Mesoscopic Computational Haemodynamics

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Chapter 2

Model Considerations

"Life is short, Art is long"

Hippocrates

Haemodynamics comprises three major problems: the physics of pressure and flow in the circulation, its role in the living systems and the use of this knowledge for diagnostic and clinical activities. This chapter is concerned with the physical principles of the mechanics of the circulation in large blood vessels. The governing equations of motion are studied and major flow characteristics in simplified geometries are investigated. Most of the brief treatment in this chapter follows some of that available in literature (McDonald, 1974; Pontrelli, 1998)

2.1 Blood

Blood is a suspension of formed blood cells and some liquid particles (the chylomicrons) in an aqueous solution (the plasma). The most important mechanical property of blood that influences its motion is the apparent viscosity η, which relates the shear rate γ and the shear stress σ. If this relationship satisfies the Newton's law of viscosity

$$\sigma = -\eta\,\gamma \tag{2.1}$$

where the viscosity η is independent of the shear rate γ, the fluid is known to be Newtonian. In this sense, blood is a non-Newtonian fluid, especially when the shear rate is small, in small vessels and arterioles. Experimentally, it has been reported that when the shear rate is about $1000\ sec^{-1}$, a typical value in large vessels, the non-Newtonian behaviour becomes insignificant and the apparent viscosity asymptotes to a value in the range 3 – 4 cP[1] (Caro *et al.*, 1978), while for low shear rate ($\gamma < 1\ sec^{-1}$) it rises steeply. The red cells are in part responsible for the non-Newtonian behaviour. More details can be found in literature (e.g. Caro *et al.*, 1978). The rheological properties of

[1]The poise (P) is the CGS unit of viscosity. $1P = 1\ g\ cm^{-1} sec^{-1}$. The centipoise (cP) is one hundredth of a Poise.

non-Newtonian fluids are quite different from those of the Newtonian ones. The shear rate dependent viscosity, normal stress differences, secondary flows, stress relaxation and creep are all challenging behaviours that need to be handled carefully. Numerous empirical models for the viscosity of non-Newtonian fluids have been proposed (e.g. Chrochet and Walters, 1983; Pontrelli, 1997). These can be categorised into two main groups (see e.g. Bird, Stewart and Lightfoot, 1960); two-parameter models (e.g. Bingham model and Ostwald-de Waele model, known as the power law) and three-parameter models (e.g. Ellis model and Reiner-Philippoff model). For blood, the viscosity depends mainly on the protein concentration of the plasma, the deformability of the blood cells, and the tendency of blood cells to aggregate (Fung, 1993). Consequently, the viscosity of blood varies with the shear rate of the flow. It increases with decreasing shear rate[1], increasing haematocrit, decreasing temperature, and with the tendency of cells to aggregate. Additional factors may affect the viscosity in micro-vessels.

For some unsteady flows, such as blood flow in the human circulation, the liquid generally demonstrates both a viscous and an elastic effect, both of which determine the stress-strain relationship. Such liquids are called viscoelastic. Blood plasma shows viscosity, while whole blood is both viscous and elastic. The viscosity is related to the energy dissipated during flow, while elasticity is related to the energy stored during flow due to orientation and deformation of red blood cells (Thurston, 1972; Lowe and Barbenel, 1988; Kasser *et al.*, 1989; Sharpa *et al.*, 1996). The Newtonian model can be generalised into $\sigma = \eta(A)A$ where $A = L + L^T$ with $L = \nabla\vec{v}$ and

$$\eta(A) = \eta_\infty + (\eta_o - \eta_\infty)\left[\frac{1 + log(1+\Gamma\dot{\gamma})}{1+\Gamma\,\dot{\gamma}}\right] \tag{2.2}$$

where $\dot{\gamma} = \sqrt{\frac{tr(A^2)}{2}}$, η_o and η_∞ are the asymptotic apparent viscosities as $\dot{\gamma} \to 0$ and ∞ respectively, and Γ is a positive material constant (dimension of time) representing the degree of shear-thinning. The dot over a variable denotes the substantial derivative D/Dt given by $D/Dt = \partial/\partial t + \vec{v}\cdot\nabla$.

Another model for viscosity is the Oldroyed-B model (Oldroyd, 1950 and 1958) three-parameter shear-thinning model, given by

$$\sigma + \lambda_1\ (\dot{\sigma} - L\sigma - \sigma L^T) = \eta(A + \lambda_2(\dot{A} - LA - AL^T)) \tag{2.3}$$

in which η is a constant, λ_1 and λ_2 are two constants usually known as the relaxation and retardation constants, respectively.

