# A homogeneous bioreactor model reproducing waste column data

## Considering a minimum set of dominant reactions

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### General assumptions:

- Homogeneous, perfectly mixed, (scale: 0.75 $m^3$)
- pCO2 and pH2 are constant and low
- All VFA is converted immediately to acetic acid
- Chemical reactions in equilibrium at all times
- Lumped buffer system, $NaHPO_4^-$ (in blue)

### (Bio)chemical parameters (optimized):

| | | |
|---|---|---|
| $k_{hyd}$ | 0.0026 $day^{-1}$ | Substrate specific |
| $\mu^{max}$ | 0.079 $day^{-1}$ | Biologic intrinsic |
| $K_s$ | 0.0003 mol $L^{-1}$ | Biologic intrinsic |
| $IC_{x,meth}$ | 0.004 mol $L^{-1}$ | Initial concentration |
| $IC_{C27H41O19N}$ | 0.095 mol $L^{-1}$ | Initial concentration |
| $IC_{C2H4O2}$ | 0.4 mol $L^{-1}$ | Initial concentration |
| $C_{NaHPO4}^-$ | 0.9 mol $L^{-1}$ | Lumped buffer |

### Kinetics (MATLAB)

1. Hydrolysis, acedo- and acetogenesis (lumped):

$$1C_{27}H_4O_{19}N+5.87H_2O+0.06H^+ \rightarrow 11C_2H_4O_2+0.23CO_2+4.67CH_{1.8}O_{0.5}N_{0.2}+0.06NH_4^+$$

$$\frac{dC_{s,hyd}}{dt}=k_{hyd}\cdot C_{s,hyd}$$ Rate limiting step

2. Acetic acid methanogenesis:

$$1C_2H_4O_2+0.02NH_4^+ \rightarrow 0.95CO_2+0.94CH_4+0.10CH_{1.8}O_{0.5}N_{0.2}+0.05H_2O+0.02H^+$$

$$\mu_{meth}=\mu_{meth}^{max}\cdot\frac{C_{s,meth}}{K_{s,meth}+C_{s,meth}}$$

### Chemical equilibria (ORCHESTRA)

$C_2H_4O_2 \rightleftarrows C_2H_3O_2^- + H^+$ $\quad NH_4^+ \rightleftarrows NH_3 + H^+$

$H_2CO_3 \rightleftarrows HCO_3^- + H^+ \rightleftarrows CO_3^{2-} + H^+$ $\quad H_2O \rightleftarrows OH^- + H^+$

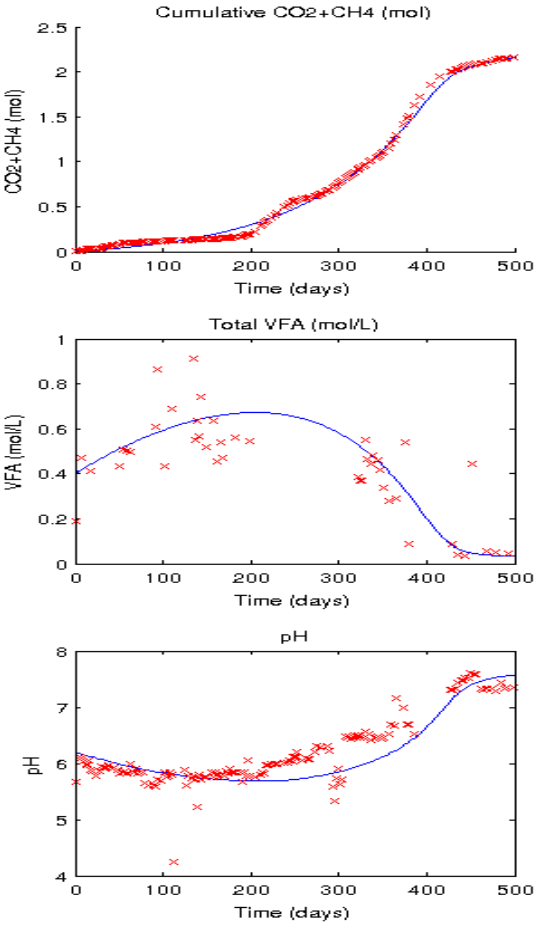
$NaCO_3 \rightleftarrows Na^+ + CO_3^{-2}$ $\quad NaHCO_3 \rightleftarrows Na^+ + HCO_3^-$ $\quad NaHPO_4^- \rightleftarrows Na^+ + HPO_4^-$

$H_3PO_4 \rightleftarrows H_2PO_4^- + H^+ \rightleftarrows HPO_4^{2-} + H^+ \rightleftarrows PO_4^{3-} + H^+$ $\quad NaC_2H_3O_2 \rightleftarrows Na^+ + C_2H_3O_2^-$

### Parameter optimization (DREAM)

Optimization of model parameters within biochemical relevant ranges for experimental pH, VFA and biogas data.

### Results




Experimental data from dissertation of R. Valencia Vazquez 2008

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