile flow with $U_{red} = 10$, computed at $Re = 225$. (a) Two-dimensional energy growth envelopes, $G(\tau)$, as a function of relative time. The maximum growth over all starting phases tested is $G_0^{max} = 6.50 \times 10^3$ at $(\tau/T = 0.52, t_0/T = 0.375)$. (b) Logarithmic contours of energy growth envelopes as a function of time interval τ and starting phase t_0 .

growth envelopes, $G(\tau)$, as a function of relative time at $Re = 225$. The maximum growth over all starting phases observed is $G_0^{max} = 6.50 \times 10^3$, which occurs at $\tau_0^{max}/T = 0.52$ for the phase $t_0/T = 0.375$. Two important observations can be made from this result. First, this value of growth is 2 orders of magnitude higher than the case where the starting phase lies at the onset of the pulse. Second, from these data, it is possible to identify the appearance of two local maximum growth in distinct areas, featuring a bimodal dependence, with one around $(\tau + t_0)/T \approx 0.875$ and the other around $(\tau + t_0)/T \approx 1.875$. Figure 6.8(b) illustrates a contour plot of $\log G(\tau, t_0)$. We can clearly see the two peaks of maximum growth, being at $t_0/T \approx 0.375$ and $t_0/T \approx 0.5$. Similar results were reported for a pulsatile flow with $U_{red} = 10$ in a straight tube with an axisymmetric stenosis (BLACKBURN; SHERWIN; BARKLEY, 2008).

Another aspect worth discussing is the energy level of the optimal growth through each period cycle. At the end of the two periods of each starting phase t_0 , we marked the optimal growth and their position in time by a single point in figure 6.8(a). All starting phases considered in our study revealed approximately the same value of optimal growth after each period. Therefore, we can conclude that the optimal growth of each optimal initial perturbation is preserved along the pulse cycle, because independently of the starting phase the perturbations go through all points in the cycle and in each part they acquire and lose energy until achieve the same level.

Figure 6.9 illustrates the two-dimensional logarithmic contours of energy at the end of each period, computed at $Re = 225$. Two important observations can be made concerning the optimal initial perturbations and their evolution at each cycle. First, the shape and location of the

initial conditions at the end of each period are identical for all starting phases; in other words, the initial conditions at $\tau = T$ and $\tau = 2T$ have the same modes for all starting phases as shown in figure 6.9(a,c), respectively. Remembering that all starting phases had the same optimal growth at the end of each period (Figure 6.8(a)), in figure 6.9(b,d), the evolution of the initial conditions presented the same optimal perturbation growth outcomes after each cycle. Hence, it is believed that all starting phases suffered the same mean flow, so that the initial conditions were convected downstream the throat by the same distance and so achieve the same energy growth. Secondly, it is remarkable that the time-dependent flow did not exert influence on the optimal mode after each period, although the initial conditions are equal in each starting phase. Therefore, the geometric aspects may be the main responsible in the evolution process of the disturbance, since after each period the perturbations are influenced by the same mean flow. In the chapter 5, we reported that the flow regime plays a key role in the sense of how the perturbation exchanges energy with the base flow. However, the location where the initial perturbations are formed and their shapes will establish how far the disturbances will be convected as well as how long they will exchange energy with the base flow. This perfectly agrees with our results, if we consider that our flow regime is completed at the end of each period for a pulsatile flow. Since the initial conditions for all starting phases are equals, it leads to the conclusion that at the end of the period all initial conditions shall have the same optimal growth and mode.

Now we focus on the shape and location of the optimal modes at the end of each period. In figure 6.9(a), it can be seen that the initial condition at $\tau = T$ presents most of the energy at the shear layers in the throat and around the separated flow; however, there is also a bit of energy upstream the throat. Besides that, the perturbation depicts chevron-shaped contours upstream the throat as well as in the shear layers, featuring a sinuous disturbance. This sinuous initial perturbation around the shear layers was also found in others shear flows for steady and pulsatile flows (BLACKBURN; BARKLEY; SHERWIN, 2008; BLACKBURN; SHERWIN; BARKLEY, 2008; CANTWELL; BARKLEY; BLACKBURN, 2010; GRIFFITH et al., 2010). Figure 6.9(b) shows the optimal perturbation growth outcome at $\tau = T$ corresponding to the initial condition shown in figure 6.9(a). As expected from a initial condition with a chevron-shaped pattern, the evolution of the optimal perturbation is a wave packet, which becomes a series of spanwise counter-rotating rolls as indicated by the velocity field vectors. It should be noted that the minimal energy is located in the centre of the rollers, being advected downstream following the centreline of the channel. The evolution of shear layers giving rise to spanwise counter-rotating rolls was also obtained in a backward-facing step (BLACKBURN; BARKLEY; SHERWIN, 2008), in a two-dimensional plane Couette and Poiseuille flows (FARRELL, 1988) and in a constricted channel for symmetric and asymmetric flows (Chapter 5). It should be noted that the counter-

Figure 6.9: Plots of two-dimensional logarithmic contours of energy at the end of each period, computed at $Re = 225$. (a,c) Optimal initial perturbation. (b,d) Optimal perturbation growth outcome. The vectors represent the velocity field.

rotating rolls were only observed when the initial conditions presented chevron-shaped pattern. On the other hand, the initial condition at $\tau = 2T$ did not exhibit a sinuous disturbance with chevron-shaped pattern. However, it is also located mainly at the shear layers with a mild energy upstream the throat, but it is more intense and presents a energy distribution more stretched upstream and downstream the throat than at $\tau = T$. Figure 6.9(d) shows the optimal perturbation growth outcome at $\tau = 2T$ corresponding to the initial condition illustrated in figure 6.9(c). It is remarkable that the optimal mode stayed close to the throat even after two periods, although some part had gone with the base flow and lost their energy. As mentioned above, due to the absence of the chevron-shaped pattern there is no wave packet propagating downstream the throat.

6.3.4.2 Dependence on Reynolds number for starting phase at $t_0/T = 0$

Now that we have investigated the two-dimensional transient energy growth with respect to the starting phase, we will examine the dependence of optimal growth on Reynolds number and time horizon. Figure 6.10 summarizes the optimal energy growth of two-dimensional optimal initial perturbations for starting phase at $t_0/T = 0$ (the beginning of the pulse cycle time). Figure 6.10(a) illustrates the optimal envelopes, $G(\tau)$, versus time horizon for Reynolds numbers

from 45 up to 270. We recall, just to be clear, that each point in figure 6.10(a) corresponds to the energy growth of the optimal initial condition for a specific time τ . So that, the maximum energy growth among all optimal initial perturbations is $G_0^{max}(270) = 3.08 \times 10^2$, which occurs at $\tau_0^{max}/T = 0.90$. On the other hand there is no growth at $Re = 45$ for any time. For the symmetric steady flow with $Re = 270$, we found a maximum growth of $G_0^{max} = 2.01 \times 10^2$ at $\tau = 5.77$. Hence, although the pulsatile base flow is more complex, for a starting phase at $t_0/T = 0$, the maximum growth is just slightly higher than the symmetric steady flow, having the same order of magnitude.

Figure 6.10(b) shows the optimal growth logarithmic contours in the (τ, Re) plane. The solid and dashed lines represent regions with $G \geq 1$ and $G < 1$, respectively. So, the lighter regions above the line where $\log G = 0$ are where the optimal growth is larger than unity. In addition, the dotted lines indicate the three local of maximum growth as a function of τ in figure 6.10(a,b). Since the pulsatile flow introduces a complexity in the base flow compared to steady cases, it is expected that different types of optimal initial conditions reveal in the pulsatile flow, such that their energies are exchanged with the base flow in distinct manners. It can be seen in figure 6.10 that each local of maximum growth has a specific optimal initial perturbation and growth rate which establishes its dynamic, however the initial conditions will be analyzed later. Analyzing figure 6.10(b), the critical Reynolds number, Re_E , which the optimal growth first exceeds unity is obtained when $\partial G(\tau, Re_E)/\partial \tau|_{\tau=0} = 0$, it means that when the line $\log G = 0$ intercept the Re -axis we find Re_E . The critical value for the smallest growth is $Re_E = 54.0$ for two-dimensional perturbations. This value is higher than that found for a symmetric steady flow (see §5.2.4.3), which is interesting due to the higher complexity of the pulsatile base flow.

Figure 6.10(c,d) plots the variation of the maximum growth and the time of maximum growth against Re . The peak growth were classified by order in which they appear in figure 6.10(a). The $\log G_0^{max}$ and τ_0^{max} grow linearly with Re for all three groups of peak growth, in addition it is clear that each local maximum growth reveals at distinct distances from the throat, so that the initial conditions have different ways to exchange energy with the flow, which explain why each initial condition has different growth rate. Moreover, it is possible to see that the Reynolds number affect all initial conditions in the same way, such that the higher the Reynolds number the higher the maximum growth and time of maximum growth at least for the range of Re performed in this chapter.

