Mathematical modeling of solutes transportation in arterial blood flow

Nawal Hussein Balal Siddig

Ahfad University for Women- Omdurman –Sudan

Abstract In this paper, the solutes transport mechanism was studied from mathematical view. Three models were established to model and analyze solutes transportation inside arteries, in arterial lumen and though arterial walls. The Navier-stokes equations were used with the second and the third models, to model blood velocity and pressure. Blood is considered to be viscous incompressible, Newtonian in large arteries and Non-Newtonian in the capillaries.

Introduction

Study of blood flow, pulse, pressure, wave propagation, and transport phenomena in the circulatory system had began over two centuries ago, but recently, problems in engineering, biological sciences, computational sciences and physical sciences are using increasingly sophisticated mathematical techniques. Mathematical modeling of solutes transport and solutes absorption processes – by the arterial wall – is very important nowadays because it helps in understanding of the relationship between the mechanism of blood flow, the nourishing of the inner arterial wall by solutes and the diseases that can occur when the process of solute transport is for some reasons disturbed.

Transport Equations:

Transport equations are equations which describe transport phenomena such as heat transfer, mass transfer, fluid, waves, momentum transfer and others.

A generic transport equation that describes transport phenomena is constructed as:

$$\frac{\partial \phi}{\partial t} + \nabla . f(t, x, \phi, \nabla \phi) = g(t, x, \phi), \tag{1}$$

Where:

ϕ =   is a quantity to be transferred
f =   is called the flux
t =   is the time
g =   is the source.

Equation (1) clearly indicates that all transfer processes express a certain conservation law (for all dependent variables).

In general, the transport phenomena are controlled by two mechanical processes, convection and diffusion. But bio-transport processes go beyond these two processes that it can occur via blood vessels by contraction and dilation [1].

Since this paper is concerned with the solutes transport phenomenon in arteries, this section will discuss the solute transport in blood flow and arterial walls.

The most important micro-size particles for biofluid dynamics applications are (blood dynamics) :

- Platelets for blood clotting after injury.
- Red blood cells for carrying of oxygen to body tissue and organs.
- Monocytes: members of the white blood cell group.

- Endothelial cells for lining of all blood vessels for regulating.
- Epithelial cells: regulating lining inner organ walls.

The particles transport inside/across cells is done by concentration gradients (diffusion) while particles transport in blood vessels is done by pressure gradient. In blood, the transport of dissolved species include the following:

- Gases like oxygen, carbon dioxide (CO_2).
- Liquids like lymphate.
- Electrolytes, i.e. charged biological molecules
- Nutrients
- Waste products

The solute transport process in blood occurs across membranes such as arterial walls, driven by blood or by osmotic pressure difference and concentration gradient.

The mass transport of species in the arterial lumen is described mathematically by the following three dimensional convection-diffusion equations as:

$$\frac{\partial C}{\partial t} + u.\nabla C = -D\nabla^2 C \qquad , \qquad (2)$$

Where:

C = is the concentration of species

u = is the blood velocity vector

D = is the diffusivity of species in the blood

For transport analysis of microcirculation region with consideration of a representative blood capillary with a thin membrane wall and a homogeneous soft tissue, with a constant concentration C_T, the following assumptions should be taken into consideration during model proposing :

- $C = C\,(x,t)$ only,
- $Q/A = \bar{u}$ is the area-averaged constant blood velocity,
- Axial diffusion is negligible,
- The transfer coefficient $B \equiv PS / \forall_S$ is constant, then accordingly, the governing equation for species mass transfer between the capillary blood vessel and the tissue is written as:

$$\frac{\partial C}{\partial t} + \bar{u}\frac{\partial C}{\partial t} = B(C - C_T), \qquad (3)$$

Where:

C_T = is the concentration of the soft tissue.

