# Supporting Information for

## Evaluating Enhanced Sulfate Reduction and Optimized Volatile Fatty Acids (VFA) Composition in Anaerobic Reactor by Fe (III) Addition

Yiwen Liu[1], Yaobin Zhang[2,*] and Bing-Jie Ni[1,*]

[1]Advanced Water Management Centre, The University of Queensland, St Lucia, QLD 4072, Australia

[2]Key Laboratory of Industrial Ecology and Environmental Engineering, Ministry of Education, School of Environmental Science and Technology, Dalian University of Technology, Dalian 116024, China

***Corresponding authors:**

Bing-Jie Ni, P +61 7 33463230; F +61 7 33654726; E-mail: b.ni@uq.edu.au

Yaobin Zhang, P +86 411 84706460; F +86 411 84706263; E-mail: zhangyb@dlut.edu.cn

**The following are included as supporting information for this paper:**

number of pages: 10

number of figures: 0

number of tables: 6

**Table S1. The Definition and Units of Model Components**

| Variable | Definition | Unit |
|---|---|---|
| $S_{su}$ | Sugar | g COD/$m^3$ |
| $S_{bu}$ | Butyrate acid | g COD/$m^3$ |
| $S_{bu-}$ | Butyrate | g COD/$m^3$ |
| $S_{pro}$ | Propionate acid | g COD/$m^3$ |
| $S_{pro-}$ | Propionate | g COD/$m^3$ |
| $S_{ac}$ | Acetate acid | g COD/$m^3$ |
| $S_{ac-}$ | Acetate | g COD/$m^3$ |
| $S_{h2}$ | Hydrogen in wastewater | g COD/$m^3$ |
| $S_{h2,g}$ | Hydrogen in gas phase | g COD/$m^3$ |
| $S_{co2}$ | Carbon dioxide in wastewater | mM |
| $S_{hco3}$ | Bicarbonate | mM |
| $S_{co2,g}$ | Carbon dioxide in gas phase | mM |
| $S_{nh3}$ | Ammonia | g N/$m^3$ |
| $S_{nh4}$ | Ammonium | g N/$m^3$ |
| $S_{SO4}$ | Sulfate | g S/$m^3$ |
| $S_{H2S}$ | $H_2S$ in wastewater | g S/$m^3$ |
| $S_{HS}$ | $HS^-$ in wastewater | g S/$m^3$ |
| $S_{H2S,g}$ | $H_2S$ in gas phase | g S/$m^3$ |
| $S_{h+}$ | Hydrogen ion | mM |
| $S_{Cat}$ | Metallic cation | mM |
| $S_{An}$ | Metallic anion | mM |
| $S_{Fe2}$ | $Fe^{2+}$ | g Fe/$m^3$ |
| $X_{Fe3}$ | $Fe_2O_3$ | g Fe/$m^3$ |
| $S_{Fe3}$ | $Fe^{3+}$ | g Fe/$m^3$ |
| $X_{FeS}$ | Iron-sulfide precipitation | g /$m^3$ |
| $X_S$ | Readily biodegradable COD | g COD/$m^3$ |
| $X_I$ | Inert particular COD | g COD/$m^3$ |
| $X_{su}$ | Sugar degraders | g COD/$m^3$ |
| $X_{bu}$ | Butyrate degraders | g COD/$m^3$ |
| $X_{pro}$ | Propionate degraders | g COD/$m^3$ |
| $X_{IRB,bu}$ | IRB grown on butyrate | g COD/$m^3$ |
| $X_{IRB,pro}$ | IRB grown on propionate | g COD/$m^3$ |
| $X_{IRB,ac}$ | IRB grown on acetate | g COD/$m^3$ |
| $X_{IRB,h}$ | IRB grown on hydrogen | g COD/$m^3$ |
| $X_{SRB,bu}$ | SRB grown on butyrate | g COD/$m^3$ |
| $X_{SRB,pr}$ | SRB grown on propionate | g COD/$m^3$ |
| $X_{SRB,ac}$ | SRB grown on acetate | g COD/$m^3$ |
| $X_{SRB,h}$ | SRB grown on hydrogen | g COD/$m^3$ |
| $S_{IC}$ | Total inorganic carbon | mM |
| $S_{IN}$ | Total inorganic nitrogen | g N/$m^3$ |
| $S_{oH-}$ | Hydroxide ion | mM |