The $\log G_0^{max}$ is plotted in figure 6.10(e) as a function of τ_0^{max} . As expected, the $\log G_0^{max}$ grows linearly with τ_0^{max} in each group of local maxima growth. From this analysis, we are able to conclude that the pulsatile base flow demonstrates the same linear growth be-

Figure 6.10: Dependence on Reynolds number of the two-dimensional transient energy growth for $t_0/T = 0$. (a) Energy growth envelopes, $G(\tau)$, as a function of τ for Reynolds number varying from 45 up to 270. (b) Logarithmic contours plot for two-dimensional optimal energy growth, $G(\tau, Re)$, as a function of τ and Re . The critical Reynolds number for the first growth is $Re_E = 54.0$. The dotted-line curves shows the local of maxima energy growth as a function of τ . Variation of maximum growth (c) and time (d) as a function of Re . (e) Maximum energy growth as a function of time of maximum growth. The $\log G_0^{max}$ grows linearly with τ_0^{max} in each group of local maxima growth.

Figure 6.11: Plots of two-dimensional logarithmic contours of energy for starting phase at $t_0/T = 0$, computed at $Re = 225$. Optimal initial perturbations (at the top) and Optimal perturbation growth outcomes (at the bottom). The vectors represent the velocity field.

haviour as occurred for the steady flows. However, due to the flow complexity it triggers more than one initial condition which leads to different local maxima growth.

We now consider the structures of the optimal initial perturbations and their evolutions in an effort to understand which are the convective mechanism behind each group of local maxima growth in figure 6.10. The optimal initial perturbations and their respective optimal modes are plotted in figure 6.11 by logarithmic contours of energy for $\beta = 0$ and starting phase at $t_0/T = 0$. It can be seen that, there are remarkable differences between the three initial conditions. For the *first peaks*, the optimal initial perturbations have chevron-shaped pattern, featuring a sinuous disturbance, but they are not so intense compared to the *second*

peaks in which this pattern appears upstream and downstream the throat. Thus, both of the initial conditions became wave packets composed by series of spanwise counter-rotating rolls. Looking at the *third peaks*, in figure 6.11(c), we can see that the initial condition did not present a sinuous disturbance, as a consequence its evolution did not become a wave packet, in addition, the maximum growth is close to the throat. It is worth noting that, unlike the steady flows, the higher the Reynolds number the farther downstream the throat the initial conditions reach their maxima growth for $\beta = 0$. In the pulsatile flow, there are some initial conditions which have their maximum growth close to the throat even for the highest Reynolds number used.

6.3.4.3 Dependence on Reynolds number for starting phase at $t_0/T = 0.375$

We now extend the analysis for Re -dependence to another starting phase and compare the findings. Figure 6.12 summarizes the optimal energy growth for two-dimensional initial perturbations for starting phase $t_0/T = 0.375$. Optimal energy envelopes against time horizon for Reynolds numbers from 45 to 270 are shown in figure 6.12(a). The maximum energy growth among all optimal initial conditions is $G_0^{max}(270) = 3.65 \times 10^4$ which occurs at $\tau_0^{max}/T = 0.55$, in addition, all energy growth curves have a positive slope for short time. Optimal growth logarithmic contours in the (τ, Re) plane are shown in figure 6.12(b). In this case, we can also identify three groups of local maxima growth, so that the dotted lines indicate the three local of maximum growth as a function of τ in figure 6.12(a,b). The critical value for the smallest growth is $Re_E = 31.5$ for two-dimensional optimal initial perturbations. It should be noted that the Re_E for starting phase at $t_0/T = 0.375$ is higher than at $t_0/T = 0$. Furthermore, the maximum energy growth found at $Re = 270$ for $t_0/T = 0.375$ is also higher than at $t_0/T = 0$. Therefore, we conclude that the shift in the starting phase of the initial condition does not only affect the maximum growth at each Reynolds number but also the critical Reynolds number for the smallest growth.

Variation of maximum growth and time of maximum growth as functions of Re are plotted in figure 6.12(c,d). As happened for starting phase at $t_0/T = 0$, the system presents three groups of local maxima growth. As previously done, the peaks growth were classified by order in which they appeared in figure 6.12(a). An important aspect to notice is that the growth rate of the maximum growth for the *first* and *second peaks* at the starting phases $t_0/T = 0.375$ and the *second peaks* at $t_0/T = 0$ are practically the same. In these three cases, the disturbance exchanges energy with the base flow with the same rate when the Reynolds number is varied, even having different optimal initial perturbations in each group of local maxima growth.

Figure 6.12(e) shows the $\log G_0^{max}$ against τ_0^{max} . Again, we found that the $\log G_0^{max}$

Figure 6.12: Dependence on Reynolds number of the two-dimensional transient energy growth for $t_0/T = 0.375$. (a) Energy growth envelopes, $G(\tau)$, as functions of τ for Reynolds number varying from 45 to 270. (b) Logarithmic contours plot for two-dimensional optimal energy growth, $G(\tau, Re)$, as functions of τ and Re . The critical Reynolds number for the first growth is $Re_E = 31.5$. The dotted-line curves shows the local of maxima energy growth as a function of τ . Variation of maximum growth (c) and time (d) as a function of Re . (e) Maximum energy growth as a function of time of maximum growth. The $\log G_0^{max}$ grows linearly with τ_0^{max} in each group of local maxima growth.

Figure 6.13: Plots of two-dimensional logarithmic contours of energy for starting phase at $t_0/T = 0.375$, computed at $Re = 225$. Optimal initial perturbations (at the top) and Optimal perturbation growth outcomes (at the bottom). The vectors represent the velocity field.

grows linearly with τ_0^{max} in each group of local maxima growth. It is remarkable that each group of local maxima growth has a constant growth rate in both starting phase at $t_0/T = 0$ and $t_0/T = 0.375$. In chapter 5, we also reported that the maximum growth increases exponentially with time of maximum growth with Reynolds number as a parameter for symmetric and asymmetric flows in a constricted channel. Furthermore, Blackburn, Sherwin & Barkley (2008) found the same results for a steady flow in a stenotic pipe. Hence, constant growth rates which relates maximum growth with the time that it occurs using Reynolds number as a parameter could be a pattern for any flow regime in confined flows.

Following the discussion about the structures of the optimal initial perturbations and

their evolution of the starting phase at $\tau/T = 0$. Figure 6.13 illustrates the logarithmic contours of energy for $\beta = 0$ and starting phase at $\tau/T = 0.375$, computed at $Re = 225$. Looking at the initial conditions, it is possible to see that they are mostly concentrated and energetic downstream the throat in the flow separation with a sharp chevron-shaped pattern. This happens because the initial conditions were applied shortly after the peak velocity when the flow was being ejected through the constriction during the formation of the separated flow as shown in figure 6.3.

Analyzing the optimal initial perturbations throughout this paper, we can identify that the quantity of chevron-shaped in the initial conditions upstream and downstream the throat are intrinsically related to the number of counter-rotating rolls which give rise in the wave packet as can be seen in the the figures 6.11 and 6.13, so that each chevron-shaped upstream and downstream the throat contribute to one counter-rotating roll.

6.3.4.4 Dependence on spanwise wavenumber

Going one step further in our analysis, we now present a detailed investigation of the three-dimensional case. So, at this stage, the perturbations are allowed to vary in the homogeneous direction with an additional parameter $\beta = 2\pi/L_z$, the spanwise wavenumber, for a fixed Reynolds number. Here we adopted starting phase at $t_0/T = 0.375$ because it exhibited the highest maximum energy growth for the two-dimensional case.

Figure 6.14 summarizes the optimal energy growth for three-dimensional perturbations. Figure 6.14(a) plots the transient energy growth, $G(\tau, \beta)$, against spanwise wavenumber β and time τ . It is possible to see that, for the smaller β the optimal transient curves are very similar, suggesting that the optimal initial perturbations evolve in a similar way. However, for the higher β there is a drastic change of the maximum growth and time of maximum growth as also observed for the asymmetric steady flow (see §5.3.4.3) and in a backward-facing step (BLACKBURN; BARKLEY; SHERWIN, 2008). Thus, although the flow regimes are quite distinct, this suggest that the geometry has a strong influence in the sense of bound the energy growth, so that it could model the energy growth of a initial condition. Figure 6.14(b) depicts a close-up of figure 6.14(a) for short times with β from 0 to 15 in steps of 1. As observed for steady flows in a constricted channel (Chapter 5), in a axisymmetric pipe (BLACKBURN; SHERWIN; BARKLEY, 2008) and flow past a circular cilinder (ABDESSEMED et al., 2009), first the optimal growth are higher for the higher β and then shortly after the smaller β exceed their energy.

