CHEN 3220 Project 1 – Part 1
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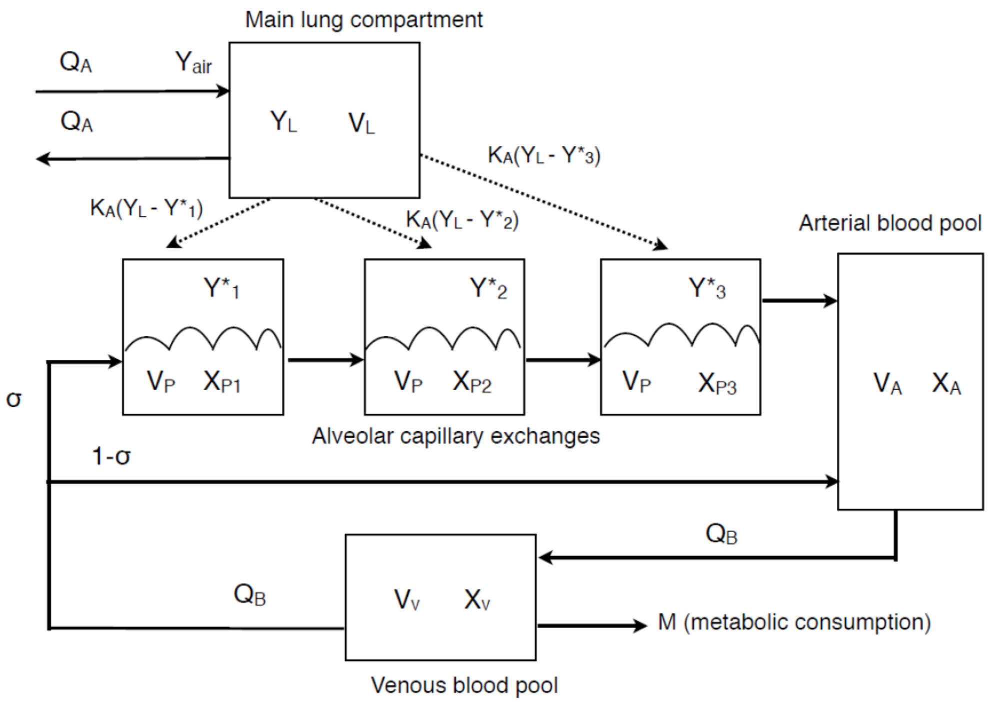
MODELING OXYGEN FLOW IN THE CIRCULATORY SYSTEM

PROBLEM STATEMENT

The objective of this project is to correctly use a mathematical model to derive and solve the accompanying calculations, specifically using a model of oxygen flow in the respiratory system. Given the model of oxygen flow depicted below, we are asked to predict the transient and steady-state behavior of oxygen concentrations in the main lung compartment, the alveolar capillaries, the venous blood pool, and the arterial blood pool.



A. THE TRANSIENT MATERIAL BALANCE

The approach to solving the problem is to derive the mass balances in the six compartments, in terms of variables $Y_L, X_{P1}, X_{P2}, X_{P3}, X_A, X_V$. Where the accumulation term can be expressed in terms of volume and molar fraction as follows:

$$accum = \frac{d(VX)}{dt} = V\frac{dX}{dT} + X\frac{dV}{dT}$$

Where X is the molar fraction of O_2 (can also be expressed as Y) and V is the volume, both specific terms to each of the six compartment (control volumes).

In addition, the following assumptions were made when working with the above mathematical model of the system:

1. Physical and chemical details of the cells involved in the respiratory tract are ignored.
2. Strictly speaking, mass is conserved, not volume. By equating the volume of a certain mass of oxygen in air to the volume of that mass of oxygen in blood, we assume the density of oxygen is

the same in each of those mixtures. Further, we assume that the addition of oxygen does not change the volume of the blood.

3. Assumes that each compartment in the scheme can be modeled using a well-stirred tank. This obviously implies that the contents of the compartment are well mixed and, less obviously, that the composition of the outlet stream is the same as the composition of the contents of the tank.
4. Assumes inspiration and expiration can be modeled using a sinusoidal function.
5. Assume volumes of pulmonary pools are all equal.
6. Given the mathematical expression for Y_j^*, $X_{Pj} \leq 0.20155\ \ ml\ O2/ml\ blood$ no matter how high the molar fraction of oxygen is in the main lung compartment.