C = is the species concentration

$\bar{u}$ = is the blood velocity vector

B = is a constant,

       $B = PS / \forall_B$ (4)

P = is the membrane permeability

S = is the surface area of species mass, transfer between capillary and tissue and $S = d\pi L$

$\forall_B$ = is the blood volume

d = is the capillary diameter

x = is the capillary length, $o \leq x \leq 1$ [2].

Equation (3) can be solved, according to the suitable initial and boundary conditions, using math software programs like MATlAB, Flex PDE,FMS or other types. The numerical solution can be achieved if the values $\bar{u}$, B and C_T are known with the constants. The following diagram illustrates the previous mentioned transport process of species between the capillary and the tissue.
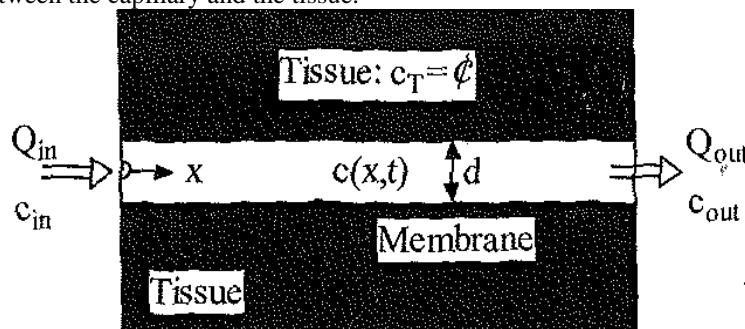
Figure 1: Mass transfer between tissue and a capillary of diameter d and length $o \leq x \leq 1$

According to the fact that, solutes dynamics is directly related to the blood dynamics, the following two mathematical models are constructed to model solutes in arteries as:

The First Model:

Is called the wall-free model. In this model, the Navier-Stokes equations for incompressible fluids are used to model the blood motion. These equations have been used with an advection-diffusion process that models the solute dynamics. They were first used to model oxygen and lipoprotein absorption processes. The main assumptions for construction of the model are:

    i) The blood velocity provides the convective field of the solute equation.

    ii) The permeability, controlling the absorption process of the solute through the wall, is a suitable function of the shear stress exerted by the blood on the arterial wall. Mathematically, step (ii) indicates that the boundary conditions, for the solute equation on the wall are related to the blood velocity field.

    iii) The diffusion of the solutes is represented by a diffusivity tensor which is considered to be a function of the shear rate.

    iv) The solute dynamics "inside" the arterial wall has been neglected.

The wall-free model can defined by the following two systems.

$$\begin{cases} \dfrac{\partial u}{\partial t} + (u.\nabla)u - v\,\Delta u + \nabla p = f, \ x \in \Omega_f, \ t > 0 \\[2mm] \nabla.u = 0, \ x \in \Omega_f, \ t > 0 \\[2mm] u = b \ on \ \partial\Omega_f\,|\Gamma_w, \ u = 0 \ on \ \Gamma_w, \, t > 0, \\[2mm] u = u_0 \ with \ \nabla.u_0 = 0, \ x \in \Omega_f, \ t = 0 \end{cases} \tag{5}$$

$$\frac{\dot{\partial} C_f}{\partial t} - \nabla.(\mu_f \,\nabla C_f) + u.\nabla C_f = f_f, \ x \in \Omega_f, \ t > 0 \tag{6}$$

The boundary conditions are:

$$\begin{cases} (a) \ n.(\mu_f \,\nabla C_f) + \xi\,C_f = \xi K_w \ on \ \Gamma_w, \, t > 0 \\[2mm] (b) \ C_f = 0 \ on \ \partial\Omega_f \setminus \Gamma_w, \ t > 0 \\[2mm] C_f = C_{f,0}, \ x \in \Omega_f, \ t = 0 \end{cases} \tag{7}$$

Where

$\Omega_f \subset R^d$ (d = 2,3): represents lumen of a given vascular district. The boundary of Ω_f is assumed to be composed by different part (the proximal section Γ_{up})

Γ_{up}: is the proximal section, that is, the up stream part of the vascular district (with respect to heart and blood flow).