The global maximum growth occurs for the two-dimensional case at $t_0/T = 0.375$, but, this was not the case for $t_0/T = 0$, as shown in figure 6.15. Therefore, although the

Figure 6.14: Dependence on spanwise wavenumber of the three-dimensional transient energy growth for starting phase at $t_0/T = 0.375$, computed at $Re = 225$. (a) Surface plot of energy growth envelopes, $G(\tau, \beta)$, as function of spanwise wavenumber β and time τ . (b) Cut of (a) for short times with β from 0 to 15 in steps of 1.

evolution dynamics of the optimal modes are almost preserved for each starting phase when the spanwise wavenumber is slightly varied, a starting phase shift can change the spanwise wavenumber of the dominant perturbation.

Variation of local maximum growth and time of maximum growth as a function of β are shown in figure 6.16, emphasizing two different branches of local maxima. It is clear that the local maxima suffer a drastic fall for higher spanwise wavenumber, mainly in the time of maximum growth. The *first branch* lies in the smaller spanwise wavenumber, which exhibited the highest local maxima. Increasing the spanwise wavenumber until $\beta = 4.5$, there is a split up between the *first* and *second branches*. It is noteworthy that this same local maxima behavior with spanwise wavenumber was also observed for the asymmetric steady flow (Figure 5.20), with

Figure 6.15: Comparison of two- and three-dimensional optimal energy growth, $G(\tau)$, as a function of relative time at $Re = 225$.

the split up between the branches happening around the same spanwise wavenumber. However, here we just found two instead of three branches of local maxima. Besides that, it should be noted that, when $\beta \geq 5$ we also observed a change in the maximum growth behaviour as shown in figures 5.10 and 5.11. Hence, we can infer that the geometry play a key role in the sense of how the initial conditions involve, as well as changes its instability mechanism. These two branches are classified by the optimal modes, related to each maximum growth.

Figure 6.16(a) shows the variation of local maximum growth against β . It can be seen that the *second branch* decreases linearly with a rate given by $\partial \log G_{\beta}^{max} / \partial \beta = -0.071$. It is a notable result, because this is the same rate that was found in the asymmetric steady flow for the *second branch*. Moreover, it is not intuitive that, two very distinct flow regimes can have the same exponential decrease rate at high β . As previously mentioned, although the symmetric and asymmetric steady flows are flow regimes before and after primary instability, the *third branch* of the asymmetric flow and the symmetric flow also exhibit the same exponential decrease rate with β . The most interesting aspect of these results is that we were able to recover the exponential decrease rate of the *second* and *third branches* of the asymmetric flow from the *second branch* of a pulsatile flow and at high values of β of the symmetric flow, respectively. Thus, in this particular geometry, we find two mechanisms which are dictated by the two exponential decrease rate. In addition, it is remarkable that, although the Reynolds numbers are different in each flow regime, we found similar exponential decrease rates. Therefore, it suggests that the geometry is crucial in establishing the energy exchange between the optimal modes and the base flows, being the unique parameter among all analyzed which remained unchanged.

Figure 6.17 depicts $\log G_{\beta}^{max}$ as a function of τ_{β}^{max} . As happened for the asymmetric

Figure 6.16: Variation of local maxima as a function of spanwise wavenumber of the pulsatile flow for a starting phase at $t_0/T = 0.375$, computed at $Re = 225$. There are two different branches of local maxima. (a) Maximum growth as a function of β . (b) Maximum time as a function of β . The local maxima in the *second branch* decrease in a linear rate for the higher β .

steady flow, there is no global correlation between the local maxima for the pulsatile flow (Figure 6.17(a)). However, at high β , they collapse onto a straight line, so that we can define a linear relationship between $\log G_\beta^{max}$ and τ_β^{max} which is written below

$$\log G_\beta^{max} \simeq 1.000\tau_\beta^{max}. \quad (6.3)$$

Again, we have a constant growth rate for the higher spanwise wavenumber, but here it is restricted from $\beta = 11$ to 20 , because there is an early deviation from the linearity for β higher than 20 (Figure 6.17(b)). So, it is another evidence that does not matter which flow regime is

Figure 6.17: (a) Maximum energy growth as a function of time of maximum growth for a starting phase at $t_0/T = 0.375$, computed at $Re = 225$; (b) close-up of (a) for short times of the local time of maximum growth. There is a constant growth rate which relates maximum growth and time of maximum growth for the higher β in the *second branch*.

being simulated, it could be a pattern of any flow regime in a constricted channel.

In order to understand the convective mechanisms in the three-dimensional case for starting phase at $t_0/T = 0.375$. Figure 6.18 illustrates three-dimensional optimal modes at $Re = 225$. Streamwise velocity iso-surfaces for the optimal initial perturbations are shown at the left-hand side and vorticity iso-surfaces of the optimal perturbation growth outcomes corresponding to the initial conditions are shown at the right-hand side. The optimal mode from the *first branch* is shown in figure 6.18(a). As expected, due to the similar evolution dynamics of the optimal modes, it presents the same structure with a strong chevron-shaped pattern downstream the constriction. In addition, again the sinuous disturbance becomes a wave packet when the initial perturbation evolves. Taking now the optimal mode which were

Figure 6.18: Plots of three-dimensional optimal perturbations before primary instability for starting phase at $t_0/T = 0.375$, computed at $Re = 225$. Streamwise velocity iso-surfaces of the optimal initial perturbation (left-hand side). Vorticity iso-surfaces of the optimal perturbation growth outcomes (right-hand side). The pictures at the top show a side view and those at the bottom show a top view.

generated after $\beta \geq 4.5$ (*second branch*). Although the pulsatile flow suffers a great change in the time of maximum growth from the *first* to the *second branch* (Figure 6.16), it did not modify the shape of their optimal initial perturbations. In addition, as occurred for the optimal modes at high β for the steady case, the optimal mode manifested its optimal growth at the shear layers.

7 PAEDIATRIC VENTRICULAR ASSIST DEVICES

We now change the subject to the numerical modelling and simulation of the paediatric ventricular assist device (PVAD). This work was motivated by a collaboration of the NDF with the Bioengineering laboratory of the Heart Institute of the Medical School of the University of São Paulo and was supported by the FAPESP Project (2012/50283-6).

PVADs are confectioned with geometry and materials similar to those used in adult versions, but in general, present high rates of hemolysis and thrombus formation, which remains an obstacle to the development of these devices. Hence, the development of methodologies for optimizing PVADs is of fundamental importance to obtain a device for long-term use.

In this chapter, a brief literature review about the main topics related to the PVAD will be presented. First, in §7.1, some topics about anatomy and physiology that are important for the project and their relationship to the VAD are explored. Afterwards, in §7.2, the main causes of thrombus formation, hemolysis and clotting in a biological context are described. Next, in §7.3, we briefly discuss the approach of treating the blood as a Newtonian fluid, the validity of this hypothesis and its limitations. After that, in §7.4, the main characteristics of the pulsatile ventricular assist devices are presented, as well as some dimensional and operational features of the VADs, in addition, a quantitative analyses about the causes of thrombus formation and hemolysis in the VADs are delineated. Finally, the haemodynamic metric used to study the blood flow inside the PVAD is presented in §7.5.

7.1 The Heart as a Pump

The structural and functional features of the cardiovascular system can be evaluated by measures applied to any mechanical hydraulic system. The shape, displacement and forces generated by the heart, as well as the main mechanical features of the blood vessels, can be analyzed in terms of the variation of size, pressure and flow. In this context, we will present the principal structural and functional features of the heart, elucidating the functional relation to VADs.

Figure 7.1: Principal structures of the heart. Extracted from Loon (2005).

7.1.1 Structure of the Heart

The heart may be described as a double pump, which moves the blood sequentially through the pulmonary circulation (right side) and systemic circulation (left side) (Figure 7.1). The thickness of each cardiac chamber is directly related to its function. The atria, which has to stand low internal pressures, have walls that are relatively thin. On the other hand, the action of the ventricles develop higher pressures in the flow, so their walls are considerably thicker. In this case, the left ventricle is responsible for the high pressure of the systemic circulation, having walls that are thicker than those of the right ventricle, which do not need to develop very high pressures to pump blood through the pulmonary circulation.

Children with advanced heart failure, which result in failure of the left, right or both ventricle are candidates for implantation of a PVAD. This device has the function of pumping blood to the systemic or pulmonary circulation to aid the left or right ventricles, respectively.

Note that the correct heart function depends on the efficiency of the heart valves, responsible for separating the chambers. In the heart, four important valves are found, being two between atria and ventricles (called mitral and tricuspid valves) and two in the outflow tracts of the ventricles (called pulmonary and aortic valves). The opening of the atrioventricular valves and closing of the pulmonary and aortic valves allows the blood flow from the atria to the respective ventricles, during the ventricular relaxation (diastole); the closing of the atrioventricular valves and opening of the pulmonary and aortic valves allows the blood flow from the right ventricle to the pulmonary artery and from the left ventricle to the aortic artery, which occurs during ventricular contraction (systole) (AIRES, 2008).