The differential equations from the material balances are derived on each compartment below.

Main Lung Compartment

$$accum = Q_A Y_{air} - Q_A Y_L - K_A(Y_L - Y_1^*) - K_A(Y_L - Y_2^*) - K_A(Y_L - Y_3^*) = \alpha$$

Where the following equation applies for Y_1^*, Y_2^*, Y_3^*:

$$Y_1^*, Y_2^*, Y_3^* \equiv Y_j^* = \frac{.00032X_{Pj}}{.20155 - X_{Pj}} + \left(11.27X_{Pj}\right)\left(.055X_{Pj}\right)$$

Also the following parameters:

$$Q_A = 4500\frac{ml\ air}{minute}$$
$$Y_{air} = .2$$
$$Y_L = \ .142\frac{ml\ O_2}{ml\ gas}$$
$$K_A = 3050\frac{ml\ air}{minute}$$
$$Y_L(t=0) = .142\frac{ml\ O_2}{ml\ gas}$$

Checking the units:

$$\frac{ml\ O_2}{minute} = \left[\frac{ml\ air}{minute} * \frac{ml\ O_2}{ml\ air}\right] - \left[\frac{ml\ air}{minute} * \frac{ml\ O_2}{ml\ air}\right] - \left[\frac{ml\ air}{minute}\left(\frac{ml\ O_2}{ml\ air} - \frac{ml\ O_2}{ml\ air}\right)\right] - \left[\frac{ml\ air}{minute}\left(\frac{ml\ O_2}{ml\ air} - \frac{ml\ O_2}{ml\ air}\right)\right] - \left[\frac{ml\ air}{minute}\left(\frac{ml\ O_2}{ml\ air} - \frac{ml\ O_2}{ml\ air}\right)\right]$$

Where:

$$accum = \frac{d(V_L Y_L)}{dt} = V_L\frac{dY_L}{dt} + Y_L\frac{dV_L}{dT}$$

Substituting the expression for $accum = \alpha$ into the expression, we obtain the transient material balance:

$$V_L\frac{dY_L}{dt} = \alpha - Y_L\frac{dV_L}{dt}$$

The differential equation:

$$\frac{dY_L(X_{P1}, X_{P2}, X_{P3})}{dt} = \frac{1}{V_L}\left(\alpha - Y_L\frac{dV_L}{dt}\right)$$

Where α is an equation defined above and the expression for V_L, where $\tau = 5\ seconds$:

$$V_L = 2700 + 260\cos\left(\frac{2\pi t}{\tau}\right) = [ml]$$

Alveoli 1

$$accum = \sigma Q_B X_V + K_A(Y_L - Y_1^*) - \sigma Q_B X_{P1}$$

And the following parameters:

$$\sigma = .99$$
$$Q_B = 5500\frac{ml\ blood}{minute}$$
$$X_V(t=0) = .150\frac{ml\ O_2}{ml\ blood}$$
$$X_{P1}(t=0) = .165\frac{ml\ O_2}{ml\ blood}$$

Checking the units:

$$\frac{ml\ O_2}{minute} = \left[\frac{ml\ blood}{minute} * \frac{ml\ O_2}{ml\ blood}\right] + \left[\frac{ml\ air}{minute}\left(\frac{ml\ O_2}{ml\ air} - \frac{ml\ O_2}{ml\ air}\right)\right] - \left[\frac{ml\ blood}{minute} * \frac{ml\ O_2}{ml\ blood}\right]$$

The transient material balance:

$$accum = \frac{d(V_P X_{P1})}{dt} = V_P\frac{dX_{P1}}{dt} + X_{P1}\frac{dV_P}{dt}$$

Simplifying because there is no change in alveoli volume, $V_P = 22\ ml$ and $\frac{dV_p}{dt} = 0$ in the second term:

$$accum = \frac{d(V_P X_{P1})}{dt} = V_P\frac{dX_{P1}}{dt}$$

The differential equation:

$$\frac{dX_{P1}(X_V, Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_V + K_A(Y_L - Y_1^*) - \sigma Q_B X_{P1}]$$