Γ_{dw}: is the desital section which represents the part of Ω_f corresponding to the arterial wall.

Γ_w: is the part of Ω_f corresponding to the arterial wall.

$\Omega_f = \Gamma_w \ U \ \Gamma_{up} \ U \ \Gamma_{dw}$ as shown in (Fig. 2...)

$u(t,x) \in R^d$ = denotes the velocity field of the blood.

$p(t,x)$ = is the kinematic pressure: the ratio between the pressure and the blood density.

$C_f(t,x)$ = Denotes the concentration of the considered solute, for example O_2 and lipoproteins, in the blood.

$K_w(t,x), x \in \Gamma_w$: Denotes the solute concentration on the arterial wall Γ_w.

v = is the diffusivity tensor.

ξ = is the arterial wall permeability.

f = is a possible forcing term, for the blood velocity (e.g. the gravity force).

f_f = Represents a possible forcing term for the solute concentration (e.g. the effect of chemical reaction of the solute with other substances dissolved in blood).

μ_f = is the diffusivity tensor.

Journal of Scientific and Engineering Research

The following assumption and hypotheses were introduced into the model.
1. The blood is assumed to be a Newtonian fluid with a constant kinematic viscosity, v,
2. The arterial wall is assumed to be rigid.
3. The boundary conditions in (7) indicates that the flux in solute entering or leaving the blood domain through Γ_w is related the difference of concentration across the boundary by the arterial wall permeability ξ.
4. The diffusivity μ_f is a function of the rate of deformation tensor *d*, such that:

$$d_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \; i, j = 1, 2, \ldots d, \qquad\qquad\qquad (8)$$

The consideration is:

$$(\mu_f)_{ij} = \mu_{fo}\,(\delta_{ij} + D\,|d_{ij}|^{\in}, \; i, j = 1,2,\ldots..d \qquad\qquad\qquad (9)$$

Where:

$\mu_{of}, D, \in$:   Are positive coefficients depend on the specific solute and on the concentration of the red blood cells, which is assumed to be constant.

δ_{ij} :   is the Kronecker identity tensor.

The wall permeability ξ has been modeled as a function of the shear stress $\sigma(u)$ which induced by the blood flow in the arterial wall, and $\sigma(u) = t. \, T_{(u)}.n$

Where:

$T(u)$ =   is the local stress tensor defined as: $T(u) = 3\, vd$

n, T =   Are the normal and tangential unit vector on T_w respectively.

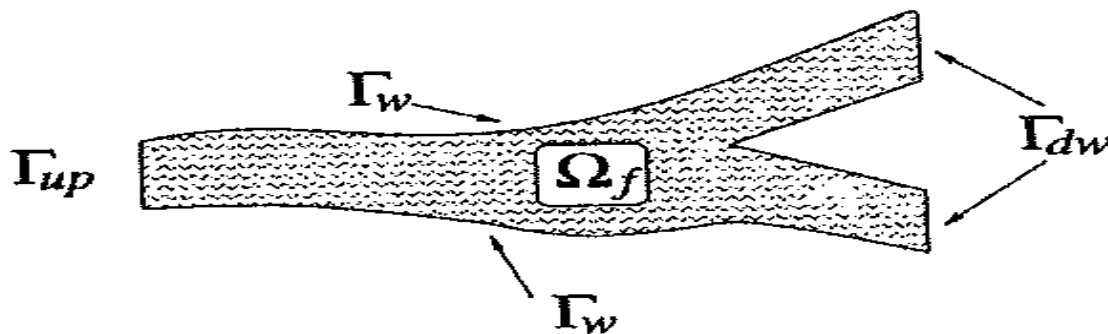The following figure illustrates the wall-free model description.

