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Mathematical modelling of intraoperative gas exchange in extracorporeal oxygenation

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Abstract: During cardiopulmonary bypass surgery, a key role is played by the oxygen and carbon-dioxide exchange between the body and the oxygenator. In this work, we present a preliminary mathematical model of this gas exchange and show some results based on experimental data in piglets.

I. Introduction

Several studies have indicated that cardiopulmonary bypass (CPB) during surgical correction of congenital heart defects may contribute to white matter injuries in neonates [1,2]. The underlying mechanisms responsible for these injuries remain poorly understood, largely because MR imaging cannot be performed intraoperatively, since conventional CPB systems are not safe for use near an MR scanner. In previous work, we addressed this limitation by developing an MR-conditional heart-lung machine (HLM) that enables MR imaging during CPB procedures [3,4]. Using this system, we conducted in-vivo experiments on piglets to obtain preliminary data [5]. However, the available dataset is not sufficient to fully explain the causes of the observed neurological damage. To overcome this issue, we aim at creating a full data-informed model of the relevant physiological processes. As a first step towards this goal, in this work we focus on the oxygen (O_2) and carbon dioxide (CO_2) exchange within the oxygenator of the MR-conditional HLM. Specifically, we build upon the mathematical model introduced by [6], which describes the O_2 and CO_2 exchange within a hollow fiber membrane oxygenator, and estimate the O_2 and CO_2 contents and partial pressures on the venous side using the initial values on the arterial side and the HLM settings.

II. Material and methods

We start by considering Eqs. (9) and (12) of [6] yielding the O_2 transfer rate (OTR) and CO_2 transfer rate (CTR):

$$OTR = \dot{Q}_B(CaO_2 - CvO_2) \tag{1}$$

$$CTR = \dot{Q}_B(CvCO_2 - CaCO_2) \tag{2}$$

where $\dot{Q}_B$ (L/min) is the blood flow rate, and CxO_2 and $CxCO_2$ (mL/L blood) are the O_2 and CO_2 contents on the arterial and venous sides if $x = a$, and $x = v$, respectively. Next, we note by Fick's law [7] that

$$CvO_2 = CaO_2 - \frac{\dot{V}O_2}{\dot{Q}_B} \tag{3}$$

$$CvCO_2 = CaCO_2 + \frac{\dot{V}CO_2}{\dot{Q}_B} \tag{4}$$

where $\dot{V}O_2$ and $\dot{V}CO_2$ (mL/min) are the O_2 consumption and CO_2 production, which can be calculated starting from body weight (BW, which is around 15 kg for piglets) and temperature T (°C) from [7] and [8]:

$$\dot{V}O_2 = 32.394 \cdot BW^{0.375} \cdot 4 \cdot 10^{-7} \cdot T^{4.077} \tag{5}$$

$$\dot{V}CO_2 = 5.9319 \cdot BW^{0.75} \cdot 4 \cdot 10^{-7} \cdot T^{4.077} \tag{6}$$

By combining (3) with (5) and (4) with (6), we obtain that $OTR = \dot{V}O_2$ and $CTR = \dot{V}CO_2$. We can now derive the unknown partial pressures on the venous side, PvO_2 and $PvCO_2$ (mmHg). At the start of the operation, we measure the partial pressures on the arterial sides, namely PaO_2 and $PaCO_2$ for O_2 and CO_2, respectively. The values for the venous side, PvO_2 and $PvCO_2$, are computed from (3), (4) using mathematical models for O_2 and CO_2 contents ([6] Eqs. (4), (7)) as follows. By using $x \in \{a, v\}$ for either arterial or venous side, we have:

$$CxO_2 = 10(1.34 \cdot tHb \cdot SxO_2 + PxO_2 \cdot \alpha_{O_2} \cdot \left(1 - \frac{Hct}{100}\right)) \tag{7}$$

$$CxCO_2 = 22.6 \cdot \alpha_{CO_2} \cdot PxCO_2 \cdot 10^{pH_x - pK} \cdot (1 - \frac{0.0289 \cdot tHb}{(3.352 - 0.0046 \cdot SxO_2)(8.142 - pH_x)}) \tag{8}$$

where Hct (%) and tHb (g/dL) are the measured hematocrit and the hemoglobin content, respectively, and $pK = 6.0907$ is the apparent dissociation coefficient of the CO_2/HCO_3^- system. The solubility coefficients α_{O_2} (mL O_2/dL blood/mmHg) and α_{CO_2} (mmol CO_2/L blood/mmHg), oxygen saturation SxO_2 and pH are computed from the partial pressures as follows [6,9]:

$$\alpha_{O_2} = 0.1358(0.0276 \cdot e^{-0.0361T} + 0.0143) \tag{9}$$

$$\alpha_{CO_2} = 0.05874(0.9454 \cdot e^{-0.0625T} + 0.6539 \cdot e^{-0.012T}) \tag{10}$$

$$SxO_2 = \frac{{PxO_2}^{2.9}}{{PxO_2}^{2.9} + {PxO_{2,50}}^{2.9}} \quad (11)$$

$$PxO_{2,50} = 32.558 \cdot 10^{\left(-0.266\left(ln(40) - ln(PxCO_2)\right)\right)} \quad (12)$$

$$pH_x = 6.1 + log_{10}\left(\frac{PxCO_2 - 16.08}{0.03 \cdot PxCO_2}\right) \quad (13)$$

where the last relation implies that $[HCO_3^-] = PxCO_2 - 16.08$ derived from experimental data.

