Acid-Base Physiology

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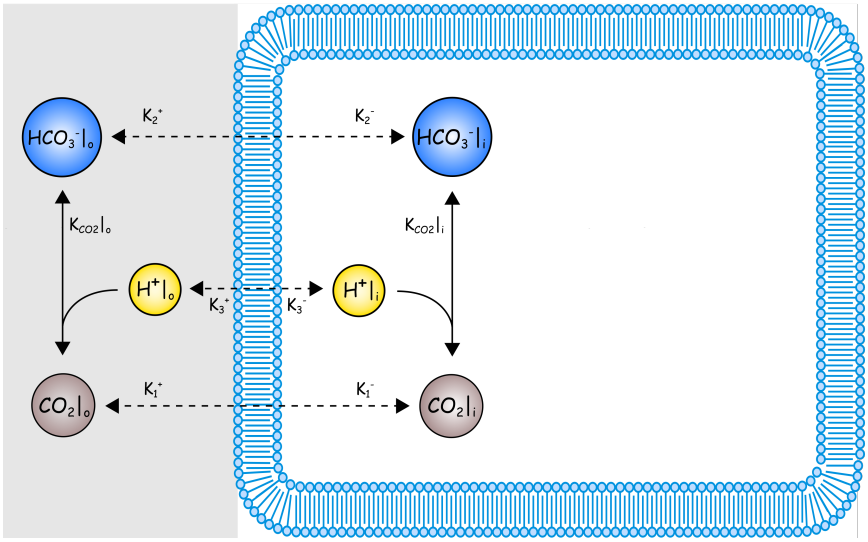
1 Bond Graph Modelling

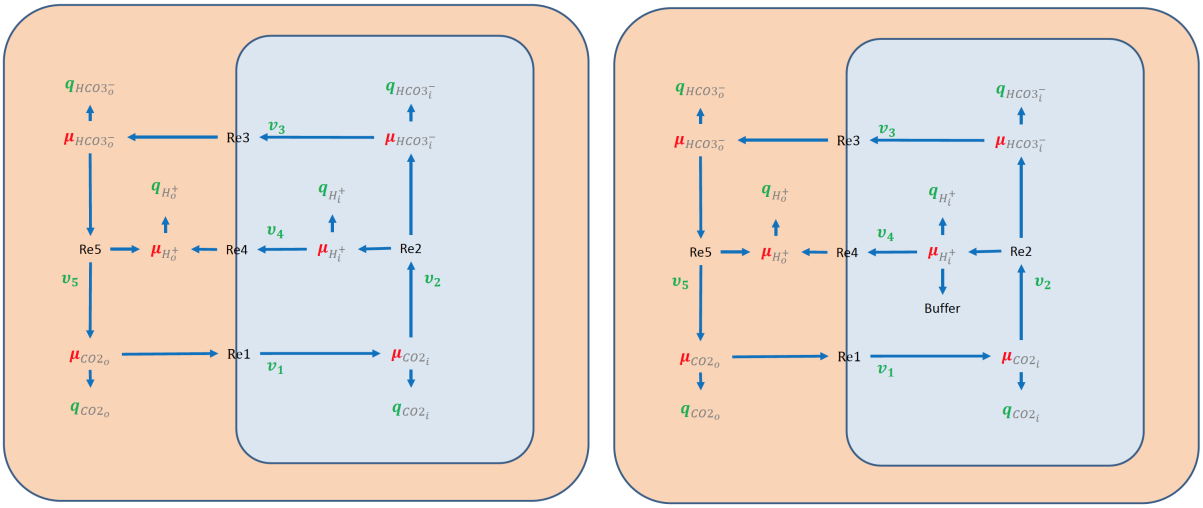
1.1 The biomolecular cycle

The biomolecular cycle of carbonic dioxide experiment is adopted from Boron and De Weer, 1976.