The general function of all these valves is to prevent retrograde blood flow or regurgitation. In order to provide good heart efficiency the valves should exert minor resistance to the flow in the opening phase and therefore their leaflets are extremely thin. Their geometry and morphology are such that the leaflets have sufficient tangential stiffness to withstand the pressures to which they are exposed in the closed situation, although the mitral and tricuspid valves also need cords (chordae tendineae) to prevent the valves from prolapsing (LOON, 2005).

7.1.2 Pressure in the Arterial system

The blood pressure in the arterial system is generated and maintained by the interaction between the cardiac driving force, the elastic expansion capacity and the resistance to blood flow carried predominantly by arterioles and arteries of diameter less than 200 μm . This combination allows a system with an intermittent pump to manage supra-atmospheric pressures permanently. Although it is constantly in the upper atmospheric levels, blood pressure in the arterial system oscillates between a maximum and a minimum level, thus, has pulsatile nature. The maximum pressure is reached during systole, and the minimum level during diastole, which is why they are called systolic and diastolic pressure, respectively. The systolic pressure is generated by cardiac systole, and its level depends mainly on factors such: 1) the intrinsic contractile capacity of the cardiac muscle (contractility); 2) the degree of stretching of myocardial fibers (Frank-Starling principle); 3) blood volume present in the left ventricle prior to contraction; 4) resistance against which the heart ejects blood (afterload), mechanism that activate the self-regulation of the heart muscle; and 5) the frequency of the beats that influence the volume per minute of blood ejected by the heart (AIRES, 2008).

7.1.3 Volume-Pressure Diagram

The volume of blood ejected by the ventricle depends on the volume of blood present in the left ventricle at end-diastole (end-diastolic volume). Therefore, according to this relationship, known as the *Frank-Starling mechanism of the heart*, in each cardiac cycle the volume ejected by the heart into the aorta during systole is equal to the volume of blood in the heart received from venous return.

Figure 7.2 shows the volume-pressure diagram of the human heart. The systolic and diastolic pressure curves represent the active and passive pressures of the left ventricle, respectively, as a function of the end-diastolic volume. The arrows, forming an anti-clockwise loop, represent the pressure-volume relation in the left ventricle during the four phases of a cardiac

Figure 7.2: Volume-Pressure Diagram. Relationship between left ventricular volume and intraventricular pressure during diastole and systole. Thick red lines demonstrate changes in intraventricular volume and pressure during the normal cardiac cycle. EW, net external work. Extracted from (GUYTON; HALL, 2006).

cycle.

The end of the period of filling determines end-diastolic volume, which occurs under very low intraventricular pressure. The stretch to which the ventricular walls are submitted at the end of diastole is called preload. The diastolic stretch has a fundamental role in regulating the systolic performance of the heart chambers. At the beginning of the systole the intraventricular pressure rises sharply, with no volume change since the rise of pressure inside the ventricle determines the closing of the mitral valve. Since the aortic valve remains closed, this phase of the cardiac cycle is denominated isovolumic contraction. Insofar as the ventricular contraction progresses, there comes a point at which the intraventricular pressure exceeds the pressure within the aorta. At this moment, the aortic valve opens and blood is quickly ejected into the arterial system. This is the phase of ejection. At the end of ventricular ejection, the pressure falls within the ventricular chamber, which determines the closure of the aortic valve. A part of the blood remains in the ventricular cavity, determining the end-systolic volume of the left ventricle. Finally, the ventricle relaxes sharply, without variation of volume, because the mitral and aortic valves are closed. This phase is called isovolumic relaxation, which closes the cycle (AIRES, 2008).

Figure 7.3: The pressure transients in the left ventricle, left atrium and aorta during one cardiac cycle. Closure and opening of the aortic and mitral valve are shown at the top. Phases of the cardiac cycle: (1) Atrial Systole; (2) Isovolumic Contraction; (3) Ejection; (4) Isovolumic Relaxation; (5) Ventricular Filling. Adapted from (LOON, 2005)

7.1.4 Cardiac Cycle

The pumping action of the heart is reflected in the volume and pressure changes that occur in each cardiac chamber and large arteries when the heart finishes each cycle. Figure 7.3 shows the temporal relation between atrial, ventricular and aortic pressures that occur in the left side of the heart. In this figure, it can be seen that the valves are opened due to a high pressure gradient in the left ventricle, and an open connection between the atrium and aorta is never established, resulting in an efficient pump function.

With the implantation of the VAD, two new valves are introduced, one in the left ventricle and another one in the aorta (figure 7.4). Consequently, the aortic valve is no longer used because in the process of filling of the left ventricle the blood will flow to the VAD and will be ejected directly into the aorta, partially modifying the cardiac cycle. Closure and opening of the valves of the VAD will be established by gradients of pressure created by the new dynamics of the flow, in which the pulsatile pump does the role of the contraction of the left ventricle in the ejection phase.

Figure 7.4: Implantation of the InCor VAD. Adapted from (INCOR, 2012)

7.2 Hemostasis and Thrombosis

The thrombus formation, hemolysis and clotting are some of the main problems in the use of a VAD and they constitute serious challenges for its development and optimization. Therefore, a brief discussion about their causes in a biological context will be made in this section.

Normal hemostasis comprises a series of regulated processes that maintain blood in a fluid, clot-free state in normal vessels while rapidly forming a localized hemostatic plug at the side of vascular injury. The pathologic counterpart of hemostasis is thrombosis, the formation of blood clot (thrombus) within intact vessels.

The three principal biological alterations which lead to thrombus formation (called Virchow's triad) are:

- Endothelial Injury
- Abnormal Blood Flow
- Hypercoagulability

Thrombi can develop anywhere in the cardiovascular system, as for example, in the heart chambers, valves, arteries or capillaries. The size and shape of thrombi depend on the site of origin and its cause. Arterial or cardiac thrombi typically arise at sites of endothelial injury or turbulence; venous thrombi characteristically occur at sites of stasis. Thrombi are focally attached to the underlying vascular surface and tend to propagate toward the heart; thus, arterial thrombi grow in a retrograde direction from the point of attachment, while venous thrombi extend in the direction of blood flow. The propagating portion of a thrombus tends to be poorly attached and

therefore prone to fragmentation and migration through the blood as an embolus. For more detailed information on the biological aspects of hemodynamic disturbances and thromboembolic diseases see Kumar et al. (2010).

7.3 Dynamic Properties of the Blood

In this section, we will address the issue of the use of blood as a Newtonian fluid in VADs and limitations of this approximation.

Blood is a viscoelastic fluid that behaves as a Newtonian fluid at shear rates above 500 s^{-1} . At shear rates lower than 50 s^{-1} , the viscosity of blood increases exponentially due to the formation of large aggregates of erythrocytes. As shear rate increases, the erythrocytes are dispersed and aligned in the direction of the flow (STUART; KENNY, 1980). Consequently, the use of a Newtonian fluid is often justified on the grounds that blood hemolysis is a result of strong shear flows and turbulence, which are characterized by high shear rates (DEUTSCH et al., 2006), that are regularly found in VADs for adults, due to the action of the pulsatile chamber and strong jet to the outlet.

In Bachmann et al. (2000), it was observed that in a PVAD of 15 cm^3 the majority of points in the device have a shear rate of 408 s^{-1} for the Newtonian fluid and 265 s^{-1} for non-Newtonian fluid. The measurements were made using laser doppler velocimetry (LDV). Both of these values are below the critical shear rate of 500 s^{-1} , for which a Newtonian fluid behaviour can be assumed for the blood. Nevertheless, in devices for adults with chamber volume equal to 70 cc the shear rates are on the order of $10,000 \text{ s}^{-1}$ in the central pump region and $25,000 \text{ s}^{-1}$ near the valves (BALDWIN et al., 1988). On the other hand, the PVAD of the Heart Institute that we will study has a volume of 30 cm^3 , i.e., it has a volume intermediate among the devices found in the market. Thus, a detailed study of the flow field and shear rates inside the device must be performed in a first analysis to find out if the approach of the blood as a Newtonian fluid is plausible; otherwise, the use of a non-Newtonian fluid model will be required.

Consequently, as discussed in section 7.4.2, shear rates lower than 500 s^{-1} also generate another problem in the PVAD, because they increase thrombus formation and deposition on the surface of the device. Therefore, preliminary measures during the project will be critical to better understand the possible challenges that will appear during its development.

Finally, it is worth mentioning the high fidelity of the results obtained in (MEDVITZ et al., 2007; MEDVITZ et al., 2009) with CFD, using a Newtonian fluid in a VAD for adults. The methodology was validated with experimental data obtained from particle image velocimetry

Figure 7.5: (a) Ventricular assist device, cannulas and valve. (b) Control unit. Adapted from Galantier (2007).

(PIV).

