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APPENDIX A: CELLULAR KINETICS - TABLE 1

Biochemical rate coefficients (v_{ij}) and kinetic rate equations (ρ_j) for particulate components ($i=1-12$; $j=1-19$)

| Component \rightarrow | i | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | Kinetic Rates (ρ_j , kg COD \cdot m $^{-3}$ \cdot d $^{-1}$) |
|-------------------------|-----------------------------|---------------------------|---------------------------------|--------------------------|------------------------------------|------------------------------------|--------------------------------------|-----------------------------------|------------------------------|-----------------------------|---------------------------------------|---|------------------------------------|---|
| j | Process \downarrow | S_{1i} | S_{2i} | S_{3i} | S_{4i} | S_{5i} | S_{6i} | S_{7i} | S_{8i} | S_{9i} | S_{10i} | S_{11i} | S_{12i} | |
| 1 | Disintegration | | | | | | | | | | $-\sum_{i=1}^{12} C_{i,1}$ | $-\sum_{i=1}^{12} N_{i,1}$ | $f_{D,1}$ | $k_{d,1} \cdot X_1$ |
| 2 | Hydrolysis of carbohydrates | 1 | | | | | | | | | $-\sum_{i=1}^{12} C_{i,2}$ | | | $K_{hyd,2} \cdot X_2$ |
| 3 | Hydrolysis of proteins | | 1 | | | | | | | | $-\sum_{i=1}^{12} C_{i,3}$ | | | $K_{hyd,3} \cdot X_3$ |
| 4 | Hydrolysis of lipids | $1-f_{h,4}$ | | $f_{h,4}$ | | | | | | | $-\sum_{i=1}^{12} C_{i,4}$ | | | $K_{hyd,4} \cdot X_4$ |
| 5 | Uptake of Sugars | -1 | | | | $(1-Y_{5,5}) \cdot f_{5,5}$ | $(1-Y_{5,6}) \cdot f_{5,6}$ | $(1-Y_{5,7}) \cdot f_{5,7}$ | $(1-Y_{5,8}) \cdot f_{5,8}$ | | $-\sum_{i=1}^{12} C_{i,5}$ | $-(Y_{5,5}) \cdot N_{5,5}$ | | $k_{5,5} \frac{S_{1,5}}{K_{1,5} + S_{1,5} + S_{5,5}} \cdot X_{5,5} \cdot I_5$ |
| 6 | Uptake of Amino Acids | | -1 | | $(1-Y_{6,4}) \cdot f_{6,4}$ | $(1-Y_{6,5}) \cdot f_{6,5}$ | $(1-Y_{6,6}) \cdot f_{6,6}$ | $(1-Y_{6,7}) \cdot f_{6,7}$ | $(1-Y_{6,8}) \cdot f_{6,8}$ | | $-\sum_{i=1}^{12} C_{i,6}$ | $-\sum_{i=1}^{12} N_{i,6}$ | | $k_{6,6} \frac{S_{2,6}}{K_{2,6} + S_{2,6} + S_{6,6}} \cdot X_{6,6} \cdot I_6$ |
| 7 | Uptake of LCFA | | | -1 | | | | $(1-Y_{7,7}) \cdot 0.7$ | $(1-Y_{7,8}) \cdot 0.3$ | | $-\sum_{i=1}^{12} C_{i,7}$ | $-(Y_{7,7}) \cdot N_{7,7}$ | | $k_{7,7} \frac{S_{3,7}}{K_{3,7} + S_{3,7} + S_{7,7}} \cdot X_{7,7} \cdot I_7$ |