**Table S2. Stoichiometric Matrix for the Developed Model**

| | $S_{su}$ | $S_{bu}$ | $S_{pro}$ | $S_{ac}$ | $S_{h2}$ | $S_{SO4}$ | $S_{H2S}$ | $S_{IC}$ | $S_{IN}$ | $X_{Fe3}$ | $S_{Fe3}$ | $S_{Fe2}$ | $X_{FeS}$ | $X_S$ | $X_I$ | $X_{su}$ | $X_{bu}$ | $X_{pro}$ | $X_{SRB,bu}$ | $X_{SRB,pr}$ | $X_{SRB,ac}$ | $X_{SRB,h}$ | $X_{IRB,bu}$ | $X_{IRB,pr}$ | $X_{IRB,ac}$ | $X_{IRB,h}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | COD | COD | COD | COD | COD | S | S | C | N | Fe | Fe | Fe | FeS | COD | COD | COD | COD | COD | COD | COD | COD | COD | COD | COD | COD | COD |
| 1 | 1 | | | | | | | | | | | | | -1 | | | | | | | | | | | | |
| 2 | -1 | *f1*(1-$Y_{su}$) | *f2*(1-$Y_{su}$) | *f3*(1-$Y_{su}$) | *f4*(1-$Y_{su}$) | | | $-\sum c(C_i)\cdot v_{i,4}$ | $-Y_{su}c(N_{bio})$ | | | | | | | $Y_{su}$ | | | | | | | | | | |
| 3 | | -1 | *f5*(1-$Y_{bu}$) | *f6*(1-$Y_{bu}$) | | | | | $-Y_{c4}c(N_{bio})$ | | | | | | | | $Y_{bu}$ | | | | | | | | | |
| 4 | | | -1 | *f7*(1-$Y_{pro}$) | *f8*(1-$Y_{pro}$) | | | $-\sum c(C_i)\cdot v_{i,4}$ | $-Y_{pr}c(N_{bio})$ | | | | | | | | | $Y_{pro}$ | | | | | | | | |
| 5 | | -1 | | | | $-\frac{1-Y_{SRB,bu}}{2}$ | $\frac{1-Y_{SRB,bu}}{2}$ | | $-Y_{SRB,bu}c(N_{bio})$ | | | | | | | | | | $Y_{SRB,bu}$ | | | | | | | | |
| 6 | | | -1 | | | $-\frac{1-Y_{SRB,pr}}{2}$ | $\frac{1-Y_{SRB,pr}}{2}$ | $-\sum c(C_i)\cdot v_{i,4}$ | $-Y_{SRB,pr}c(N_{bio})$ | | | | | | | | | | | $Y_{SRB,pr}$ | | | | | | | |
| 7 | | | | -1 | | $-\frac{1-Y_{SRB,ac}}{2}$ | $\frac{1-Y_{SRB,ac}}{2}$ | $-\sum c(C_i)\cdot v_{i,4}$ | $-Y_{SRB,ac}c(N_{bio})$ | | | | | | | | | | | | $Y_{SRB,ac}$ | | | | | | |
| 8 | | | | | -1 | $-\frac{1-Y_{SRB,h}}{2}$ | $\frac{1-Y_{SRB,h}}{2}$ | $-\sum c(C_i)\cdot v_{i,4}$ | $-Y_{SRB,h}c(N_{bio})$ | | | | | | | | | | | | | $Y_{SRB,h}$ | | | | | |
| 9 | | -1 | | | | | | | $-Y_{IRB}c(N_{bio})$ | | $-7(1-Y_{IRB})$ | $7(1-Y_{IRB})$ | | | | | | | | | | | $Y_{IRB}$ | | | | |
| 10 | | | -1 | | | | | $-\sum c(C_i)\cdot v_{i,4}$ | $-Y_{IRB}c(N_{bio})$ | | $-7(1-Y_{IRB})$ | $7(1-Y_{IRB})$ | | | | | | | | | | | | $Y_{IRB}$ | | | |
| 11 | | | | -1 | | | | $-\sum c(C_i)\cdot v_{i,4}$ | $-Y_{IRB}c(N_{bio})$ | | $-7(1-Y_{IRB})$ | $7(1-Y_{IRB})$ | | | | | | | | | | | | | $Y_{IRB}$ | | |
| 12 | | | | | -1 | | | $-\sum c(C_i)\cdot v_{i,4}$ | $-Y_{IRB}c(N_{bio})$ | | $-7(1-Y_{IRB})$ | $7(1-Y_{IRB})$ | | | | | | | | | | | | | | | $Y_{IRB}$ |
| 13 | | | | | | | | | | -1 | 1 | | | | | | | | | | | | | | | |
| 14 | | | | | | | -1 | | | | | *-η1* | *η2* | | | | | | | | | | | | | |
| 15 | | | | | | | | | | | | | | 0.9 | 0.1 | -1 | | | | | | | | | | |
| 16 | | | | | | | | | | | | | | 0.9 | 0.1 | | -1 | | | | | | | | | |
| 17 | | | | | | | | | | | | | | 0.9 | 0.1 | | | -1 | | | | | | | | |
| 18 | | | | | | | | | | | | | | 0.9 | 0.1 | | | | -1 | | | | | | | |
| 19 | | | | | | | | | | | | | | 0.9 | 0.1 | | | | | -1 | | | | | | |
| 20 | | | | | | | | | | | | | | 0.9 | 0.1 | | | | | | -1 | | | | | |
| 21 | | | | | | | | | | | | | | 0.9 | 0.1 | | | | | | | -1 | | | | |
| 22 | | | | | | | | | | | | | | 0.9 | 0.1 | | | | | | | | -1 | | | |
| 23 | | | | | | | | | | | | | | 0.9 | 0.1 | | | | | | | | | -1 | | |
| 24 | | | | | | | | | | | | | | 0.9 | 0.1 | | | | | | | | | | -1 | |
| 25 | | | | | | | | | | | | | | 0.9 | 0.1 | | | | | | | | | | | -1 |