7.4 Ventricular Assist Device

The VAD system for paracorporeal use of the Heart Institute University of Sao Paulo Medical School Hospital has the following units: pulsatile pump, special cannulas and a mobile unit for control and monitoring of the pulsatile pump (Figure 7.5).

The pulsatile pump is a disposable ventricular orthosis, constructed with biocompatible material. This pump comprises two chambers: pneumatic and sanguine, separated by a medical grade polyurethane flexible diaphragm to act as a blood contacting surface. The blood chamber has variable volume and contains one inlet and one outlet, at which connectors for cannulas and bovine pericardial valve prostheses are accommodated, ensuring a unidirectional flow through the device. The control unit can be operated in four modes for better use of the PVAD, and is composed by a electropneumatic system and a microcomputer. The modes of operation are:

- Asynchronous: Manual selection of frequency and ejection time.
- Auto (full-to-empty): Frequency and flow are adjusted automatically by venous return.
- Synchronous: Synchronized by the R wave of the electrocardiogram (ECG) signal with adjustable rate (1:1 to 1:16).
- Emergency: Manual selection of frequency and ejection time.

for more information about the device, the reader should consult (INCOR, 2015).

Figure 7.6: The InCor PVAD prototype.

For the design of the computational and experimental model we will use a PVAD prototype manufactured according to specifications of the Department of Bioengineering of the Heart Institute (Figure 7.6).

VADs intended for either adults or children use of the same materials and principles of operation. However, the differences in their geometries, such as smaller volume in the blood chambers with a higher ratio between surface area and blood volume, and smaller diameter of the valves orifices provide more blood surface contacting and lower blood flow, respectively, in PVADs. These factors influence the flow features, because they generate turbulence and high WSS during long periods of the pumping cycle, causing hemolysis or pre-rupture of red blood cells (SUTERA; MEHRJANDI, 1975). At the same time, substances released from the red cells during hemolysis influence platelet activation, which combined with regions of stagnant flow or low WSS in the vicinity of the solid walls cause thrombus formation (DAVID; THOMAS; WALKER, 2001).

The non-physiologic flow patterns generated in the device are considered one of the major culprits in enhancing the hemostatic response by chronically activating platelets, yet in the lack of an appropriate methodology, this becomes the biggest obstacle in optimizing the device at the stage of research and development (BLUESTEIN; CHANDRAN; MANNING, 2010).

7.4.1 Dimensional Analysis

In the present section, we will discuss some dimensional and operational features of the VADs that can naturally be represented as dimensionless quantities, e.g., the Reynolds and Strouhal numbers, which determine the nature of the flow. The Reynold and Strouhal numbers can be

define respectively as

$$St = \frac{UD_i}{\nu} \quad (7.1)$$

and

$$St = \frac{UT}{D_i}, \quad (7.2)$$

where U is the reference flow velocity, T is the cardiac cycle as reference time and D_i is the diameter of the mitral port as reference length.

Following the same analysis developed in (BACHMANN et al., 2000) for dimensionless quantities, if we choose the diastolic duration as 50% of the cardiac cycle and consider the cross-sectional area of the mitral valve (inlet port) as $1/4\pi D_i^2$, so the frequency of the cardiac cycle is $f = 0.5T$, and consequently U can be evaluated from the average cardiac output Q . The average flow rate during the diastole is twice the cardiac output, since the fluid get inside the device for only half part of the cardiac cycle. Then, the equation for the average flow velocity during the diastole is $U = 8Q/\pi D_i^2$. It is noteworthy that, $Q = f \cdot SV$, where SV is the stroke volume. Assuming that the non-Newtonian nature of blood does not introduce any additional parameters, the “global” fluid dynamics of the system is described by the Reynolds and Strouhal numbers. If we substitute the expressions analyzed here for a diastolic duration of 50% in the equations (7.1) and (7.2) we have

$$Re = \left(\frac{8}{\pi\nu} \right) \frac{f \cdot SV}{D_i} \quad (7.3)$$

and

$$St = \left(\frac{4}{\pi} \right) \frac{SV}{D_i^3}. \quad (7.4)$$

The values for the Reynolds and Strouhal numbers for VADs from InCor and the Pennsylvania State University (Penn State) operating at 70 beats per minute (for 50% diastolic duration) and kinematic viscosity of $3.77 \times 10^{-6} \text{ m}^2/\text{s}$ are presented in table 7.1. The Reynolds number is a strong function of pump size and therefore is reduced in the pediatric pump. The elevated St seen with the Penn State 15 cc pump reflects the fact that the inlet port was undersized relative to a geometrically similar design (BACHMANN et al., 2000). In addition, it is worthy noting that Bachmann et al. (2000) reported that Strouhal numbers out of the range from 4 to 7 may indicate improper vortex formation and the possibility of poor wall washing, being the Strouhal number an essential parameter to evaluated VADs. Therefore, the reduction of the size of the VADs for the use in children alter the internal flow field, and it is suggested that fluid dynamic factors are responsible for the high degree of thrombus formation observed in PVADs.

Table 7.1: Comparison of the Reynolds and Strouhal numbers of the VADs.

Pump size	Re	St
InCor 65 cc device	2049	5,3
InCor 30 cc device	1075	3,6
InCor 15 cc device	695	3.9
Penn State 70 cc device	2482	8,3
Penn State 50 cc device	1054	4.5
Penn State 15 cc device	1567	45,8

7.4.2 Quantitative Analysis of Thrombus Formation and Hemolysis in VADs

In this section, we will deal with mechanical aspects of the flow in blood pumps, which contribute for thrombus formation and hemolysis.

As mentioned previously, thrombosis, the destruction of red blood cells (hemolysis), and clotting formation must be avoided in artificial blood pumps to achieve long-term clinical success. Daily et al. (1996) pointed out that the thrombogenicity of assist devices can be attributed to (1) the coagulability of the blood, (2) the properties of the blood contacting surfaces, and (3) fluid dynamic factors. The relationship of these to the fluid mechanics, velocity, shear and wall shear rates, and turbulence is the major impetus for flow studies in blood pumps. None of these phenomena is completely understood. A hemolysis potential curve from the National Heart, Lung, and Blood Institute, which relates shear stress and exposure time to red cell, white cell, and platelet lysis has been available since 1985 (DEUTSCH et al., 2006).

Hubbell & McIntire (1986) reported that the critical shear rate for which clotting is maximum on segmented polyurethane, the material used for the blood sac, is 500 s^{-1} . Below this value, it is believed that convective transport mechanisms to the surface increase with decreasing shear rate, yielding an increase in thrombus formation and deposition. Above the critical value, although more blood is potentially damaged, wall shear forces exceed adhesion forces, and clotting factors are washed away from the surface. Thrombus depositions are subsequently reduced with increases in shear beyond 500 s^{-1} .

Pulsatile pumps are characterized by inlet jets that set up a rotational “washing” pattern during filling. Because blood cells are viscoelastic, they can tolerate high stresses for short exposure times without hemolysis. For example, an exposure time of more than 0.1 ms at a shear stress of $10,000 \text{ dynes/cm}^2$ will produce red cell lysis as will 1500 dynes/cm^2 for times over 100 s (DEUTSCH et al., 2006). Sustained turbulent stresses above 4000 dynes/cm^2 created by a submerged jet can also damage blood cells (SALLAM; HWANG, 1987). However, platelet

activation and the initiation of the clotting process may occur at even lower stresses (DEUTSCH et al., 2006).

The measurement of hemolysis directly through quantification of plasma-free hemoglobin, involving human blood in a VAD of 100 cc, indicating that the degree of hemolysis is a function of the operating condition of the ventricle was found by Jarvis, Tarbell & Frangos (1991). For example, 90 bpm produced a third more hemolysis than did 60 bpm, with both at 50% systolic duration.

7.5 Haemodynamic metric

Now we will present the haemodynamic metrics used to study the blood flow inside the PVAD.

The wall shear stress is the tangential force exerted by the flowing blood on the device walls. Since, the blood was considered as a Newtonian fluid in this thesis, the shear stress is proportional to the gradient of the velocity (shear rate), so we can define the shear stress vector as

$$\vec{\tau}_w = [\mu(\nabla \mathbf{u}) \cdot \hat{\mathbf{n}}]_{wall}, \quad (7.5)$$

where μ is the dynamic viscosity. Consequently, the wall shear rate (WSR) is

$$\text{WSR} = \frac{\vec{\tau}_w}{\mu} = [(\nabla \mathbf{u}) \cdot \hat{\mathbf{n}}]_{wall}. \quad (7.6)$$

In the last decades, time-averaged metrics have been extensively applied in order to understand diseases in biological system caused by flow-related mechanism (PEIFFER; SHERWIN; WEINBERG, 2013; MOHAMIED et al., 2014). An important metric to analyze the wall shear rate in a time-dependent environment, which occurs in VADs, is the time-average wall shear rate (TAWSR) which is calculated using the following definition

$$\text{TAWSR} = \frac{1}{T} \frac{1}{\mu} \int_0^T |\vec{\tau}_w| dt. \quad (7.7)$$

The TAWSR can be considered as the time-average of the WSR magnitude.

