

# 1 Discretization

## 1.1 Discretizing governing equation with central difference approximation

Starting equation

$$\frac{D_{NO}}{r} \frac{d}{dr} \left( r \frac{dC_{NO}}{dr} \right) + R_{NO} = 0 \quad (1)$$

Simplify

$$D_{NO} \frac{d^2 C_{NO}}{dr^2} + \frac{D_{NO}}{r} \frac{dC_{NO}}{dr} = -R_{NO} \quad (2)$$

Compare to form

$$u'' + P(r)u' = F(r) \quad (3)$$

$$u = C_{NO}, \quad P(r) = \frac{1}{r}, \quad F(r) = -\frac{R_{NO}}{D_{NO}} \quad (4)$$

Taylor expansion

$$\begin{aligned} u_{i+1} &= u_i + u'_i \Delta r + \frac{1}{2} u''_i \Delta r^2, \\ u_{i-1} &= u_i - u'_i \Delta r + \frac{1}{2} u''_i \Delta r^2 \end{aligned}$$

Central difference

$$\begin{aligned} u'_i &= \frac{u_{i+1} - u_{i-1}}{2\Delta r}, \\ u''_i &= \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta r^2} \end{aligned}$$

Sub back into Eq. (3)

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + P_i \frac{u_{i+1} - u_{i-1}}{2h} = F_i, \quad h = \Delta r \quad (5)$$

where index  $i$  starts at 1.

Rearrange, let  $a_i = \frac{h}{2} P_i$

$$(1 - a_i) u_{i-1} + (-2) u_i + (1 + a_i) u_{i+1} = h^2 F_i \quad (6)$$

$$(-2) u_i = -(1 - a_i) u_{i-1} - (1 + a_i) u_{i+1} + h^2 F_i \quad (7)$$

$$u_i = -\frac{1}{2} \left( -(1 - a_i) u_{i-1} - (1 + a_i) u_{i+1} + h^2 F_i \right) \quad (8)$$

## 1.2 Discretization schemes for boundary condition

### 1.2.1 Use imaginary node and correction term

$$\frac{u_2 - u_0}{2h} = 0 \rightarrow u_0 = u_2 \quad (9)$$

$$\frac{u_{end+1} - u_{end-1}}{2h} = 0 \rightarrow u_{end+1} = u_{end-1} \quad (10)$$

Substitute into Eq. (3) when  $i = 1$

$$(-2) u_1 = -2u_2 + \frac{1}{2} h^2 F_1 \quad (11)$$

Substitute into Eq. (3) when  $i = end$

$$(-2) u_{end} = -(1 - a_{end}) u_{end-1} - (1 + a_{end}) u_{end+1} + h^2 F_{end} \quad (12)$$

$$(-2) u_{end} = -2u_{end-1} + h^2 F_{end} \quad (13)$$

### 1.2.2 Use second-order one-sided forward/backward approximation

From [1]:

$$\frac{-3u_1 + 4u_2 - u_3}{2h} = 0 \rightarrow -3u_1 + 4u_2 - u_3 = 0 \quad (14)$$

$$\frac{3u_{end} - 4u_{end-1} + u_{end-2}}{2h} = 0 \rightarrow 3u_{end} - 4u_{end-1} + u_{end-2} = 0 \quad (15)$$

## 2 Solution algorithm

### 2.1 Gauss-Seidel

From [2]:

$$u_i^{k+1} = -\frac{1}{2} \left( -(1 - a_i) u_{i-1}^{k+1} - (1 + a_i) u_{i+1}^k + h^2 F_i \right) \quad (16)$$

### 2.2 Successive overrelaxation method

$$-\frac{2}{\omega} u_i^{k+1} = -(1 - a_i) u_{i-1}^{k+1} - (1 + a_i) u_{i+1}^k + h^2 F_i - \left( \frac{2}{\omega} - 2 \right) u_i^k \quad (17)$$

Alternative formula [3]:

$$\mathbf{u}^{k+1} = \left( \frac{1}{\omega} D + L \right)^{-1} \left\{ \left[ \left( \frac{1}{\omega} - 1 \right) D - U \right] \mathbf{u}^k + \mathbf{f} \right\} \quad (18)$$