**Table S3. Process Kinetic Rate Equations for the Developed Model**

| Process | Kinetics rates expressions |
|---|---|
| 1. Hydrolysis | $k_{hydro}X_{su}$ |
| 2. Uptake of sugar | $k_{su}\frac{S_{su}}{K_{su}+S_{su}}X_{su}I_1$ |
| 3. Uptake of butyrate acid | $k_{bu}\frac{S_{bu}}{K_{\mathrm{bu}}+S_{bu}}X_{bu}I_2I_{h2s,bu}$ |
| 4. Uptake of propionate acid | $k_{pro}\frac{S_{pro}}{K_{pro}+S_{pro}}X_{pro}I_2I_{h2s,pro}$ |
| 5. Butyrate-based sulfidogenesis | $k_{SRB,bu}\frac{S_{bu}}{K_{SRB,bu}+S_{bu}}\frac{S_{SO4}}{K_{SO4}+S_{SO4}}X_{SRB,bu}I_{pH}I_{h2s,SRB,bu}P_{Fe3}$ |
| 6. Propionate-based sulfidogenesis | $k_{SRB,pro}\frac{S_{pro}}{K_{SRB,pro}+S_{pro}}\frac{S_{SO4}}{K_{SO4}+S_{SO4}}X_{SRB,pro}I_{pH}I_{h2s,SRB,pro}P_{Fe3}$ |
| 7. Acetate-based sulfidogenesis | $k_{SRB,ac}\frac{S_{ac}}{K_{SRB,ac}+S_{ac}}\frac{S_{SO4}}{K_{SO4}+S_{SO4}}X_{SRB,ac}I_{pH}I_{h2s,SRB,ac}P_{Fe3}$ |
| 8. Hydrogenotrophic sulfidogenesis | $k_{SRB,h}\frac{S_h}{K_{SRB,h}+S_h}\frac{S_{SO4}}{K_{SO4}+S_{SO4}}X_{SRB,h}I_{pH}I_{h2s,SRB,h}P_{Fe3}$ |
| 9. Butyrate-based iron reduction | $k_{IRB,bu}\frac{S_{bu}}{K_{IRB,bu}+S_{bu}}\frac{S_{Fe3}}{K_{Fe3^+}+S_{Fe3}}X_{IRB,bu}I_{pH}I_{h2s,IRB}$ |
| 10. Propionate-based iron reduction | $k_{IRB,pro}\frac{S_{pro}}{K_{IRB,pro}+S_{pro}}\frac{S_{Fe3}}{K_{Fe3^+}+S_{Fe3}}X_{IRB,pro}I_{pH}I_{h2s,IRB}$ |
| 11. Acetate-based iron reduction | $k_{IRB,ac}\frac{S_{ac}}{K_{IRB,ac}+S_{ac}}\frac{S_{Fe3}}{K_{Fe3^+}+S_{Fe3}}X_{IRB,ac}I_{pH}I_{h2s,IRB}$ |
| 12. Hydrogenotrophic iron reduction | $k_{IRB,h}\frac{S_h}{K_{IRB,h}+S_h}\frac{S_{Fe3}}{K_{Fe3^+}+S_{Fe3}}X_{IRB,h}I_{pH}I_{h2s,IRB}$ |
| 13. $Fe_2O_3$ corrosion | $k_{Fe}\frac{X_{Fe3}}{K_{Fe3}+X_{Fe3}}$ |
| 14. Sulfide precipitation | $k_{pre}S_{H2S}S_{Fe2}$ |