A recently accepted model for blood viscosity is that proposed by Pontrelli (1998), which combines the generalised Newtonian model with the Oldroyd-B model which considers the creep, the normal stress and the stress relaxation effects with constant viscosity. This yields

$$\sigma + \lambda_1\ (\dot{\sigma} - L\sigma - \sigma L^T) = \eta(A)\,A + \eta_0\lambda_2(\dot{A} - L\,A - A\,L^T) \tag{2.4}$$

[1]In some fluids, known as shear-thickening fluids, viscosity increases with shear rate. In others, known as shear-thinning fluids, viscosity decreases with increasing shear rate. In blood, both thickening and thinning behaviour is observable.

where σ is the extra stress[1], $L = \nabla \vec{v}, A = L + L^T$ and the viscosity $\eta(A)$ is computed from the Generalised Newtonian model, as given by Eq.(2.2). This generalised Oldroyd-B model (GOB) captures most of the important characteristics of blood. For details on evaluations of these models, we refer to the Ph. D. thesis of Yeleswarapu (Yeleswarapu, 1996).

2.1.1 Simplifications

Experimentally, three main regions that categorise the relationship between shear rate and blood viscoelasticity have been observed:

- at low shear rate ($\gamma < 10\,sec^{-1}$) the cells are clustered in large aggregates with diminishing nature as the shear rate is increased. The viscosity and the elasticity are of $O(10^{-1})$ Poise. In this region, blood is absolutely non-Newtonian.
- at medium shear rate ($10 < \gamma < 100\,sec^{-1}$), the clusters are disintegrated and forced to be oriented. The viscosity is of $O(10^{-3}$–$10^{-2})$ Poise, decreasing with increasing shear rate. The elasticity is of $O(10^{-1})$ Poise but slightly less than at low shear rate.
- with increasing shear rate ($\gamma > 100\,sec^{-1}$), the cells are deformed and they tend to form layers that slide on plasma. To a fair approximation, blood can be treated as Newtonian in this region.

In this study our focus is on large blood vessels, such as the abdominal aorta in which the shear rate exceeds $100\,sec^{-1}$ and therefore, to the first approximation, we consider blood to be Newtonian. Available numerical studies on non-Newtonian behaviour have shown minor influences on the flow in large vessels (e.g. Gijsen *et al.*, 1999; Cole *et al.*, 2002). We also assume that blood is an isotropic, homogeneous and incompressible fluid.

2.2 Fluid-Structure Interaction

The walls of an artery are distensible tubes of complex elastic behaviour. The diameter of the vessel varies with the pulsating pressure. Being elastic, it also propagates pressure and flow waves generated by the heart at a velocity of magnitude mainly determined by the elastic parameters of the wall and the pressure gradient. It is to be noted that, the distensibility of wall vessels is essential for the wave to propagate, as for a fluid like blood flowing in a rigid tube, the wave would unrealistically propagate with the speed of sound in blood (about 1500 m/sec) (McDonald, 1974).
However, fluid-structure interaction is rather a challenge in haemodynamics. This is due to the complex structure of the arterial wall (fibrous elastin and collagen supported in a fluid) and its *elastomer* behaviour[2]. With the advances in Computa-

[1] The Caushy stress tensor is $T = -pI + \sigma$ with p the pressure.
[2] Elastomers are easily extensible

tional Fluid Dynamics (CFD) and development of computing power, studies on fluid-structure interactions have been reported. In lattice BGK models, this field is under development (Chopard and Marconi, 2002) and only a few applications are present in the literature (e.g. Fang *et al.*, 2002; Hoekstra *et al.*, 2003). The promising future of new imaging techniques such as magnetic resonance elastography (Weaver, 2001) may allow accurate estimation of elastic properties of the vessels and motivate the need for more complex simulation models. However, the Poisson ratio[1] for arterial walls is approximately 0.5, making the deformation nearly isovolumetric.
In large vessels, such as the aorta and the carotid, a maximum change of 10% in the vessel diameter is expected. This results in the same change in the Womersley parameter ($\alpha = R\sqrt{\frac{\omega}{\nu}}$, with ω the angular frequency and ν the kinematic viscosity) and the Reynolds number ($R_e = UD/\nu$ with U the velocity and D the diameter). For the aorta under resting conditions, the Womersley parameter is 16 if the wall is rigid and is in the range $14.5 - 17.6$ under elastic assumption, while the Reynolds number is 1150 for rigid wall approximation and is in the range 1035–1265. The effect is therefore quite minor for large arteries. Therefore, to first approximation, rigid wall assumption is reasonably valid in large arteries.