## 3 Governing equation in individual compartment

### 3.1 Nitric oxide

RBC core  $r_0 < r < r_1$

$$\frac{D_{NO}}{r} \frac{d}{dr} \left( r \frac{dC_{NO}}{dr} \right) - \lambda_{core} C_{NO} = 0$$

$$F_i = \frac{\lambda_{core} u_i}{D_{NO}}$$

CFL  $r_1 < r < r_2$

$$\frac{D_{NO}}{r} \frac{d}{dr} \left( r \frac{dC_{NO}}{dr} \right) = 0$$

$$F_i = \frac{0}{D_{NO}}$$

EC  $r_2 < r < r_3$

$$\frac{D_{NO}}{r} \frac{d}{dr} \left( r \frac{dC_{NO}}{dr} \right) + R_{NO} = 0$$

$$F_i = -\frac{R_{NO_{max}}}{D_{NO}} \frac{P_{O_2}}{P_{O_2} + K_{m,eNOS}}$$

VW  $r_3 < r < r_4$

$$\frac{D_{NO}}{r} \frac{d}{dr} \left( r \frac{dC_{NO}}{dr} \right) - \lambda_{vw} C_{NO} = 0$$

$$F_i = \frac{\lambda_{vw} u_i}{D_{NO}}$$

T  $r_4 < r < r_5$

$$\frac{D_{NO}}{r} \frac{d}{dr} \left( r \frac{dC_{NO}}{dr} \right) - \lambda_t C_{NO} = 0$$

$$F_i = \frac{\lambda_t u_i}{D_{NO}}$$

#### 3.1.1 NO matrix

$$A = \begin{bmatrix} -3 & 4 & -1 & \cdots & \cdots & \cdots & 0 \\ 1 + a_2 & -2 & 1 - a_2 & 0 & \cdots & \cdots & \vdots \\ 0 & 1 - a_3 & -2 & 1 + a_3 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & 1 - a_{n-2} & -2 & 1 + a_{n-2} & 0 \\ \vdots & \cdots & \cdots & 0 & 1 - a_{n-1} & -2 & 1 + a_{n-1} \\ 0 & \cdots & \cdots & \cdots & 1 & -4 & 3 \end{bmatrix}, \mathbf{\tilde{u}} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_i \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix}, F = \begin{bmatrix} 0 \\ h^2 F_2 \\ h^2 F_3 \\ \vdots \\ h^2 F_i \\ \vdots \\ h^2 F_{n-1} \\ 0 \end{bmatrix} \quad (19)$$

## 3.2 Oxygen

RBC core  $r_0 < r < r_1$

$$P_{O_2} = 70$$

CFL  $r_1 < r < r_2$

$$\alpha \frac{D_{O_2}}{r} \frac{d}{dr} \left( r \frac{dP_{O_2}}{dr} \right) = 0$$

$$G_i = \frac{0}{\alpha D_{O_2}}$$

EC  $r_2 < r < r_3$

$$\alpha \frac{D_{O_2}}{r} \frac{d}{dr} \left( r \frac{dP_{O_2}}{dr} \right) - R_{NO} = 0$$

$$G_i = \frac{R_{NO_{max}}}{\alpha D_{O_2}} \frac{P_{O_2}}{P_{O_2} + K_{m,eNOS}}$$

VW  $r_3 < r < r_4$

$$\alpha \frac{D_{O_2}}{r} \frac{d}{dr} \left( r \frac{dP_{O_2}}{dr} \right) - Q_{O_2 \max VW} \frac{P_{O_2}}{P_{O_2} + appK_m} = 0$$

$$appK_m = K_m \left( 1 + \frac{C_{NO}}{C_{ref}} \right) \quad (20)$$

$$G_i = \frac{Q_{O_2 \max VW}}{\alpha D_{O_2}} \frac{P_{O_2}}{P_{O_2} + K_m \left( 1 + \frac{u_i}{C_{ref}} \right)}$$

T  $r_4 < r < r_5$

$$\alpha \frac{D_{O_2}}{r} \frac{d}{dr} \left( r \frac{dP_{O_2}}{dr} \right) - Q_{O_2 \max T} \frac{P_{O_2}}{P_{O_2} + appK_m} = 0$$

$$appK_m = K_m \left( 1 + \frac{C_{NO}}{C_{ref}} \right) \quad (21)$$

$$G_i = \frac{Q_{O_2 \max T}}{\alpha D_{O_2}} \frac{P_{O_2}}{P_{O_2} + K_m \left( 1 + \frac{u_i}{C_{ref}} \right)}$$

### 3.2.1 O<sub>2</sub> matrix

$$A = \begin{bmatrix} 1 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ 1 - a_{r_1+1} & -2 & 1 + a_{r_1+1} & 0 & \cdots & \cdots & 0 \\ 0 & 1 - a_{r_1+2} & -2 & 1 + a_{r_1+2} & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & 1 - a_{n-2} & -2 & 1 + a_{n-2} & 0 \\ \vdots & \cdots & \cdots & 0 & 1 - a_{n-1} & -2 & 1 + a_{n-1} \\ 0 & \cdots & \cdots & \cdots & 1 & -4 & 3 \end{bmatrix}, \tilde{\mathbf{v}} = \begin{bmatrix} v_{r_1} \\ v_{r_1+1} \\ \vdots \\ v_i \\ \vdots \\ v_{n-1} \\ v_n \end{bmatrix}, B = \begin{bmatrix} 70 \\ h^2 G_{r_1+1} \\ \vdots \\ h^2 G_i \\ \vdots \\ h^2 G_{n-1} \\ 0 \end{bmatrix} \quad (22)$$