| | |
|---|---|
| 15. Decay of $X_{su}$ | $k_{dec,su}X_{su}$ |
| 16. Decay of $X_{bu}$ | $k_{dec,bu}X_{bu}$ |
| 17. Decay of $X_{pro}$ | $k_{dec,pro}X_{pro}$ |
| 18. Decay of $X_{SRB,bu}$ | $k_{dec,SRB,bu}X_{SRB,bu}$ |
| 19. Decay of $X_{SRB,pr}$ | $k_{dec,SRB,pro}X_{SRB,pro}$ |
| 20. Decay of $X_{SRB,ac}$ | $k_{dec,SRB,ac}X_{SRB,ac}$ |
| 21. Decay of $X_{SRB,h}$ | $k_{dec,SRB,h}X_{SRB,h}$ |
| 22. Decay of $X_{IRB,bu}$ | $k_{dec,IRB}X_{IRB,bu}$ |
| 23. Decay of $X_{IRB,pr}$ | $k_{dec,IRB}X_{IRB,pro}$ |
| 24. Decay of $X_{IRB,ac}$ | $k_{dec,IRB}X_{IRB,ac}$ |
| 25. Decay of $X_{IRB,h}$ | $k_{dec,IRB}X_{IRB,h}$ |
| $P_{fe3}=\frac{X_{fe3}}{K_{p,fe}}+1$ and $I_{h2s}=1-\frac{S_{h2s}}{K_{h2s}}$ | |

**Table S4. Acid-base Reactions of the Developed Model**

| Equation |
| --- |
| $S_{Cat} + S_{nh4}/14 + S_{h+} 2*S_{Fe2} + 3*S_{Fe3} - S_{hco3} - S_{ac-}/64 - S_{pro-}/112 - S_{bu-}/160 - S_{oH-} - 2*S_{SO4}/32 - S_{HS}/32 - S_{An} = 0$ |
| $S_{oH-} * S_h = Kw$ |
| $S_{bu-}*(K_{a,bu+} S_{h+}) - K_{a,bu}*(S_{bu-} + S_{bu}) = 0$ |
| $S_{pro-}*(K_{a,pro+} S_{h+}) - K_{a,pro}*(S_{pro-} + S_{pro}) = 0$ |
| $S_{ac-}*(K_{a,ac+} S_{h+}) - K_{a,ac}*(S_{ac-} + S_{ac}) = 0$ |
| $S_{hco3-}*(K_{a,co2+} S_{h+}) - K_{a,co2}*(S_{hco3-} + S_{co2}) = 0$ |
| $S_{nh4-}*(K_{a,nh4+} S_{h+}) - K_{a,nh4}*(S_{nh4} + S_{nh3}) = 0$ |
| $S_{hs}*(K_{a,h2s+} S_{h+}) - K_{a,h2s}*(S_{hs} + S_{h2s}) = 0$ |