2.3 Equations of Motion

Even with the above simplifications, it is still difficult to mathematically describe the mechanics of the circulation for the whole body. One way to study this complex system is to consider flow in an isolated single segment. The whole system may be studied using electric network similarity (see e.g. Berger, 1993).
For an isothermal fluid, the equations of conservation of mass and momentum fully describe the macroscopic behaviour of the viscous flow. The rate of mass accumulation is always equal to the difference between the rate of incoming and outgoing masses. This leads to the well known equation of continuity

$$\frac{D\rho}{Dt} + \rho(\nabla \cdot \vec{v}) = 0 \tag{2.5}$$

which simplifies to

$$\nabla \cdot \vec{v} = 0 \tag{2.6}$$

for incompressible fluids. The conservation of momentum follows from Newton's second principle: Mass per unit volume times acceleration is equal to the sum of three forces; the pressure force, the viscous force and, if exists, the external force, all per unit volume

$$\rho\frac{D\vec{v}}{Dt} = -\vec{\nabla}p - \vec{\nabla}\cdot\sigma + \rho\vec{G} \tag{2.7}$$

In these equations, ρ is the density ($\rho = 1.05 gm/cm^3$ for blood), D/Dt is the substantial derivative, p is the pressure, σ is the stress tensor (symmetric and second order) and

[1]It is the ratio of transverse to longitudinal strain

$\vec{G}$ is the external force. There are five unknowns (velocity components, pressure and density) in four equations. It follows that one more equation is needed to uniquely determine the solution of the system. This equation is provided by applying a boundary condition. Boundary conditions are equations in the unknowns, holding only in three dimensions (any three of x, y, z, t in Cartesian coordinate system). The general specifying equation for the boundary conditions may be written in the form

$$F(p, \rho, \vec{v}, x, y, z, t) = 0 . \tag{2.8}$$

Assigning a boundary condition to the equations of motion results in a simplified set of equations suitable for a specific type of flow problems. For example, assuming constant density and viscosity results in the celebrated Navier-Stokes equations for incompressible Newtonian fluids

$$\rho \frac{D\,\vec{v}}{D\,t} = -\vec{\nabla} p + \mu \vec{\nabla}^2 \vec{v} + \rho \vec{G}, \tag{2.9}$$

and for negligible viscous effects, $\vec{\nabla} \cdot \sigma = 0$, this reduces to the Euler equation

$$\rho \frac{D\vec{v}}{Dt} = -\vec{\nabla} p + \rho \vec{G}. \tag{2.10}$$

The energy equation will not be used in this study and therefore, is not presented here. We assume that the system is isothermal. In this study, analytic solutions for the used benchmarks will be presented whenever needed. It is understood that the equations presented here are the fundamental equations used to derive these solutions and therefore, it will not be necessary to derive the analytical solutions for these benchmarks.

2.3.1 The Boltzmann Equation

From a CFD point of view, the Navier-Stokes equations are adequate enough to describe macroscopic fluid flow phenomena through simple structures. As mentioned in the introduction, there is always a need to go more complex in order to understand the complexity of nature. Going complex may involve a choice of going microscopic up to the molecular dynamics, or even more.
In kinetic theory, an alternative description for monatomic gas dynamics is given through the Boltzmann equation (Boltzmann, 1872)

$$\frac{\partial f}{\partial t} + \vec{\xi} \cdot \frac{\partial f}{\partial \vec{x}} + \vec{G} \cdot \frac{\partial f}{\partial \vec{\xi}} = Q(f, f) \tag{2.11}$$

where $f = f(\vec{x}, \vec{\xi}, t)$ is the distribution function, $\vec{x}$ and $\vec{\xi}$ are the position and velocity vectors of a molecule, $\vec{G}$ is the force per unit mass acting on the molecule, $Q(f, f)$ is the quadratic collision operator and t the time. This equation can be used to describe fluids in the limit of small mean free path between molecular collisions, which enters the equation as a collision rate. This implies that f should not be far from the Maxwellian[1]

$$g = \rho(2\pi RT)^{-D/2}\, exp[-\ (\vec{u} - \vec{\xi})^2/2RT] \tag{2.12}$$

where R is the ideal gas constant, T the absolute temperature of the fluid, D the spatial dimension and $\vec{u} - \vec{\xi}$ is the peculiar speed. The speed of sound in kinetic theory is defined as (Chapman and Cowling, 1970)

$$c_s = \sqrt{\gamma R\ T} \tag{2.13}$$

with $\gamma = 1 + 2/D$ the ratio of specific heats. By applying conservation laws to the Boltzmann equation, and assuming that f is Maxwellian, one can derive the compressible Euler equation for the hydrodynamic variables.