1.2 Bond Graph models

We built two separate bond graph models of the carbon dioxide experiment from Boron and De Weer, 1976. The model on the left side shows the condition that there is no intracellular buffering power ($\beta = 0$ mM), and the one on the right side shows the situation that we have intracellular buffering power ($\beta = -26$ mM). We simulated the buffering power in the bond graph model using a sink element for the protons inside the cell.



1.3 Parameters

The corresponding rated constants, κ are computed as discussed by Gawthrop et al. (2015a) and listed in the Table 1. The thermodynamic constants, K of six substances are evaluated and given in Table 2. Reactions $Re1$ and $Re3$ are corresponding to CO2 diffusion and HCO3 diffusion through the membrane. Reactions $Re2$ and $Re5$ are presenting

CO2 hydration in intracellular and extracellular environment, respectively. Finally, reaction $Re4$ acts as the proton pump in the apical side of the membrane. The rated constants for $Re4$ and $Re5$ are set to zero to simulate the condition that there is no pumping protons out of the membrane, and we have artificial sea water with constant pH.

Table 1: Reaction Parameters

Reaction	κ
Re1	6e−5
Re2	4050
Re3	5e−9
Re4	0
Re5	0

Table 2: Species Parameters

Species	K
$CO_2(int)$	0.00000926
$HCO_3^-(int)$	0.108
$H^+(int)$	0.108
$CO_2(ext)$	0.00000926
$HCO_3^-(ext)$	0.108
$H^+(ext)$	0.108

2 Simulation

Figure 1 shows the results from Boron's paper using the equations in Boron and De Weer, 1976 and implementing them in CellML.

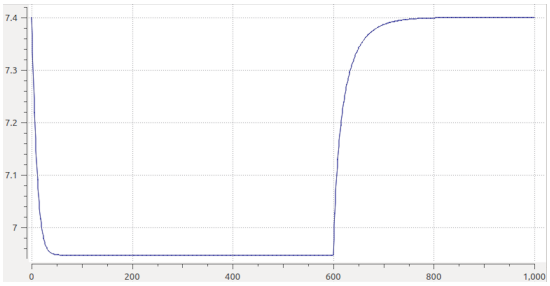


Figure 1: Intracellular pH, based on Boron and De Weer, 1976.

Figure 2 shows the results for the bond graph model when we have no buffering power inside the cell. It can be seen the pH dropped to 4.5 because there wasn't any buffer to consume the protons from CO2 hydration.

Figure 3 shows the results for the bond graph model when we incorporated a sink element inside the cell to simulate the buffering power effect. It can be seen the pH has a similar value to the results presented in Boron and De Weer, 1976.

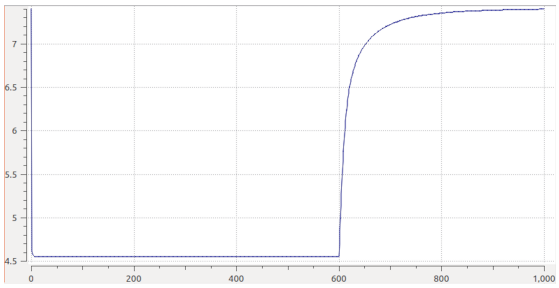


Figure 2: Intracellular pH, based on bond graph model without considering buffering power.

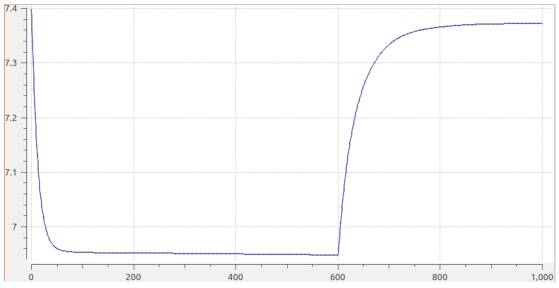


Figure 3: Intracellular pH, based on bond graph model with buffering power.