Ultimately, PvO_2 and $PvCO_2$ are obtained from solving (3) and (4) substituting (7) – (13). The two nonlinear equations are solved in MATLAB setting the constraints $5 < PvO_2 < 200$ mmHg and $10 < PvCO_2 < 100$ mmHg (to ensure numerically stable and clinically plausible estimates under surgical conditions [10]) using the interior-point method implemented by "fmincon".

III. Results and discussion

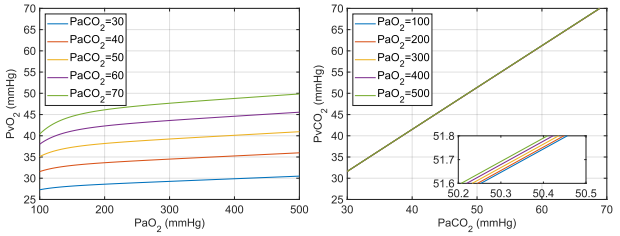

Figure 1: Predicted behavior of simulated venous partial pressures against arterial ones, oxygen part (left) and carbon dioxide part (right). We set T=35 °C, tHb=10.3 g/dL, Hct=30.9%, BW=15 kg, $\dot{Q}_B$ = 800 mL/min, $\dot{Q}_G$= 1000 mL/min.

We start by plotting a sample behavior of our model on synthetic data in Figure 1. We depict the value of PvO_2 as a function of PaO_2 for different values of $PaCO_2$ on the left; similarly, on the right we focus on $PvCO_2$ as a function of $PaCO_2$. All other parameters are not changing. We can notice that the carbon dioxide side displays a linear behavior quite consistent across PaO_2 values, while linearity on the oxygen part emerges only after approximately $PaO_2 = 200$ mmHg, and the values of $PaCO_2$ have a notable impact.

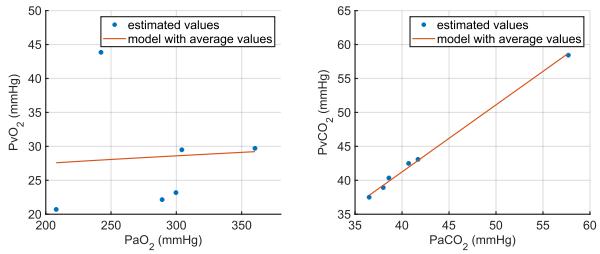

Figure 2: Estimated venous partial pressures for oxygen (left) and carbon dioxide (right) obtained from in-vivo data. The line represents the model output, obtained similarly to Figure 1, but setting the other parameters equal to the observed means throughout the experiment.

This impact is also reflected in the test on experimental data reported in Figure 2. The partial pressures of O_2 and CO_2 that are measured during one of the experiments are depicted. We compare the measurements, reported as dots, against the output obtained from our model, where T, tHb, Hct, $\dot{Q}_B$ and $\dot{Q}_G$ are set to the mean values observed throughout the experiment. We can see the substantial impact of the other parameters in the $PaO_2 - PvO_2$ model (Figure 2, left panel); in contrast, for CO_2 (Figure 2, right panel) the model captures the behavior of the data even if the values of T, tHb, Hct, $\dot{Q}_B$ and $\dot{Q}_G$ are set to their average. It can be noticed that $PaCO_2$ is maintained close to the intended range for the in-vivo study, while PaO_2 is increased above physiological levels in accordance with standard clinical practice [10]. The venous partial pressures O_2 and CO_2 fall within physiological ranges for both $PvCO_2$ (24.2 – 48.2 mmHg) and PvO_2 (24.79 – 114.17 mmHg) [11].

The main limitation of this study is the small amount of data available. With additional measurements, the model could be improved by fitting the equations shown directly to the experimental observations. Furthermore, the calculated venous partial pressures could not be validated against measured results, as no venous blood gas analysis was performed during the experiments, but the results appear physiologically consistent.

IV. Conclusions

The proposed modeling approach for estimating venous partial pressures of blood gases demonstrates promising results. The estimated values fall within physiological ranges and show good agreement with experimental data. By enabling estimation of venous partial pressures, the model also allows for the calculation of the updated arterial partial pressures, creating a comprehensive framework to predict dynamic changes in blood gas partial pressures over time.

Author's Statement

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