2.3.2 Solution of the Boltzmann Equation

As it is difficult to solve the Boltzmann equation, numerical perturbation approaches have been introduced. There are a few different ways to find asymptotic solutions for the Boltzmann equation and bridge the link between the mesoscopic Boltzmann equation and the macroscopic hydrodynamic. Examples are:

- **Hilbert expansion**: The Boltzmann equation is solved by expanding *both* the velocity distribution function and the macroscopic variables in a power-series of the Knudsen number (Cercignani, 1971; Sone *et al.*, 2000). The leading terms of the resulting equations involve the Euler equations but *not* the Navier-Stokes equations.

- **Chapmann-Enskog expansion**: Here the velocity distribution function is expanded while the macroscopic variables are not. The leading terms of the resulting equation include, in addition to the Euler equation, compressible Navier-Stokes equations, which approximate to incompressible Navier-Stokes equations in the limit of low Knudsen numbers. Higher order defects are reported (Sone *et al.*, 2000). This technique is still the most popular in the lattice Boltzmann community and will be adopted in this study, although it is more complex than the other approaches.

- **Diffusive scaling**: By considering the finite discrete velocity model of the Boltzmann equation and scaling of $\vec{x} \to \vec{x}/\varepsilon$ and $t \to t/\varepsilon^2$, the generalised lattice Boltzmann equation is obtained. Adopting the diffusive scaling and equivalent moment techniques lead directly to the incompressible Navier-Stokes equations (Inamuro *et al.*, 1997; Junk *et al.*, 2002). This way, the accuracy of the lattice Boltzmann equation can be realised as second order in space and first order in time.

[1]The Maxwellian distribution function describes equilibrium states as characterised by no heat flux or stresses other than the isotropic pressure. The Maxwellian is not an exact solution of the Boltzmann equation.

In addition to variational methods (Cercignani, 1983). More details on the solution of the Boltzmann method by means of the Chapmann-Enskog expansion are discussed in the next chapter.

2.3.3 The Hydrodynamic Stress Tensor

For its importance in haemodynamics, it is worth adding a short note about the hydrodynamic stress tensor. If a fluid is viscous, energy is dissipated during its motion due to thermodynamic irreversibility of internal friction and thermal conduction. This will affect the fluid motion. Dissipation of energy is always associated with momentum flux whose density can be described by the symmetric tensor Π_{ik} which gives the ith component of the amount of momentum flowing in unit time through unit area perpendicular to the x_k-axis. The momentum flux density tensor in a viscous fluid of mass density ρ and viscosity η moving with velocity $\vec{v}_i$ takes the form (Landau and Lifshitz, 1975)

$$\Pi_{ik} = \rho v_i v_k - \sigma_{ik} \, , \tag{2.14}$$

where

$$\sigma_{ik} = -p\delta_{ik} + \eta(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i}) = -p\delta_{ik} + 2\eta S_{ik}, \tag{2.15}$$

is the stress tensor for an incompressible fluid, p is the scalar pressure, δ_{ik} denotes the unit tensor, and

$$S_{ik} = \frac{1}{2}(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i}) \tag{2.16}$$

is the strain rate tensor. In order to estimate the stress tensor components of an incompressible fluid, derivatives of the corresponding velocity profiles are conventionally computed from the measured or simulated velocity profiles. However, the lattice Boltzmann methods obtains it directly, as will be seen in the next chapter.

2.4 Specifying Simulation Parameters

In order to simulate flow in a model representing a segment of the cardiovascular system, different input parameters must carefully be selected. Some of them are addressed here.

2.4.1 Flow Rate

As it is patient specific, choosing a flow rate for a study is not an easy task. However, for a new computational method like the lattice Boltzmann model, validation with existing studies is needed. Therefore, we have selected two existing flow rates, recently studied by Moore *et al.* (1994a) and Taylor *et al.* (1998). The two flow rates are similar in shape and their average does not differ. The shape of the flow rate will be shown together with simulation results produced by it.