8 NUMERICAL SIMULATIONS OF THE FLOW INSIDE A PVAD

This chapter address the growing need for tools to understand the haemodynamic of the In-Cor PVAD under development in the Heart Institute University of São Paulo Medical School Hospital for patients under 25 kg of body weight.

However, there is a great obstacle to the development for such models, which is the difficulty to simulate the fluid-structure interaction (FSI) between the blood and the flexible membranes of the artificial cardiac valves and diaphragm. Hence, firstly, in order to develop a model that properly represents the diaphragm motion and opening and closure of the mitral valve, a preliminary model is presented based on special boundary conditions. More specifically, the driving force and the flow direction of the diaphragm are defined by velocity distribution on the diaphragm wall, and the opening and closure of the mitral valve are performed by a velocity waveform which goes to zero in the systolic period. Previous work by Medvitz et al. (2007) studied a piston motion model based on a physiologic flow waveform observed during experiments and valve closure was modeled by locally increasing the viscosity during the closed phase, which was validated by comparing simulation results with particle image velocimetry (PIV).

The aim of this chapter is to study the blood flow in a 35 cc PVAD, which was based on the InCor PVAD geometry, by means of computational fluid dynamics (CFD). We intend to contribute to a better understanding of the flow field within the device, and its relation to thrombus formation and deposition on its surface and occurrence of hemolysis which are the greatest obstacles to its development. The pneumatic PVAD was operated at rates of 120 bpm, 90 bpm and 60 bpm with a fixed diastolic duration of 2/3 of the cardiac cycle time to understand the differences of the fluid motion in each condition. However, the mitral and aortic valves were removed from the geometry model. Flow patterns, velocity fields, WSR and time-average wall shear rates (TAWSR) were analyzed to evaluate the performance of the device.

In §8.1, there are the methodology approaches for the computational simulations, such as the diaphragm model, a detailed description of the pump cycle and geometry discretization.

Figure 8.1: The PVAD geometry

The main findings are described in §8.2.

8.1 Methodology

8.1.1 Problem description

The computational simulations of the flow inside the 35 cc PVAD was performed at three different operating conditions. The PVAD was operated at rates of 120 bpm, 90 bpm and 60 bpm to explore the aspects of the fluid motion in each condition. We employed a diastolic duration of $2/3$ of the cardiac cycle time for all cases. The mitral and aortic valves were removed (22 mm mitral and 14 mm aortic), so that there was no obstruction to the flow to get inside the device (Figure 8.1).

8.1.2 Computational simulations

An unsteady three-dimensional computational fluid dynamics (CFD) model was developed to assess the performance of the 35 cc PVAD. In this study, blood was treated as an incompressible Newtonian fluid. Numerical simulations were carried out using the Spectral/hp Element Method (KARNIADAKIS; SHERWIN, 2005). For the cases investigated in this work, blood is governed by the Navier-Stokes equations (Equations (2.1)).

Figure 8.2: Velocity waveforms applied at the diaphragm and inlet as a function of time.

8.1.3 Diaphragm model

The flexible membrane that separates the pneumatic and sanguine chambers was modeled in a fixed position. Therefore, the diaphragm was dealt by special boundary conditions to represent the diaphragm motion. In other words, the driving force and the flow direction were defined by velocity distribution on the diaphragm wall as follows

$$\mathbf{u}_{wall}(x, z, t) = u_{diaphragm}(t) \left(1 - \frac{x^2 + z^2}{R_d^2} \right) \hat{\mathbf{y}} \quad (8.1)$$

where $u_{diaphragm}(t)$ is the diaphragm velocity, x and z are the Cartesian coordinates on the plane of the diaphragm with origin in the diaphragm center, R_d is the radius of the region of the diaphragm that is allowed to move and $\hat{\mathbf{y}}$ is the versor component along the y direction.

8.1.4 Pump cycle

Figure 8.2 shows velocity waveforms which were applied at the diaphragm and inlet as a function of time and normalized by the mean inlet velocity u_m . From these two waveforms we can easily see the systolic and diastolic periods, in order to simulate the cardiac cycle. Firstly, the diaphragm pushes the blood out of the chamber through the aortic port, while the mitral port remains closed. Afterward, at the diastole, the mitral port is opened and the blood is allowed to enter the chamber and 35 cc is injected within the pump, while the diaphragm velocity is negative. Two important points related to diaphragm negative velocity are noteworthy, in order to justify this modeling. First, in our geometry the diaphragm is a flat surface; however when the diaphragm is in its diastolic position it is curved and can store part of the volume which

Figure 8.3: Force coefficients as a function of time when the device is operated at a rate of 120 bpm, using $P = 5$.

gets inside the chamber. So, in this way, 20% of the the fluid is taken out of the chamber in the diastole. Second, the force with which the diaphragm pushes the fluid towards itself, when it returns to the diastolic position can be thought as a velocity distribution to simulate the suction. The opening and closure of the aortic valve was not modeled, so that the aortic port remains open at the whole cycle. So we can define the diaphragm and inlet velocity as follows

$$u_{diaphragm}(t) = \begin{cases} A_{di} \sin(\frac{3\pi t}{T}) & \text{if } 0 \leq t/T < \frac{T}{3} \\ A_{do} \sin(\frac{3\pi t}{2T} - \frac{\pi}{2}) & \text{if } \frac{T}{3} \leq t/T < T \end{cases} \quad (8.2)$$

and

$$u_{inlet}(t) = \begin{cases} 0 & \text{if } 0 \leq t/T < \frac{T}{3} \\ A_i \sin(\frac{3\pi t}{2T} - \frac{\pi}{2}) & \text{if } \frac{T}{3} \leq t/T < T \end{cases} \quad (8.3)$$

where $u_{inlet}(t)$ is the inlet velocity, A_{di} is the positive velocity amplitude of the diaphragm, A_{do} is the negative velocity amplitude of the diaphragm and A_i is the inlet velocity amplitude.

8.1.5 Discretization

The Spectral/ hp element method was applied to simulate blood flow inside the device, which requires that the computational domain is subdivided into elements. The total number of volume elements constructed for the PVAD were 31355 and all of them are tetrahedrons (Figure 8.4). Since high-order polynomials can represent the solution within each element of the mesh, the mesh generated in this study was made relatively coarse. The same mesh was used for all simulations even for different operating conditions. Convergence of the solutions was verified

Figure 8.4: Computational mesh of the PVAD

calculating the root mean square (RMS) value of the force coefficients on the device surface in the eighth cardiac cycle. The force coefficients as functions of time when the device was operated at a rate of 120 bpm are shown in figure 8.3. Then the polynomial order, P , was increased within each element to achieve a satisfactory numerical error. The convergence analysis for the three operating conditions are shown in tables 8.1, 8.2 and 8.3. It can be seen that with 5^{th} order polynomials (i.e. 6^{th} order accuracy in space), which corresponds in terms of degrees of freedom to meshes of approximately 3.9 million tetrahedral elements, the convergence is reached with uncertainty less than 1% in all cases. Hence, the computation simulations were performed using $P = 5$.

The triangular external faces of the tetrahedral elements were curved using SPHERIGON patches (VOLINO; MAGNENAT-THALMAN, 1998), following a method developed by Plata (2010). Therefore, although the mesh had elements with large sizes the surface mesh was curvilinear.

8.1.6 Modeling parameters and boundary conditions

The fluid properties were chosen to match the blood analog fluid usually employed in the in vitro experiments. We assume the blood density $\rho = 1099.84 \text{ kg/m}^3$ (FERRARA et al., 2010), the kinematic viscosity $\nu = 0.03 \text{ cm}^2/\text{s}$ (FERRARA et al., 2010) and the diameter of the mitral port $D_i = 2.2 \text{ cm}$.

The values for the Reynolds and Strouhal numbers at the three operating conditions analyzed are showed in table 8.4. Note that the Strouhal numbers are equal for all cases because it only depends on the geometric parameters. Therefore, regardless of the characteristic length chosen, the Strouhal number will be preserved in geometrically similar pumps. The pressure

Table 8.1: The effect of the spectral element polynomial order P on force coefficients at the surface of the PVAD for 120 bpm.

P	fx_{rms}	% diff	fy_{rms}	% diff	fz_{rms}	% diff	ft_{rms}	% diff
6	544.41	—	5153.86	—	1313.79	—	2412.60	—
5	548.54	-0.76	5195.98	-0.81	1324.87	-0.84	2425.86	-0.54
4	552.76	-1.53	5256.52	-1.99	1339.02	-1.92	2487.62	-3.10
3	572.29	-5.12	5419.85	-5.16	1383.59	-5.31	2646.69	-9.70

Table 8.2: The effect of the spectral element polynomial order P on force coefficients at the surface of the PVAD for 90 bpm.

