

Starting equations

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

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

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

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

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)

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

where index i starts at 1.

Rearrange

$$\left(1 - \frac{h}{2} P_i\right) u_{i-1} + (-2)u_i + \left(1 + \frac{h}{2} P_i\right) u_{i+1} = h^2 F_i \quad (6)$$

$$(-2)u_i = -\left(1 - \frac{h}{2} P_i\right) u_{i-1} - \left(1 + \frac{h}{2} P_i\right) u_{i+1} + h^2 F_i \quad (7)$$

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

Use imaginary node to approximate Neumann BCs:

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

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

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

$$u_1 = -2u_2 + h^2 F_1 \quad (11)$$

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

$$u_{end} = -\left(1 - \frac{h}{2} P_{end}\right) u_{end-1} - \left(1 + \frac{h}{2} P_{end}\right) u_{end+1} + h^2 F_{end} \quad (12)$$

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

Solving over iterations

$$u_i^{k+1} = -\frac{1}{2} \left(-\left(1 - \frac{h}{2} P_i\right) u_{i-1}^{k+1} - \left(1 + \frac{h}{2} P_i\right) u_{i+1}^k + h^2 F_i \right) \quad (14)$$

Split into 5 sections. Solutions are in the general form $A\tilde{\mathbf{u}} = B$.

Let $a_i = \frac{h}{2} P_i$.

RBC core $r_0 < r < r_1$

Governing equation:

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

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

Boundary condition:

$$\begin{aligned} u'(0) &= 0 \rightarrow u_1 = u_2, \\ u'_{RBC}(r_1) &= \sigma, \sigma = u'_{CFL}(r_1) \end{aligned}$$

Using second-order accurate one-sided difference approximation, j represents indexes in CFL domain.

$$\sigma = \frac{-3u_j + 4u_{j+1} - u_{j+2}}{2h},$$

$$\frac{3u_i - 4u_{i-1} + u_{i-2}}{2h} = \sigma,$$

$$3u_i - 4u_{i-1} + u_{i-2} = 2h\sigma$$

$$A = \begin{bmatrix} -2 & 1+a_2 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 1-a_3 & -2 & 1+a_3 & \ddots & & & & \vdots \\ 0 & 1-a_4 & -2 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & \ddots & \ddots & -2 & 1+a_{n-3} & 0 & 0 \\ \vdots & & & \ddots & 1-a_{n-2} & -2 & 1+a_{n-2} & 0 \\ \vdots & \cdots & \cdots & \cdots & 0 & 1-a_{n-1} & -2 & 1+a_{n-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & 1 & -4 & 3 \end{bmatrix}, \tilde{\mathbf{u}} = \begin{bmatrix} u_2 \\ u_3 \\ \vdots \\ u_i \\ \vdots \\ u_n \end{bmatrix}, B = \begin{bmatrix} h^2 F_2 - (1-a_2)u_1 \\ h^2 F_3 \\ \vdots \\ h^2 F_i \\ \vdots \\ h^2 F_{n-1} \\ 2h\sigma \end{bmatrix} \quad (15)$$

CFL $r_1 < r < r_2$
Governing equation

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

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

Boundary condition:

$$u_{CFL}(r_1) = u_{RBC}(r_1),$$

$$u'_{CFL}(r_2) = \phi, \phi = u'_{EC}(r_2),$$

Using one-sided difference approximation again, i is CFL, j is RBC.

$$\phi = \frac{-3u_k + 4u_{k+1} - u_{k+2}}{2h},$$

$$\frac{3u_i - 4u_{i-1} + u_{i-2}}{2h} = \phi,$$

$$3u_i - 4u_{i-1} + u_{i-2} = 2h\phi$$

$$A = \begin{bmatrix} -2 & 1+a_2 & 0 & & & & & 0 \\ 1-a_3 & -2 & 1+a_3 & \ddots & & & & \vdots \\ 0 & 1-a_4 & -2 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & \ddots & \ddots & -2 & 1+a_{n-3} & 0 & 0 \\ \vdots & & & \ddots & 1-a_{n-2} & -2 & 1+a_{n-2} & 0 \\ \vdots & \cdots & \cdots & \cdots & 0 & 1-a_{n-1} & -2 & 1+a_{n-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & 1 & -4 & 3 \end{bmatrix}, \tilde{\mathbf{u}} = \begin{bmatrix} u_2 \\ u_3 \\ \vdots \\ u_i \\ \vdots \\ u_n \end{bmatrix}, B = \begin{bmatrix} h^2 F_2 - (1-a_2)u_1 \\ h^2 F_3 \\ \vdots \\ h^2 F_i \\ \vdots \\ h^2 F_{n-1} \\ 2h\phi \end{bmatrix} \quad (16)$$

EC $r_2 < r < r_3$ is same method as CFL, only difference is in the R_{NO} term.

