Carbon dioxide pH BG model

The formation of bicarobonate (HCO_3^-) from CO_2 is given by $CO_2 + H_2O \underset{k_2}{\overset{k_1}{\rightleftharpoons}} HCO_3^- + H^+$.

The Bond Graph equivalent of this reaction can be represented as

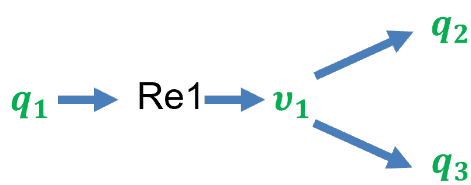

Figure 1: Bond Graph representation of the above reaction (Taken from Peter's Acid-Base notes)

where

$$q_1 = [CO_2] = sp_{CO_2} \tag{1}$$
$$q_2 = \left[HCO_3^-\right] \tag{2}$$
$$q_3 = \left[H^+\right] = 10^{-pH} \tag{3}$$

The bond graph system of equations are:

$$v_1 = -\kappa_1 K_1 q_1 + \kappa_1 K_2 K_3 q_2 q_3 \tag{4}$$
$$\dot{q_1} = -v_1 \tag{5}$$
$$\dot{q_2} = v_1 \tag{6}$$
$$\dot{q_3} = v_1 \tag{7}$$

For initial concetrations: $q_1 = 0.00003 \times 40 = 0.0012\,mol$, $q_2 = 0.024\,mol$, $q_3 = 10^{-(7.4)} = 3.98e^{-8}\,mol$, we assume at steady state $k_1 = k_2 = \frac{q_2 q_3}{q_1}$. The bond graph parameters κ_1, $K_1 - K_3$ can be found by solving the following system

$$k_1 = \kappa_1 K_1 \tag{8}$$
$$k_2 = \kappa_1 K_2 K_3 \tag{9}$$
$$1 = \frac{K_1}{K_2 K_3} \tag{10}$$

which can be written in matrix form

$$ln \begin{bmatrix} k_1 \\ k_2 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & -1 & -1 \end{bmatrix} ln \begin{bmatrix} \kappa_1 \\ K_1 \\ K_2 \\ K_3 \end{bmatrix}. \tag{11}$$

Given the pH of the erythrocyte we can calculate the equivalent pH of the plasma (pHp) as well as the pK values for the erythrocyte ($pKHCO3$) and the plasma ($pKHCO3$p) via (or vice versa by re-writing the equations):

$$pHp = pH - log(3.094 - 0.335pHp) \tag{12}$$
$$pKHCO3 = pH - log\left(\frac{q_2}{q_1}\right) \tag{13}$$
$$pKHCO3p = pKHCO3 \tag{14}$$

We also assume the partial pressures of CO_2 in the plasma and erythrocyte are equal. By using the definition of the solubility coefficients in plasma ($\alpha_p = 0.225$) and erythrocyte ($\alpha_e = 0.191$), we can calculate the $[CO2_p] = \frac{\alpha_p}{\alpha_e}[CO2]$. Additionally the bicarbonate concentration in the plasma can be found using

$$[HCO3_p] = [CO2_p]\,10^{(pHp-pKHCO3p)} \tag{15}$$

At normal conditions, the hemoglobin concentrations in plasma ($Hb_p = 9.3mmol/l$) and erythrocyte ($Hb_e = 21mmol/l$) gives the total buffer base fraction in the erythrocyte $f_e = Hb_p/Hb_e$. Given $f_p + f_e = 1$, we can find the total CO_2 (CO_{2T}) in both plasma and erthrocyte as

$$CO_{2T} = (CO2_p + HCO3_p)f_p + (CO_2 + HCO3)f_e \tag{16}$$

This model is largely adapted from [1]

References

[1] Stephen Edward Rees, Steen Andreassen, R Hovorka, and ER Carson. A dynamic model of carbon dioxide transport in the blood. *IFAC Proceedings Volumes*, 30(2):57–62, 1997.