P	fx_{rms}	% diff	fy_{rms}	% diff	fz_{rms}	% diff	ft_{rms}	% diff
6	409.83	—	3886.28	—	990.60	—	1802.78	—
5	411.04	-0.30	3892.14	-0.15	992.44	-0.19	1819.33	-0.92
4	413.82	-0.97	3933.54	-1.22	1002.01	-1.15	1857.45	-3.03
3	429.28	-4.75	4082.55	-5.05	1041.89	-5.17	2008.04	-11.39

Table 8.3: The effect of the spectral element polynomial order P on force coefficients at the surface of the PVAD for 60 bpm.

P	fx_{rms}	% diff	fy_{rms}	% diff	fz_{rms}	% diff	ft_{rms}	% diff
5	274.68	—	2605.85	—	664.35	—	1219.28	—
4	276.14	-0.53	2628.85	-0.88	669.63	-0.80	1223.93	-0.38
3	281.94	-2.64	2675.34	-2.66	682.45	-2.72	1305.80	-7.10

Table 8.4: Comparison of the Reynolds and Strouhal numbers for different operating condition

Operating condition	Re	St
120 bpm	2025	4.2
90 bpm	1519	4.2
60 bpm	1013	4.2

and the velocity gradient were set to zero at the outlet boundary condition. No-slip condition was imposed at the device walls.

8.2 Results and discussion

Figure 8.5 shows the fluid dynamics within the PVAD at operating condition of 120 bpm during a cardiac cycle. At peak systole, when the mitral port was closed and the ejection on the diaphragm was maximum, the fluid was pushed out of the chamber straight to the outflow as

Figure 8.5: Colour maps of velocity magnitude (m/s) at 120 bpm close to (a) peak systole ($t/T = 0.15$) and (b) peak diastole ($t/T = 0.65$). The slices were taken to 35 degrees from the plane xz . The vectors represent the velocity field.

shown in figure 8.5(a). Afterward, at peak diastole, the mitral port was opened and the fluid was ejected inside the chamber; however, in our model the aortic port remains open at the diastole, so that the flow can take two paths. The first of them, the fluid goes directly to the outflow with separated flow at the right wall of the outflow. The second of them, the fluid penetrates more deeply inside the chamber as showed in figure 8.5(b). An important aspect to notice about the model is that, during the systolic period the ejection of fluid out of the chamber is not too strong. It mainly occurs because the diastolic volume does not remain inside the chamber so that less fluid is ejected during the systolic period.

Figure 8.6 illustrates the TAWSR distribution on the PVAD surface at operating conditions of 120 bpm, 90 bpm and 60 bpm, respectively. As we can see the TAWSR pattern becomes increasingly heterogeneous mainly at the outflow region when the beat rate is increased, revealing a strong relationship between beat rate and WSR. Two important observations can be made. The first is that only at 120 bpm the WSR is acceptable at the bottom of the chamber such that it exceeds 500 s^{-1} at each spatial location for at least a part of the cardiac cycle, allowing a good wall washing pattern, although the TAWSR is lower than 500 s^{-1} in some regions as shown in figure 8.6(a). However, there is a high potential of thrombus formation and deposition on the segmented polyurethane due to the low WSR for operating condition of 60 bpm. Analyzing the instantaneous flow field, the WSR did not exceed 500 s^{-1} at any time of the cycle (figure 8.7), and the TAWSR demonstrated really low values at the bottom of the device as shown in figure 8.6(c). The second is that, high WSR is found at the outflow region with peak WSR of the order of 10^4 s^{-1} . Nevertheless this is not enough to damage the red blood cells (RBC) if exposed at short times (DEUTSCH et al., 2006; SUTERA; MEHRJANDI, 1975). However, attention must be paid in this region because we did not use valves in our model yet, which certainly will increase the WSR in most part of the device due to the strong jets imposed by

Figure 8.6: Colour maps of TAWSR (s^{-1}) on the surface of the PVAD at (a) 120 bpm , (b) 90 bpm and (c) 60 bpm.

Figure 8.7: Colour maps of WSR (s^{-1}) on the surface of the PVAD at 60 bpm close to peak diastole ($t/T = 0.65$)

Figure 8.8: Colour maps of velocity magnitude (m/s) close to the peak diastole ($t/T = 0.65$) at operating condition of 120 bpm, 90 bpm and 60 bpm, respectively from left to right in three different planes. (a) 8 mm from the base face (plane xz), (b) -8 degrees from the plane yz (inflow region), (c) 8 degrees from the plane yz (outflow region). The vectors represent the velocity field.

artificial heart valves.

In order to investigate the flow field inside the device in each operating condition, the

velocity magnitude at the base, inflow and outflow regions, close to the peak diastole ($t/T = 0.65$), are shown in figure 8.8. It can be seen that the velocity magnitude is low at the bottom of the device in all cases, which explains why the WSR is so low in this region mainly at 60 bpm (Figure 8.8(a-c)). In addition, there is a drastic fall of velocity inside the device when the beating rate is decreased from 120 bpm to 60 bpm. It should be also noted, that there is a great difference of velocity magnitude and WSR between the inflow and outflow regions which is due to the uneven diameters between them, with peak velocity magnitude of approximately 4.0 m/s at the outflow region at 120 bpm. So the smaller size of the aortic port could make it prone to high rate of hemolysis.

9 CONCLUSIONS AND OUTLOOK

Biological and bio-inspired geometries flows were investigated by means of computational fluid mechanics and the Spectral/*hp* element method was employed to solve the fluid motion equations. However, two different approaches were carried out to explore the fluid motion inside these geometries. For the constricted channel, stability analyses were performed for steady and pulsatile flows to understand transition mechanisms in these systems. On the other hand, for the paediatric ventricular assist device, a model to represent the blood flow inside the pump was developed. Therefore, the idea behind this thesis was study idealized biological geometries in order to contribute for the comprehension of possible diseases which can eventually occur in these environments.

In this chapter, the main conclusions and future works will be delineated. In §9.1 conclusions are drawn regarding the stability study in the constricted channel. Afterwards, in §9.2, the main results and future works related to the paediatric ventricular assist device are described.

9.1 Hydrodynamic stability

Results have been presented from two- and three-dimensional nonlinear simulations, and normal and non-normal stability analyses of steady and pulsatile flows in a straight channel with a smooth constriction with 50% occlusion. Linear stability analysis was employed to determine the linearly unstable regions and critical values of the flows. Knowing the flow parameters for which the flows are unstable, fully three-dimensional simulations were carried to study the transition mechanism behind the bifurcations. Motivated by the hysteretic behaviour of the transition processes of the flows, non-normal analysis was also performed with the aim of exploring further the physical mechanism behind this bifurcations. Dependence on phase, Reynolds number and spanwise wavenumber were exhaustively investigated and the convective instabilities examined. In addition, we investigated an example of bypass transition with the nonlinear effects being triggered by an optimal initial perturbation in a linearly stable region for

the asymmetric steady flow.

The primary bifurcation of the symmetric steady flow revealed an intricate character, in which the three-dimensional Fourier modes transfer their energy to the two-dimensional mode, such that there is a symmetry breaking of the flow before the transition, creating a hysteretic region. It is noteworthy that the symmetric breaking did not happen for two-dimensional simulations, being it a three-dimensional effect. Therefore, the bifurcation is due to a three-dimensional perturbation, which transfers its energy to the two-dimensional mode, leading it to nonlinear saturation and as a consequence the symmetry breaking occurs. The secondary instability (asymmetric flow) presented a subcritical behaviour of a pitchfork bifurcation and a huge hysteretic region was found, which extends far away from the critical point. Unlike what happens in the constricted channel, Rani & Sheu (2006) reported that a supercritical Hopf bifurcation was obtained for the primary instability in a backward-facing step (BARKLEY; GOMES; HENDERSON, 2002). So, although both flows are confined by parallel walls and asymmetric, they bifurcate by different paths. Hence, we can conclude that the bifurcation is notably influenced by the shear layers, since the separated flow of the backward-facing step and the constricted channel are very different.

Comparing the dependence on Reynolds number of the steady flows before and after the primary bifurcation, the two-dimensional maximum growth increased exponentially with $Re^{5/4}$ and Re , respectively. It indicates that the flow regime changes the physical mechanism which takes the optimal initial perturbations to their maxima. In addition, after the first bifurcation, when the asymmetric flow takes place, the two-dimensional maximum growth increases with a rate given by $\partial \log G_0^{max} / \partial Re = 0.0113$, being practically the same found by Blackburn, Barkley & Sherwin (2008) in the flow past a backward-facing step. On the other hand, the time of maximum growth increased with a different linear rate. Therefore, we believe that, although the geometries are different, the flow regime (asymmetric flow) and the channel geometry (common on both) play a key role in the sense of how the perturbation exchange energy with the base flow. However, the location where the growing initial perturbations are located and their shapes will establish how far the disturbances will be convected as well as how long they will exchange energy with the base flow. As a consequence of the strong correlation between maximum growth and time of maximum growth with the Reynolds number, for the symmetric and asymmetric flows, the maximum growth increased exponentially with time of maximum growth. From this correlation we conclude that in each flow regime the initial perturbations travels to their maxima with the same constant growth rate with Reynolds number as a parameter.