Figure 2: The scheme of the wall-free model

The notable points on the wall-free model is that: First it uses the concentration as the unknown of the advection diffusion problem but generally when gaseous solutes (e.g. oxygen) are involved, the equations are written in terms of the partial pressure of the solute and in this way, it is more immediate to consider different forms of the same solute such as oxygen which is present both as free solute in plasma and as a form linked to the hemoglobin. So accordingly, from mathematical view points, approximated laws can be used to make the relationship between partial pressure and concentration more linearly and this is assumed situation. Second, the analysis of the model is limited to analyze only one solute but actually in blood there are indeed many solutes. Thirdly, the model assumes the blood to be a Newtonian fluid, but as mentioned before, the whole blood is considered to be a non Newtonian fluid according to the existence of red blood cells and their deformation according to the blood vessels diameters and according to other parameters [3-8].

The Second Model:

This model is defined as the fluid-wall diffusion model. it is used for modeling of solutes dynamics " inside " the arterial wall with the considerations of the solute dynamics not only in the arterial lumen, but also in the arterial wall. The following assumptions are considered in the model construction:

i)   The computational domain is composed by the lumen $\Omega_f \subset R^d$ (d=2,3) and by Ω_w which represent the arterial wall as shown in Fig. (3).

ii)   The common interface between Ω_f and Ω_w has been denoted by $T \subset R^{d-1}$ such that:

$$\Gamma \equiv \overline{\Omega}_f \bigcap \overline{\Omega}_w \quad \text{also } \Omega \text{ was denoted as:}$$

$$\Omega = \overline{\Omega_f \bigcup \Omega_w} \quad \text{and } \partial\Omega \text{ its boundary}$$

The Navier-Stokes equations were used to describe the blood motion. Also an advection-diffusion equation was used for solute in the blood.

iii)   The advection phenomena were neglected because of the very low velocity of the solvent inside the wall. The dynamics of solute in the arterial wall is expressed by the following system:

$$\begin{cases} \dfrac{\partial C_f}{\partial t} - \nabla(\mu_f \nabla C_f) + u.\nabla C_f = f_f \ \ in \ \Omega_f, \ \ t>0, \\ C_f = 0 \ on \ \partial\Omega_f \setminus \Gamma, \ \ t>0 \end{cases} \tag{10}$$

$$\begin{cases} \dfrac{\partial C_w}{\partial t} - \nabla(\mu_w \nabla C_w) = f_w \ \ in \ \Omega_w, \ \ t>0, \\ C_w = 0 \ on \ \partial\Omega_w \setminus \Gamma, \ \ t>0 \end{cases} \tag{11}$$

Where:

$C_f(t,x)$:   Denotes the concentrations of the solute in the blood.

$C_w(t,x)$:   Is the concentration in the arterial wall and its value was considered to be a given datum on Γ, also $C_w(t,x)$ satisfies a pure diffusion equation.

$u, \ \sigma(u), \ \mu_f(u)$: Are provided by the solution of the previous model.

The following matching conditions were considered at the interface:

$$\mu_w \frac{\partial C_w}{\partial n_w} = -n_f . (\mu_f \nabla C_f) \, on \, \Gamma \tag{12}$$

$$n_f (\mu_f . \nabla C_f) + \xi (C_f - C_w) = 0 \ \ on \ \Gamma \tag{13}$$

Where:

n_f = is a unit outward normal vector on Γ with respect to Ω_f and $n_w = -n_f$.

The following points were considered:

i) μ_f is again a function of the shear rate.

ii) μ_w has been assumed to be constant.

iii) f_f represents possible forcing term for the solute dynamic in the lumen.

iv) f_w represents possible forcing term in the arterial wall, f_w may take into account the consumption of the solute by the arterial tissue.