**Table S5. Liquid Phase Yield Coefficient and Rate Equations for Liquid-Gas Reactions in the Developed Model**

| | $S_{h2}$ COD | $S_{co2}$ C | $S_{h2s}$ S | *Rate* |
|---|---|---|---|---|
| 1 | -1 | | | $k_L a(S_{h2} - K_{H,h2} RTS_{h2,g})$ |
| 2 | | -1 | | $k_L a(S_{co2} - K_{H,co2} RTS_{co2,g})$ |
| 3 | | | -1 | $k_L a(S_{h2s} - K_{H,h2s} RTS_{h2s,g})$ |

**Table S6. Kinetic and Stoichiometric Parameters of the Developed Model**

| Parameter | Definition | Values | Unit | Source |
|---|---|---|---|---|
| $k_{hydro}$ | Hydrolysis rate of $X_s$ | 1 | $d^{-1}$ | (1) |
| $k_{su}$ | Maximum uptake rate of $S_{su}$ by $X_{su}$ | 10 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (2) |
| $K_{su}$ | Half saturation constant for $S_{su}$ | 1000 | g COD $m^{-3}$ | (2) |
| $k_{bu}$ | Maximum uptake rate of $S_{bu}$ by $X_{bu}$ | 5 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (2) |
| $K_{bu}$ | Half saturation constant for $S_{bu}$ | 500 | g COD $m^{-3}$ | (2) |
| $k_{pro}$ | Maximum uptake rate of $S_{pro}$ by $X_{pro}$ | 5 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (2) |
| $K_{pro}$ | Half saturation constant for $S_{pro}$ | 500 | g COD $m^{-3}$ | (2) |
| $k_{SRB,bu}$ | Maximum uptake rate of $S_{bu}$ by $X_{SRB,bu}$ | 13.7 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (3) |
| $K_{SRB,bu}$ | Half saturation constant of $X_{SRB,bu}$ for $S_{bu}$ | 100 | g COD $m^{-3}$ | (3) |
| $k_{SRB,pro}$ | Maximum uptake rate of $S_{pro}$ by $X_{SRB,pro}$ | 13.6 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (3) |
| $K_{SRB,pro}$ | Half saturation constant of $X_{SRB,pro}$ for $S_{pro}$ | 150 | g COD $m^{-3}$ | (3) |
| $k_{SRB,ac}$ | Maximum uptake rate of $S_{ac}$ by $X_{SRB,ac}$ | 13.9 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (3) |
| $K_{SRB,ac}$ | Half saturation constant of $X_{SRB,ac}$ for $S_{ac}$ | 150 | g COD $m^{-3}$ | (3) |
| $k_{SRB,h}$ | Maximum uptake rate of $S_h$ by $X_{SRB,h}$ | 26.7 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (3) |
| $K_{SRB,h}$ | Half saturation constant of $X_{SRB,h}$ for $S_h$ | 0.1 | g COD $m^{-3}$ | (3) |
| $K_{SO4}$ | Half saturation constant for $S_{SO4}$ | 64 | g S $m^{-3}$ | (3) |
| $k_{Fe}$ | Maximum uptake rate of $Fe_2O_3$ | 40 | g Fe $m^{-3}$ | (4) |
| $K_{Fe3}$ | Uptake affinity constant for $Fe_2O_3$ | 1000 | g Fe $m^{-3}$ | (4) |
| $K_{P,Fe}$ | Promotion constant of $Fe_2O_3$ | 7000 | g Fe $m^{-3}$ | (4) |
| $k_{IRB,bu}$ | Maximum uptake rate of $S_{bu}$ by $X_{IRB,bu}$ | 5 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (5) |
| $K_{IRB,bu}$ | Half saturation constant of $X_{IRB,bu}$ for $S_{bu}$ | 200 | g COD $m^{-3}$ | (5) |
| $k_{IRB,pro}$ | Maximum uptake rate of $S_{pro}$ by $X_{IRB,pro}$ | 5 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (5) |
| $K_{IRB,pro}$ | Half saturation constant of $X_{IRB,pro}$ for $S_{pro}$ | 200 | g COD $m^{-3}$ | (5) |