## 4 Physiological parameters

Table 1: Systemic parameters and NCFL widths [4]

Aggregating conditions	Hct (%)	Diameter ( $\mu\text{m}$ )	NCFL (%)	
			Outer	Inner
Non	$44.0 \pm 1.6$	$52.5 \pm 4.7$	$14.4 \pm 2.1$	$11.1 \pm 1.1$
Normal	$42.8 \pm 1.7$	$50.0 \pm 4.7$	$21.3 \pm 3.4$	$13.5 \pm 1.2$
Hyper	$42.2 \pm 1.6$	$51.8 \pm 4.4$	$23.6 \pm 2.7$	$15.3 \pm 1.7$

### 4.1 CFL widths from mass conservation

Hematocrit measures proportion of volume of red blood cells (RBC) to total blood volume (RBC and plasma) [5]. Cell volume fraction or tube hematocrit  $H_t$  is calculated as:

$$H_t = \frac{N_c V_{eff}}{V_t} \quad (23)$$

where  $N_c$  is the number of RBCs in the tube volume  $V_t = \pi R^2 L$ ,  $R$  is the tube radius, and  $L$  is the tube length [6].

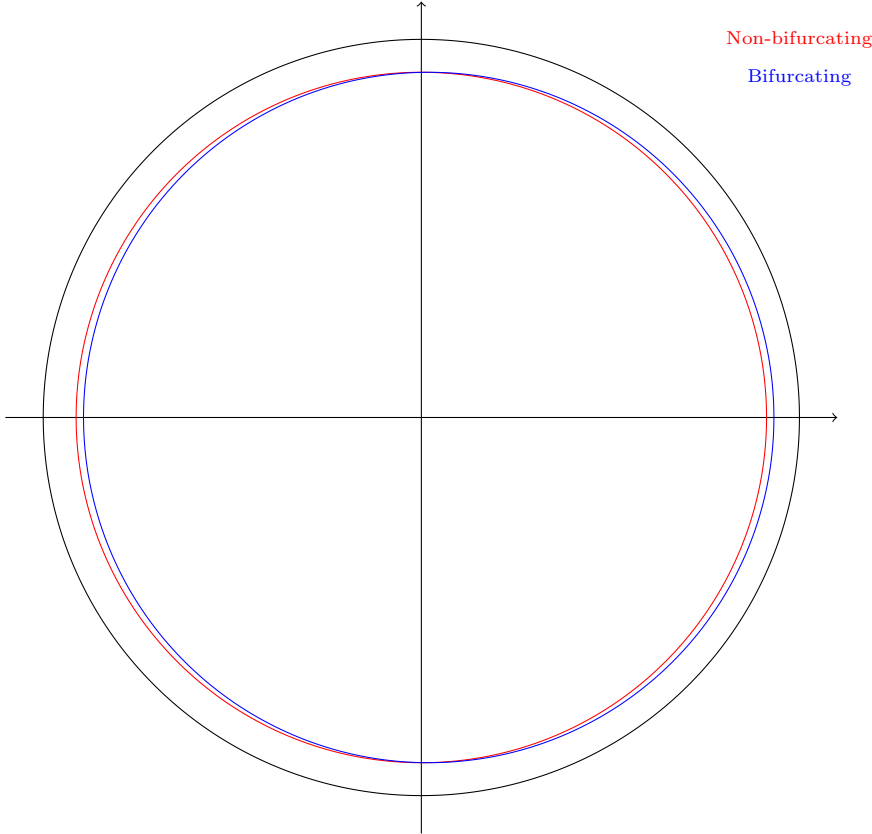
An empirical relation between  $H_t$  and  $H_d$  is given by:

$$\frac{H_t}{H_d} = H_d + (1 - H_d) (1 + 1.7e^{-0.35D} - 0.6e^{-0.01D}) \quad (24)$$

where  $D$  is the tube diameter in micrometers, and discharge hematocrit  $H_d$  is equal to systemic hematocrit [7].

Since systemic hematocrit in both cases (non-bifurcating and bifurcating flow) is the same,  $H_t$  is the same according to Eq. 24. Since  $V_t$  is the same due to constant vessel diameter,  $N_c$  assumed (?) to be the same,  $V_{eff}$  must be the same (Eq. 23).

Ignoring gravity effect and assuming symmetry, we need to find a egg / ellipse shaped graph with the same area as the circle in non-bifurcating flow.



**Assumptions:** Define normal CFL width as mean of inner and outer CFL width.

$$NCFL_{normal} = \frac{NCFL_{inner} + NCFL_{outer}}{2} \quad (25)$$

# References

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