Alveoli 2

$$accum = \sigma Q_B X_{P1} + K_A(Y_L - Y_2^*) - \sigma Q_B X_{P2}$$

Additional parameter:

$$X_{P2}(t=0) = .183\frac{ml\ O_2}{ml\ blood}$$

The transient material balance:

$$accum = \frac{d(V_P X_{P2})}{dt} = V_P\frac{dX_{P2}}{dt}$$

The differential equation:

$$\frac{dX_{P2}(X_{P1}, Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_{P1} + K_A(Y_L - Y_2^*) - \sigma Q_B X_{P2}]$$

Alveoli 3

$$accum = \sigma Q_B X_{P2} + K_A(Y_L - Y_3^*) - \sigma Q_B X_{P3}$$

Additional parameter:

$$X_{P3}(t=0) = .190\frac{ml\ O_2}{ml\ blood}$$

The transient material balance:

$$accum = \frac{d(V_P X_{P3})}{dt} = V_P\frac{dX_{P3}}{dt}$$

The differential equation:

$$\frac{dX_{P3}(X_{P2},Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_{P2} + K_A(Y_L - Y_3^*) - \sigma Q_B X_{P3}]$$

Arterial Blood Pool

$$accum = (1-\sigma)Q_B X_V + \sigma Q_B X_{P3} - Q_B X_A$$

With the additional parameter:

$$X_A(t=0) = .193\frac{ml\ O_2}{ml\ blood}$$

Checking the units:

$$\frac{ml\ O_2}{minute} = \left[\frac{ml\ blood}{minute} * \frac{ml\ O_2}{ml\ blood}\right] + \left[\frac{ml\ blood}{minute} * \frac{ml\ O_2}{ml\ blood}\right] - \left[\frac{ml\ blood}{minute} * \frac{ml\ O_2}{ml\ blood}\right]$$

The transient material balance at constant arterial blood volume, $V_A = 1700\ ml$:

$$accum = \frac{d(V_A X_A)}{dt} = V_A\frac{dX_A}{dt}$$

The differential equation:

$$\frac{dX_A(X_V,X_{P3})}{dt} = \frac{1}{V_A}[(1-\sigma)Q_B X_V + \sigma Q_B X_{P3} - Q_B X_A]$$

Venous Blood Pool

$$accum = Q_B X_A - Q_B X_V - M$$

We are given the parameter:

$$M = 230\frac{ml\ O_2}{minute}$$

Checking the units:

$$\frac{ml\ O_2}{minute} = \left[\frac{ml\ blood}{minute} * \frac{ml\ O_2}{ml\ blood}\right] - \left[\frac{ml\ blood}{minute} * \frac{ml\ O_2}{ml\ blood}\right] - \frac{ml\ O_2}{minute}$$

The transient material balance at constant $V_V = 20\ liters = 2000\ ml$:

$$accum = \frac{d(V_V X_V)}{dt} = V_V\frac{dX_V}{dt}$$

The differential equation:

$$\frac{dX_V(X_A)}{dt} = \frac{1}{V_V}[Q_B X_A - Q_B X_V - M]$$

<u>**SUMMARY FOR PART A**</u>

- ***The differential equations for each compartment***

Main lung compartment:

$$\frac{dY_L(X_{P1},X_{P2},X_{P3})}{dt} = \frac{1}{V_L}\left(\alpha - Y_L\frac{dV_L}{dt}\right)$$

Where

$$Q_A Y_{air} - Q_A Y_L - K_A(Y_L - Y_1^*) - K_A(Y_L - Y_2^*) - K_A(Y_L - Y_3^*) = \alpha$$

Put together:

$$\frac{dY_L(X_{P1},X_{P2},X_{P3})}{dt} = \frac{1}{V_L}\left(Q_A Y_{air} - Q_A Y_L - K_A(Y_L - Y_1^*) - K_A(Y_L - Y_2^*) - K_A(Y_L - Y_3^*) - Y_L\frac{dV_L}{dt}\right)$$