It is more important to remark that the flow is derived mainly by the pressure gradient and not the pressure itself. It is to be noted also that the Poiseulle formula, which relates the pressure gradient and the flow rate for steady flows, is not valid here (see McDonald, 1974 for valid relationships). In our simulations of realistic geometry, the flow rate waveform is Fourier transformed up-to the 8th harmonics (a constant + 8 sines + 8 cosines). Frequently, we also use the oscillatory components of a pressure gradient derived from a measured aortic pulse to reproduce oscillatory Womersley solution.

2.4.2 Viscosity

In a Newtonian sense, viscosity may be defined as the force required to move a unit area through a fluid to create a unit velocity gradient. Viscosity is also patient dependent and is quite sensitive to many parameters, especially the haematocrit and temperature. The value taken for blood, with a haematocrit of 45%, is acceptably taken as 4.0 cP at 37^o.

2.4.3 Dimensionless Numbers

In fluid flows, each of the pressure, viscous and transient forces dominates under certain conditions. In order to investigate the importance of each of these forces, the equations of motion are written in a dimensionless form, through defining dimensionless parameters. The major dimensionless numbers used in this study are

- **The Reynolds number** which indicates the relative significance of the viscous effect compared to the inertia effect. It is defined as

$$R_e = \frac{UD}{\nu} \tag{2.17}$$

where D is a characteristic length (such as the tube diameter), $\nu = \frac{\mu}{\rho}$ is the kinematic viscosity and U is the maximum velocity[1]. A large Reynolds number indicates that the convective inertia forces are dominant, while at low Reynolds numbers the shear forces influence the flow. The Reynolds number gives an idea about how far from turbulence we are. Experimentally, three regions can be recognised: laminar flow at low Reynolds numbers ($0 < R_e < 2300$), transient flow ($2300 < R_e < 4000$) and turbulent flow ($R_e > 4000$). For the flow in the circulation, since the geometry is not regular, the characteristic length is defined as $D = 4m = \frac{4A}{C}$ where m is the mean hydraulic depth, A is the cross section of the vessel (the vascular bed) and C is its circumference. Typical Reynolds numbers in the circulation are $R_e = 6000$ in the ascending aorta, $R_e = 1150$ in the abdominal aorta, $R_e = 500$ in the carotid artery, and can be as small as one in the arterioles. It is to be noted that, in the circulation, the Reynolds number should not be used as the only measure of the stability of the flow, as early turbulence,

[1]The Reynolds number may be also defined in terms of the average velocity.

flow mixing, vortex formation and back-flow may occur due to the complex geometry of the arterial system. The best way to describe qualitatively flow in the circulation is to call it "disturbed flow".

- **The Womersley Number** which is the ratio of the transient inertia force to the shear force

$$\alpha = \frac{D}{2}\sqrt{\frac{\omega}{\nu}} \tag{2.18}$$

  where $\omega = 2\pi f = \frac{2\pi}{T}$ is the angular frequency, with f the frequency and T the period of oscillation. If α is large, the transient inertia force dominates, while the viscous force dominates at low Womersley numbers. Typical values for the Womersley number in the circulation are $\alpha = 16$ in the abdominal aorta and $\alpha = 9$ in the carotid artery under resting conditions. Under exercise conditions, the Womersley parameter increases as a consequence of the increase in the heart rate.

- **The Strouhal Number** which determines the time available for vortex formation to occur. It is defined as

$$St = \frac{Df}{U} \tag{2.19}$$

  which can be rewritten as $St = 2\frac{\alpha^2}{\pi R_e}$. It therefore combines the influence of Reynolds and Womersley numbers. Typical values in the circulations are $St = 0.14$ in the abdominal aorta and $St = 0.10$ in the carotid artery.

- **The Mach Number** which measures the velocity of a fluid relative to the speed of sound in the fluid. It is only important when dealing with compressible fluids. Although it is accepted that blood is an incompressible fluid, the Mach number plays an important role in this study due to the compressible nature of the used lattice Boltzmann solver (see Chapter 7).

There are many other non-dimensional parameters that are useful in fluid mechanics, but in this study we will deal only with the above mentioned.
In the next chapter, we review the numerical method involved and discuss the influence of these parameters on the error behaviour of the method.