| 8 | Uptake of Valerate | | | | -1 | $(1-Y_{8,5}) \cdot 0.55$ | $(1-Y_{8,6}) \cdot 0.31$ | $(1-Y_{8,7}) \cdot 0.15$ | | | $-\sum_{i=1}^{12} C_{i,8}$ | $-(Y_{8,5}) \cdot N_{8,5}$ | | $k_{8,8} \frac{S_{4,8}}{K_{4,8} + S_{4,8} + S_{8,8}} \cdot X_{8,8} \cdot \frac{1}{1 + S_{4,8}/S_{8,8}} \cdot I_8$ |
| 9 | Uptake of Butyrate | | | | | $(1-Y_{9,5}) \cdot 0.8$ | $(1-Y_{9,6}) \cdot 0.2$ | | | | $-\sum_{i=1}^{12} C_{i,9}$ | $-(Y_{9,5}) \cdot N_{9,5}$ | | $k_{9,9} \frac{S_{5,9}}{K_{5,9} + S_{5,9} + S_{9,9}} \cdot X_{9,9} \cdot \frac{1}{1 + S_{5,9}/S_{9,9}} \cdot I_9$ |
| 10 | Uptake of Propionate | | | | | | -1 | $(1-Y_{10,6}) \cdot 0.57$ | $(1-Y_{10,7}) \cdot 0.43$ | | $-\sum_{i=1}^{12} C_{i,10}$ | $-(Y_{10,6}) \cdot N_{10,6}$ | | $k_{10,10} \frac{S_{6,10}}{K_{6,10} + S_{6,10} + S_{10,10}} \cdot X_{10,10} \cdot I_{10}$ |
| 11 | Uptake of Acetate | | | | | | | -1 | | $(1-Y_{11,9})$ | $-\sum_{i=1}^{12} C_{i,11}$ | $-(Y_{11,9}) \cdot N_{11,9}$ | | $k_{11,11} \frac{S_{7,11}}{K_{7,11} + S_{7,11} + S_{11,11}} \cdot X_{11,11} \cdot I_{11}$ |
| 12 | Uptake of Hydrogen | | | | | | | | -1 | $(1-Y_{12,9})$ | $-\sum_{i=1}^{12} C_{i,12}$ | $-(Y_{12,9}) \cdot N_{12,9}$ | | $k_{12,12} \frac{S_{8,12}}{K_{8,12} + S_{8,12} + S_{12,12}} \cdot X_{12,12} \cdot I_{12}$ |
| 13 | Decay of X_{11} | | | | | | | | | | $-\sum_{i=1}^{12} C_{i,13}$ | $-\sum_{i=1}^{12} N_{i,13}$ | | $k_{dec,13} \cdot X_{11}$ |
| 14 | Decay of X_{12} | | | | | | | | | | $-\sum_{i=1}^{12} C_{i,14}$ | $-\sum_{i=1}^{12} N_{i,14}$ | | $k_{dec,14} \cdot X_{12}$ |
| 15 | Decay of X_{13} | | | | | | | | | | $-\sum_{i=1}^{12} C_{i,15}$ | $-\sum_{i=1}^{12} N_{i,15}$ | | $k_{dec,15} \cdot X_{13}$ |
| 16 | Decay of X_{14} | | | | | | | | | | $-\sum_{i=1}^{12} C_{i,16}$ | $-\sum_{i=1}^{12} N_{i,16}$ | | $k_{dec,16} \cdot X_{14}$ |
| 17 | Decay of X_{15} | | | | | | | | | | $-\sum_{i=1}^{12} C_{i,17}$ | $-\sum_{i=1}^{12} N_{i,17}$ | | $k_{dec,17} \cdot X_{15}$ |
| 18 | Decay of X_{16} | | | | | | | | | | $-\sum_{i=1}^{12} C_{i,18}$ | $-\sum_{i=1}^{12} N_{i,18}$ | | $k_{dec,18} \cdot X_{16}$ |
| 19 | Decay of X_{17} | | | | | | | | | | $-\sum_{i=1}^{12} C_{i,19}$ | $-\sum_{i=1}^{12} N_{i,19}$ | | $k_{dec,19} \cdot X_{17}$ |
| | | Sugar (kg COD/m 3) | Amino acids (kg COD/m 3) | LCFA (kg COD/m 3) | Total Valerate (kg COD/m 3) | Total butyrate (kg COD/m 3) | Total propionate (kg COD/m 3) | Total acetate (kg COD/m 3) | Hydrogen (kg COD/m 3) | Methane (kg COD/m 3) | Inorganic Carbon (mmole C/m 3) | Inorganic Nitrogen (mmole N/m 3) | Soluble inerts (kg COD/m 3) | |

