10th March 213

A VERY simple pH control model just to get things underway. Consider carbonic anhydrase reaction:

$$CO\_{2}+H\_{2}O⇔ H\_{2}CO\_{3}⇔HCO\_{3}^{-}+H^{+}$$

Then assume carbonic acid rapidly dissociates so reaction is approximated by:

$$CO\_{2}+H\_{2}O⇔HCO\_{3}^{-}+H^{+}$$

The flux is given by

$$J=k\_{f}\left[CO\_{2}\right]-k\_{b}\left[HCO\_{3}^{-}\right]\left[H^{+}\right]$$

and the rate equations are

$$\frac{d\left[CO\_{2}\right]}{dt}=-J$$

$$\frac{d\left[HCO\_{3}^{-}\right]}{dt}=J$$

$$\frac{d\left[H^{+}\right]}{dt}=J$$

J has units mM.s-1
The forward and backward rate constants are set to: kf =0.15 s-1 and kb=0.5 (mM)-1.s-1
The initial values are C02=2mM, HCO3=0mM, H=0mM,
where CO2 is [CO2], HCO3 is [HCO3-] and H is [H+].

The CellML model is in the pHcontrol.cellml file

The integration results are shown in the pHcontrol.csv file

C code generated by CellML API from this model.

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 There are a total of 1 entries in the algebraic variable array.

 There are a total of 3 entries in each of the rate and state variable arrays.

 There are a total of 2 entries in the constant variable array.

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/\*

 \* VOI is Time in component Environment (second).

 \* STATES[0] is CO2 in component Flux (mM).

 \* STATES[1] is HCO3 in component Flux (mM).

 \* STATES[2] is H in component Flux (mM).

 \* CONSTANTS[0] is kf in component Flux (per\_second).

 \* CONSTANTS[1] is kb in component Flux (per\_mM\_per\_second).

 \* ALGEBRAIC[0] is J in component Flux (mM\_per\_second).

 \* RATES[0] is d/dt CO2 in component Flux (mM).

 \* RATES[1] is d/dt HCO3 in component Flux (mM).

 \* RATES[2] is d/dt H in component Flux (mM).

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void

initConsts(double\* CONSTANTS, double\* RATES, double \*STATES)

{

STATES[0] = 2;

STATES[1] = 0;

STATES[2] = 0;

CONSTANTS[0] = 0.15;

CONSTANTS[1] = 0.5;

}

void

computeRates(double VOI, double\* CONSTANTS, double\* RATES, double\* STATES, double\* ALGEBRAIC)

{

ALGEBRAIC[0] = CONSTANTS[0]\*STATES[0] - CONSTANTS[1]\*STATES[1]\*STATES[2];

RATES[0] = - ALGEBRAIC[0];

RATES[1] = ALGEBRAIC[0];

RATES[2] = ALGEBRAIC[0];

}

void

computeVariables(double VOI, double\* CONSTANTS, double\* RATES, double\* STATES, double\* ALGEBRAIC)

{

ALGEBRAIC[0] = CONSTANTS[0]\*STATES[0] - CONSTANTS[1]\*STATES[1]\*STATES[2];

}