Equation (2.78) has been equivalently substituted by:

$$\mu_w \frac{\partial C_f}{\partial n_w} + \xi (C_w - C_f) = 0 \ on \ \Gamma \tag{14}$$

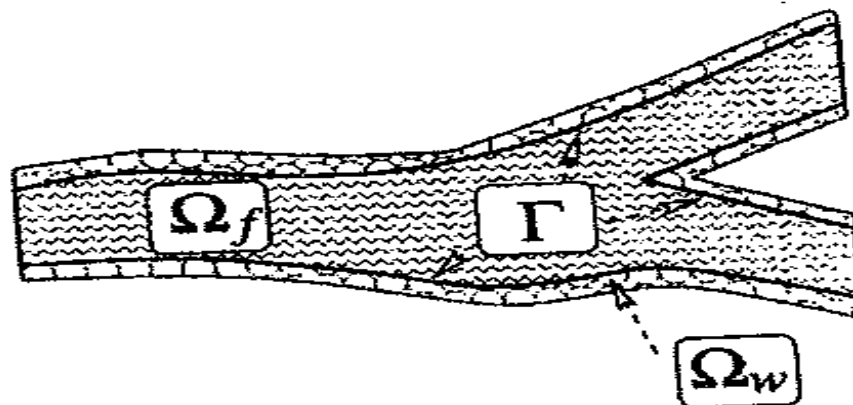The following figure illustrates the fluid-wall model.

Figure 3: Scheme of the fluid wall model

For the mathematical analysis of the two previous mentioned models see [9] .

These two models can be applied in many physiological areas with the help of computational power and rules of mathematical modeling and simulation. An example of that is their application in a Stenosis of a part of a large artery.

Discussion and Conclusion

This paper discussed the transportation phenomena of solutes in the arterial blood stream. Possible applications are in studying the relationship between the mechanism of blood flow, the nourishing of the inner arterial wall by solutes and the diseases that can occur when the process of solute transport is for some reasons disturbed and leads to a diseased conditions.

For the purpose of mathematical modeling, the blood as a biofluid, is idealized as a viscous incompressible, Newtonian in large arteries and Non-Newtonian in the capillaries because of the deformation of the red blood cells in the small arteries and the capillaries. A generic transport equation was used to describe the transport phenomena through the conversation law. A three dimensional convection-diffusion equation was used to model. The mass transport of species in the arterial lumen. Also the mass of species transfer between the capillary blood vessel and the tissue was covered by a governing equation. A couple of two models **the wall-free model and** the **fluid-wall diffusion model** - were used with the aid of Navier-Stokes equations for incompressible fluids- to model the solutes dynamics which was proved to be related to blood dynamics- with specific assumptions.

The analysis was done with the considerations of the solute dynamics not only in the arterial lumen, but also in the arterial wall.

References

[1].   Sramek, B.Bo. et al, Biomechanics of the Cardiovascular System (1995), Czech Techn Univ & Foundation for Biomechanics of Man. Czech Republic p. 209-231.

[2].   Facchini, L., Bellin, A., Toro, E., 2013d. A time-dependent mathematical model of ltration and solute exchange. application to the study of hemorrhage, in preparation.

[3].   Khakpour, M., Vafai, K., 2008a. Analysis of transport phenomena within PEM fuel cells An analytical solution. International Journal of Heat and Mass Transfer 51, 37123723.

[4].   Starling, E., 1896. On the absorption of uids from the connective tissue spaces. Journal of Physiology 19 (4), 312326.

[5].   Taylor, G., 1953. Dispersion of soluble matter in solvent owing slowly through a tube. Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences 219 (1137), 186203.

[6].   Vink, H., Duling, B., 2000. Capillary endothelial surface layer selectively reduces plasma solute distribution volume. American Journal of Physiology - Heart and Circulatory Physiology 278 (1), H285H289.

[7].   J. Waniewski, Linear approximations for the description of solute flux through the permselective membrane, J. Membr. Sci. 95 (1994)

[8].   Adamson, R., 1990. Permeability of frog mesenteric capillaries after partial pronase digestion of the endothelial glycocalyx. The Journal of Physiology 428, 113. 47, 54,

[9].   A coupled system of ODEs and quasilinear hyperbolic PDEs arising in a multiscale blood flow model. *Journal of Mathematical Analysis and Applications* **343**, 778-798, (2008).