Governing equation

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

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

Boundary condition:

$$u_{EC}(r_2) = u_{CFL}(r_2),$$

$$u'_{EC}(r_3) = \gamma, \gamma = u'_{VW}(r_3)$$

VW $r_3 < r < r_4$ is same method as CFL, only difference is in the R_{O_2} term.

Governing equation

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

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

Boundary condition:

$$u_{VW}(r_3) = u_{EC}(r_3),$$

$$u'_{VW}(r_4) = \delta, \delta = u'_T(r_4)$$

T $r_4 < r < r_5$. Combined since same governing equation. Governing equation

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

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

$$u_T(r_4) = u_{VW}(r_4),$$

$$u'(r_5) = 0 \rightarrow u_n = u_{n-1}$$

$$A = \begin{bmatrix} -2 & 1+a_2 & 0 & \cdots & \cdots & \cdots & \vdots \\ 1-a_3 & -2 & 1+a_3 & \ddots & & & \vdots \\ 0 & 1-a_4 & -2 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & -2 & 1+a_{n-3} & 0 \\ \vdots & & & \ddots & 1-a_{n-2} & -2 & 1+a_{n-2} \\ 0 & \cdots & \cdots & \cdots & 0 & 1-a_{n-1} & -2 \end{bmatrix}, \tilde{\mathbf{u}} = \begin{bmatrix} u_2 \\ u_3 \\ \vdots \\ u_i \\ \vdots \\ u_{n-1} \end{bmatrix}, B = \begin{bmatrix} h^2 F_2 - (1-a_2)u_1 \\ h^2 F_3 \\ \vdots \\ h^2 F_i \\ \vdots \\ h^2 F_{n-1} - (1+a_{n-1})u_n \end{bmatrix} \quad (17)$$

O_2 is solved using the same matrix as NO except in RBC where it has a constant partial pressure.

RBC core $r_0 < r < r_1$

$$P_{O_2} = 70$$

CFL $r_1 < r < r_2$

Governing equation

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

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

Boundary condition:

$$v_{CFL}(r_1) = v_{RBC}(r_1),$$

$$v'_{CFL}(r_2) = \phi, \phi = v'_{EC}(r_2)$$

EC $r_2 < r < r_3$
Governing equation

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

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

Boundary condition:

$$v_{EC}(r_2) = v_{CFL}(r_2),$$

$$v'_{EC}(r_3) = \gamma, \gamma = v'_{VW}(r_3)$$

VW $r_3 < r < r_4$
Governing equation

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

$$appK_m = K_m \left(1 + \frac{C_{NO}}{C_{ref}} \right) \quad (18)$$

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

Boundary condition:

$$v_{VW}(r_3) = v_{EC}(r_3),$$

$$v'_{VW}(r_4) = \delta, \delta = v'_T(r_4)$$

T $r_4 < r < r_5$
Governing equation

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

$$appK_m = K_m \left(1 + \frac{C_{NO}}{C_{ref}} \right) \quad (19)$$

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

Boundary condition:

$$v_T(r_4) = v_{VW}(r_4),$$

$$v'_T(r_5) = 0 \rightarrow v_n = v_{n-1}$$

$$A = \begin{bmatrix} -2 & 1+a_2 & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 1-a_3 & -2 & 1+a_3 & \ddots & & & & \vdots \\ 0 & 1-a_4 & -2 & \ddots & \ddots & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & & & \vdots \\ \vdots & & \ddots & \ddots & -2 & 1+a_{n-3} & 0 & 0 \\ \vdots & & & \ddots & 1-a_{n-2} & -2 & 1+a_{n-2} & 0 \\ \vdots & \cdots & \cdots & \cdots & 0 & 1-a_{n-1} & -2 & 1+a_{n-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & 1 & -4 & 3 \end{bmatrix}, \tilde{\mathbf{v}} = \begin{bmatrix} v_2 \\ v_3 \\ \vdots \\ v_i \\ \vdots \\ v_n \end{bmatrix}, B = \begin{bmatrix} h^2 G_2 - (1-a_2)v_1 \\ h^2 G_3 \\ \vdots \\ h^2 G_i \\ \vdots \\ h^2 G_{n-1} \\ 0 \end{bmatrix} \quad (20)$$