Alveoli compartment 1:

$$\frac{dX_{P1}(X_V,Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_V + K_A(Y_L - Y_1^*) - \sigma Q_B X_{P1}]$$

Alveoli compartment 2:

$$\frac{dX_{P2}(X_{P1}, Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_{P1} + K_A(Y_L - Y_2^*) - \sigma Q_B X_{P2}]$$

Alveoli compartment 3:

$$\frac{dX_{P3}(X_{P2}, Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_{P2} + K_A(Y_L - Y_3^*) - \sigma Q_B X_{P3}]$$

Arterial blood pool:

$$\frac{dX_A(X_V, X_{P3})}{dt} = \frac{1}{V_A}[(1-\sigma)Q_B X_V + \sigma Q_B X_{P3} - Q_B X_A]$$

Venous blood pool:

$$\frac{dX_V(X_A)}{dt} = \frac{1}{V_V}[Q_B X_A - Q_B X_V - M]$$

- ***Auxiliary equations to the differential equations***

  The time-dependent equation for volume of the lungs:

  $$V_L = 2700 + 260\cos\left(\frac{2\pi t}{\tau}\right)$$

  The equation for Y_j^*:

  $$Y_1^*, Y_2^*, Y_3^* \equiv Y_j^* = \frac{.00032 X_{Pj}}{.20155 - X_{Pj}} + \left(11.27 X_{Pj}\right)\left(.055 X_{Pj}\right)$$

- ***System Parameters***

· K_A= 3050 ml air/min	Mass transfer coefficient for air.
· M= 230 ml O2/min	Metabolic O2 consumption rate.
· Q_A= 4500 ml air/min	Lung ventilation rate.
· Q_B= 5500 ml blood/min	Cardiac blood output.
· V_A= 1700 ml blood	Arterial blood volume.
· Y_{air}= 0.2	Volume fraction of O2 in the input flow to the lungs.
· V_P= 22 ml	Pulmonary capillary blood volume (for each pool).
· V_V= 40 liters	Tissue volume.
· σ= 0.99	Fraction of venous blood that goes through the lungs.
· $V_L = 2700 + 260\cos\left(\frac{2\pi t}{\tau}\right)$ ml	Volume of the lungs, varying with time.
· τ= 5 seconds	Average time between breaths.

- ***Initial values at $t = 0$ for the dependent variables***

· X_A = 0.193 ml O2/ml blood	Arterial blood concentration of O2
· X_{P1} = 0.165 ml O2/ml blood	Pulmonary blood concentration of O2 in the 1st pool
· X_{P2}= 0.183 ml O2/ml blood	Pulmonary blood concentration of O2 in the 2nd pool
· X_{P3}= 0.190 ml O2/ml blood	Pulmonary blood concentration of O2 in the 3rd pool
· X_V= 0.150 ml O2/ml blood	Venous blood concentration of O2
· Y_L= 0.142 ml O2/ml gas	Lung gas volume fraction of O2

B. PERSON HOLDS BREATH AT t=0

In this scenario, the person holds his/her breath at time 0, which means that

Q_A= 0 ml air/min

$V_L = \max(2700 + 260\cos\left(\frac{2\pi t}{\tau}\right)$ ml) = 2700 + 260 = 2960 ml

$\frac{dV_L}{dt} = 0$ ml/min

Thus, while all other differential equations from Part A remain the same, the one for the main lung must be revised in order to reflect these changes.

Main Lung Compartment

Previously for Part A:

$$\frac{dY_L(X_{P1}, X_{P2}, X_{P3})}{dt} = \frac{1}{V_L}\left(Q_A Y_{air} - Q_A Y_L - K_A(Y_L - Y_1^*) - K_A(Y_L - Y_2^*) - K_A(Y_L - Y_3^*) - Y_L\frac{dV_L}{dt}\right)$$

Now, for Part B:

$$\frac{dY_L(X_{P1}, X_{P2}, X_{P3})}{dt} = \frac{1}{V_L}\left(K_A(Y_L - Y_1^*) - K_A(Y_L - Y_2^*) - K_A(Y_L - Y_3^*)\right)$$