APPENDIX B: CELLULAR KINETICS - TABLE 2

Biochemical rate coefficients ($v_{i,j}$) and kinetic rate equations (ρ_j) for particulate components ($i=13-24$; $j=1-19$)

| Component | \rightarrow | i | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | Kinetic Rates (ρ_j , kg COD \cdot m $^{-3}$ \cdot d $^{-1}$) |
|-----------|-----------------------------|--------------|--------------------------------|-----------------------------------|------------------------------|----------------------------|---|--|------------------------------------|--|---|--|---|--|-----------------------------|----------------------------|--|
| j | Process | \downarrow | X_c | X_{ch} | X_{pr} | X_h | X_m | X_{aa} | X_{lc} | X_{va} | X_{bu} | X_{prp} | X_{ac} | X_H | S_{cat} | S_{an} | |
| 1 | Disintegration | | -1 | $f_{ch,c}$ | $f_{pr,c}$ | $f_{h,c}$ | | | | | | | | $f_{X,c}$ | | | $k_{dec,c} \cdot X_c$ |
| 2 | Hydrolysis of carbohydrates | | | -1 | | | | | | | | | | | | | $K_{hyd,ca} \cdot X_{ch}$ |
| 3 | Hydrolysis of proteins | | | | -1 | | | | | | | | | | | | $K_{hyd,pr} \cdot X_{pr}$ |
| 4 | Hydrolysis of lipids | | | | | -1 | | | | | | | | | | | $K_{hyd,h} \cdot X_h$ |
| 5 | Uptake of Sugars | | | | | | Y_m | | | | | | | | | | $k_{m,m} \frac{S_m}{K_{s,m} + S_m} X_m I_1$ |
| 6 | Uptake of Amino Acids | | | | | | | Y_{aa} | | | | | | | | | $k_{m,aa} \frac{S_{aa}}{K_{s,aa} + S_{aa}} X_m I_1$ |
| 7 | Uptake of LCFA | | | | | | | | Y_{lc} | | | | | | | | $k_{m,lc} \frac{S_{lc}}{K_{s,lc} + S_{lc}} X_m I_2$ |
| 8 | Uptake of Valerate | | | | | | | | | Y_{va} | | | | | | | $k_{m,va} \frac{S_{va}}{K_{s,va} + S_{va}} X_m \frac{1}{1 + S_{va}/S_m} I_3$ |
| 9 | Uptake of Butyrate | | | | | | | | | | Y_{bu} | | | | | | $k_{m,bu} \frac{S_{bu}}{K_{s,bu} + S_{bu}} X_m \frac{1}{1 + S_{bu}/S_m} I_4$ |
| 10 | Uptake of Propionate | | | | | | | | | | | Y_{prp} | | | | | $k_{m,prp} \frac{S_{prp}}{K_{s,prp} + S_{prp}} X_m I_4$ |
| 11 | Uptake of Acetate | | | | | | | | | | | | Y_{ac} | | | | $k_{m,ac} \frac{S_{ac}}{K_{s,ac} + S_{ac}} X_m I_5$ |
| 12 | Uptake of Hydrogen | | | | | | | | | | | | | Y_{H2} | | | $k_{m,H2} \frac{S_{H2}}{K_{s,H2} + S_{H2}} X_m I_6$ |
| 13 | Decay of X_m | | 1 | | | | -1 | | | | | | | | | | $k_{dec,m} X_m$ |
| 14 | Decay of X_{ch} | | 1 | | | | | -1 | | | | | | | | | $k_{dec,ch} X_{ch}$ |
| 15 | Decay of X_h | | 1 | | | | | | -1 | | | | | | | | $k_{dec,h} X_h$ |
| 16 | Decay of X_{va} | | 1 | | | | | | | -1 | | | | | | | $k_{dec,va} X_{va}$ |
| 17 | Decay of X_{bu} | | 1 | | | | | | | | -1 | | | | | | $k_{dec,bu} X_{bu}$ |
| 18 | Decay of X_{prp} | | 1 | | | | | | | | | -1 | | | | | $k_{dec,prp} X_{prp}$ |
| 19 | Decay of X_{ac} | | 1 | | | | | | | | | | -1 | | | | $k_{dec,ac} X_{ac}$ |
| | | | 1 | | | | | | | | | | | -1 | | | $k_{dec,H2} X_{H2}$ |
| | | | Composites (kg COD/m 3) | Carbohydrates (kg COD/m 3) | Proteins (kg COD/m 3) | Lipids (kg COD/m 3) | Sugars degraders (kg COD/m 3) | Amino acids degraders (kg COD/m 3) | LCFA degraders (kg COD/m 3) | Val- & Butyrate degraders (kg COD/m 3) | Propionate degraders (kg COD/m 3) | Acetate degraders (kg COD/m 3) | Hydrogen degraders (kg COD/m 3) | Particulate inerts (kg COD/m 3) | Cations (kmole /m 3) | Anions (kmole /m 3) | |

APPENDIX C: PAPER 1

Study of inhibition in plug flow anaerobic digesters using mathematical modeling and simulation. Journal of The Institute of Incorporated Engineers, Sri Lanka, Vol 13, No 1, July 2013. (Karunaratne H.D.S.S., Rathnasiri P.G., University of Moratuwa)



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