An significant finding of this study was that it was possible to transition the flow to the top part of the hysteretic curve of the subcritical bifurcation (linearly stable region of the asymmetric steady flow) by nonlinear saturation, seeding the base flow with an optimal initial perturbation with an initial energy above a certain threshold. Another important point about this nonlinear saturated state was that, depending on the number of spanwise Fourier modes the flow establishes different transition regimes. When we performed simulations with 4 Fourier modes, the flow achieved nonlinear saturation, moreover the flow that was established is stationary. However, using 8 Fourier modes, the system reached a regime where the two- and three-dimensional modes exchange energy in an oscillatory behaviour between the saturated state and a stage of redistribution of energy which brings the energy of the three-dimensional modes down again. Hence, the modes of short wavelengths prevent the saturated state to hold. Furthermore, the two-dimensional mode is crucial for the transition processes of the primary and secondary global instabilities, because in both flow regimes the two-dimensional mode led them to the nonlinear saturated state. The energy exchange between two- and three-dimensional modes plays a very important role in this physical mechanism.

As a final thought throughout this context, we identified that the asymmetric flow in the constricted channel and in the backward-facing step bifurcate by different physical mechanisms, however it is intriguing that the two-dimensional maximum energy growth increases exponentially with Reynolds number by the same growth rate in both flows. Thus, it is another evidence that the asymmetric channel flow establishes the way how the flow exchanges energy with the perturbation, showing the importance of the geometry, even though the shear layers have different shapes. Nevertheless, the shear layers were decisive for the flow transition, with each flow exhibiting different characteristics when they bifurcate.

The transition process behind the primary bifurcation of the pulsatile flow occurs by energy transfer from the three-dimensional modes to the two-dimensional mode. This physical mechanism was also observed for the symmetric steady flow, suggesting that it can be a response of the system for flow regimes which are symmetrically ejected from the throat in a constricted channel with 50% occlusion. However, when the two-dimensional mode achieves nonlinear saturated state in both flows, they suffer different effects from the transition processes. The symmetric steady flow becomes asymmetric through the transition, but the pulsatile flow stays symmetric with respect the channel centreline. It should be also noted that the two-dimensional mode was also important in the transition process of secondary bifurcation of the asymmetric flow. Therefore, from this three transition processes, we can conclude that the two-dimensional mode plays a key role in this geometry.

However, certain points still need to be clarified with respect to the transition process of the primary instability of symmetric and pulsatile flows. First, the physical mechanism by which the three-dimensional modes transfer their energy to the two-dimensional mode was not completely explained. In addition, it should be verified if this energy transfer results from weakly non-linear effects. Third, the mechanism which stabilizes the original unstable three-dimensional modes when the two-dimensional mode grows was not investigated. Finally, it can be investigated if a finite spanwise extent with end-walls as would be done in a real experiment would exhibit a behaviour similar to that observed here.

A central outcome from non-normal analysis of the pulsatile flow is that the optimal growth is preserved along the pulse cycle periods, so that, at the end of each cycle period the optimal growth has the same energy for all starting phases, it happens because in a energy balance the optimal modes acquire and lose energy through the cycle until achieve the same level. More than that, all the optimal initial perturbations and their optimal modes also presented the same shape and location. This suggests that the optimal modes are equally affected by the mean flow.

Analyzing the dependence on Reynolds number of the optimal modes of the pulsatile flow, it was shown that, as occurred for the steady flows, there were constant growth rates which relate local maximum growth and time of maximum growth, so that the optimal modes grow to their maxima with the same growth rate. However, due to the complexity of the time-dependent flow, three different optimal initial perturbations were triggered which led to distinct growth rates in each starting phase studied. It means that there are at least three modes competing as optimal during the pulse cycle periods, although they do not manifest their peak growth at the same time. Therefore, in the pulsatile flow, we found three empirical functions for each starting phase which relates local maximum growth and time of maximum growth. If we extended this behaviour for any optimal perturbation, it suggests that every optimal mode increases in energy and time peaks by a constant growth rate, when the Reynolds number is the parameter which is varying.

When the spanwise wavenumber was increased there was a rupture in the optimal modes behaviour around $\beta = 4.5$ in the three flow regimes. This behaviour change gives rise to branches of similar optimal modes, which were marked by a drastic fall in the time of maximum growth and consequently the optimal modes started to manifest their maximum growth at the shear layers. Thus, the split up between the *first* and *second branches* occurred around $\beta = 4.5$ for the asymmetric and pulsatile flow, in addition the symmetric flow also exhibited a deviation from the linear growth, in figure 5.11, around this spanwise wavenumber, suggesting a geometry

effect. Nevertheless, the symmetric flow does not suffer a intense break at $\beta = 4.5$, as happened for the asymmetric and pulsatile flows, creating different branches.

In the three flow regimes, we found exponential decrease rates of the local maxima growth with respect to the spanwise wavenumber when its value is high. It happened because the optimal growths are associated with the shear layers and strong gradients, having their maxima growth close to the throat and afterwards they decayed quickly downstream due to diffusion effects. The shear layers effects are so remarkable that we can predict the maximum growth and time of maximum growth in each β for a determined Re . In addition, the exponential maximum growth decrease rate of the *third branch* of the asymmetric flow has practically the same rate with β found in the symmetric flow. More notable is that the *second branches* of the asymmetric and pulsatile flows also have the same exponential decrease rate, being that these branches were created by similar split up around $\beta = 4.5$. Thus, we can identify two physical mechanisms of energy exchange. This is a strong evidence that the physical mechanisms that establish the influence of the spanwise number on the local maxima growth should be the same in each case. We propose that, the main characteristic behind it is the geometry (constricted channel), due to it is the unique common feature between the three flow regimes. Therefore, it suggests that these two physical mechanisms of energy exchange are intrinsic to the constricted channel flow, because we were able to recover both mechanisms in distinct flow regimes, being that the asymmetric flow inherited both.

Another interesting finding was that each branch presented its own convective mechanism. The *second branch* was generated by velocity gradients in the shear layers and within the large recirculating region, thus the optimal initial perturbations laid concentrated at lower channel walls. On the other hand, the *third branch* took place mostly at the upper channel wall and free stream, so that the optimal modes travel mainly between the recirculating regions until reach their optimal growths. In addition, the optimal modes *second* and *third branches* did not evolve to wave packets formed by the series of spanwise counter-rotating rolls, how is normally observed in channels. Finally, in the *first branch*, the optimal initial perturbations equally spread upstream and downstream the throat.

9.2 PVAD model

The model developed for the PVAD is simple, however it was able to properly represent the three-dimensional WSR on its surface and velocity field inside the device, which give us an idea of the order of magnitude of these quantities in the prototype. Therefore, we can conclude, from

these first data, that the WSR falls significantly when the beat rate is decreased from 120 bpm to 60 bpm, which can make the use of PVAD devices at reduced beat rate not advisable, as also observed in a 15 cc PVAD by Roszelle et al. (2008). This is because of the low WSR at the device wall, which has high potential of thrombus formation and deposition on the segmented polyurethane. On the other hand, the PVAD operated at a rate of 120 bpm shows excellent results, due to the WSR was neither high enough to damage the RBC nor sufficiently low to allow thrombus deposition. However, it is worth mentioning that the difference between the inflow and outflow diameters causes a great difference of WSR in these two regions, reaching such a value that velocity magnitude achieves approximately 4.0 m/s at the outflow. It should be also noted, that valves were removed, as well as the operating features were not all considered in this model, so that the nature of the fluid dynamics inside the device is not completely represented.

Although, the preliminary model was quite promising, it still needs to be refined and made more sophisticated, in order to obtain more accurate information to propose changes in the design and improve the hydrodynamic performance of the device. Bering it in mind, in the near future, the next steps to improve the PVAD model should be to develop a method to close the aortic valve following the approach presented by (AVRAHAMI et al., 2006; AVRAHAMI; ROSENFELD; EINAV, 2006), in which the opening and closure are achieved by changes in the fluid viscosity in a region close to the valve. In addition, particle tracking can be employed to visualize the flow patterns and then obtain the haemodynamics characteristics. Once the model is developed and tested, a model for the valves should be placed in the device to maintain the unidirectional flow through the device, with the opening and closure prescribed.

A more accurate representation of the diaphragm is also of paramount importance and the use of dynamic mesh will be necessary for that. Thus, fluid-structure interaction should be incorporated in the solution of the algorithm, so the valves can open and close in response to the flow, however it will be executed in last stage of model.

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