Where

V_L =2960 ml

SUMMARY FOR PART B

- ***The differential equations for each compartment***

Main lung compartment:

$$\frac{dY_L(X_{P1}, X_{P2}, X_{P3})}{dt} = \frac{1}{V_L}\left(K_A(Y_L - Y_1^*) - K_A(Y_L - Y_2^*) - K_A(Y_L - Y_3^*)\right)$$

Alveoli compartment 1:

$$\frac{dX_{P1}(X_V, Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_V + K_A(Y_L - Y_1^*) - \sigma Q_B X_{P1}]$$

Alveoli compartment 2:

$$\frac{dX_{P2}(X_{P1}, Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_{P1} + K_A(Y_L - Y_2^*) - \sigma Q_B X_{P2}]$$

Alveoli compartment 3:

$$\frac{dX_{P3}(X_{P2}, Y_L)}{dt} = \frac{1}{V_P}[\sigma Q_B X_{P2} + K_A(Y_L - Y_3^*) - \sigma Q_B X_{P3}]$$

Arterial blood pool:

$$\frac{dX_A(X_V, X_{P3})}{dt} = \frac{1}{V_A}[(1-\sigma)Q_B X_V + \sigma Q_B X_{P3} - Q_B X_A]$$

Venous blood pool:

$$\frac{dX_V(X_A)}{dt} = \frac{1}{V_V}[Q_B X_A - Q_B X_V - M]$$

- ***Auxiliary equation to the differential equations***
  The equation for Y_j^*:
$$Y_1^*, Y_2^*, Y_3^* \equiv Y_j^* = \frac{.00032X_{Pj}}{.20155 - X_{Pj}} + (11.27X_{Pj})(.055X_{Pj})$$

- ***System Parameters***
  - K_A= 3050 ml air/min — Mass transfer coefficient for air.
  - M= 230 ml O2/min — Metabolic O2 consumption rate.
  - Q_A= 0 ml air/min — Lung ventilation rate, 0 in this scenario.
  - Q_B= 5500 ml blood/min — Cardiac blood output.
  - V_A= 1700 ml blood — Arterial blood volume.
  - Y_{air}= 0.2 — Volume fraction of O2 in the input flow to the lungs.
  - V_P= 22 ml — Pulmonary capillary blood volume (for each pool).
  - V_V= 40 liters — Tissue volume.
  - σ= 0.99 — Fraction of venous blood that goes through the lungs.
  - V_L =2960 ml — Maximum of $V_L(t)$ previous scenario; constant.
  - τ= 5 seconds — Average time between breaths.
- ***Initial values at $t = 0$ for the dependent variables***
  - X_A = 0.193 ml O2/ml blood — Arterial blood concentration of O2
  - X_{P1} = 0.165 ml O2/ml blood — Pulmonary blood concentration of O2 in the 1st pool
  - X_{P2}= 0.183 ml O2/ml blood — Pulmonary blood concentration of O2 in the 2nd pool
  - X_{P3}= 0.190 ml O2/ml blood — Pulmonary blood concentration of O2 in the 3rd pool
  - X_V= 0.150 ml O2/ml blood — Venous blood concentration of O2
  - Y_L= 0.142 ml O2/ml gas — Lung gas volume fraction of O2

APPENDIX: DEFINITION OF VARIABLES

· K_A	Mass transfer coefficient for air.
· M	Metabolic O2 consumption rate.
· Q_A	Lung ventilation rate.
· Q_B	Cardiac blood output.
· V_A	Arterial blood volume.
· Y_{air}	Volume fraction of O2 in the input flow to the lungs.
· V_P	Pulmonary capillary blood volume (for each pool).
· V_V	Tissue volume.
· σ	Fraction of venous blood that goes through the lungs.
· V_L	Volume of the lungs, varying with time.
· τ	Average time between breaths.
· X_A	Arterial blood concentration of O2
· X_{P1}	Pulmonary blood concentration of O2 in the 1st pool
· X_{P2}	Pulmonary blood concentration of O2 in the 2nd pool
· X_{P3}	Pulmonary blood concentration of O2 in the 3rd pool
· X_V	Venous blood concentration of O2
· Y_L	Lung gas volume fraction of O2