| | | | | |
|---|---|---|---|---|
| $k_{IRB,ac}$ | Maximum uptake rate of $S_{ac}$ by $X_{IRB,ac}$ | 5 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (5) |
| $K_{IRB,ac}$ | Half saturation constant of $X_{IRB,ac}$ for $S_{ac}$ | 200 | g COD $m^{-3}$ | (5) |
| $k_{IRB,h}$ | Maximum uptake rate of $S_h$ by $X_{IRB,h}$ | 5 | g COD $m^{-3}$_S/ g COD $m^{-3}$_X $d^{-1}$ | (5) |
| $K_{IRB,h}$ | Half saturation constant of $X_{IRB,h}$ for $S_h$ | 200 | g COD $m^{-3}$ | (5) |
| $K_{Fe3}^{+}$ | Uptake affinity constant for $Fe^{3+}$ by IRB | 10 | g Fe $m^{-3}$ | (4) |
| $k_{pre}$ | Precipitation rate | 1 | $m^3$ $g^{-1}$ $d^{-1}$ | (1) |
| $k_{dec,su}$ | Decay rate coefficient of $X_{su}$ | 0.02 | $d^{-1}$ | (2) |
| $k_{dec,bu}$ | Decay rate coefficient of $X_{bu}$ | 0.01 | $d^{-1}$ | (3) |
| $k_{dec,pro}$ | Decay rate coefficient of $X_{pro}$ | 0.01 | $d^{-1}$ | (3) |
| $k_{dec,SRB,bu}$ | Decay rate coefficient of $X_{SRB,bu}$ | 0.01 | $d^{-1}$ | (3) |
| $k_{dec,SRB,pro}$ | Decay rate coefficient of $X_{SRB,pro}$ | 0.01 | $d^{-1}$ | (3) |
| $k_{dec,SRB,ac}$ | Decay rate coefficient of $X_{SRB,ac}$ | 0.015 | $d^{-1}$ | (3) |
| $k_{dec,SRB,h}$ | Decay rate coefficient of $X_{SRB,h}$ | 0.01 | $d^{-1}$ | (3) |
| $k_{dec,IRB}$ | Decay rate coefficient of *IRB* | 0.01 | $d^{-1}$ | (2) |
| $f1$ | stoichiometric parameters | 0.13 | — | (2) |
| $f2$ | stoichiometric parameters | 0.27 | — | (2) |
| $f3$ | stoichiometric parameters | 0.41 | — | (2) |
| $f4$ | stoichiometric parameters | 0.19 | — | (2) |
| $f5$ | stoichiometric parameters | 0.2 | — | (2) |
| $f6$ | stoichiometric parameters | 0.8 | — | (2) |
| $f7$ | stoichiometric parameters | 0.57 | — | (2) |
| $f8$ | stoichiometric parameters | 0.43 | — | (2) |
| $\eta_1$ | stoichiometric parameters | 1.65 | — | (1) |
| $\eta_2$ | stoichiometric parameters | 2.82 | — | (1) |
| $Y_{su}$ | microorganism yield coefficient | 0.1 | g COD /g COD | (2) |
| $Y_{bu}$ | microorganism yield coefficient | 0.0366 | g COD /g COD | (3) |
| $Y_{pro}$ | microorganism yield coefficient | 0.0366 | g COD /g COD | (3) |
| $Y_{SRB,bu}$ | microorganism yield coefficient | 0.0329 | g COD /g COD | (3) |
| $Y_{SRB,ac}$ | microorganism yield coefficient | 0.0329 | g COD /g COD | (3) |
| $Y_{SRB,pro}$ | microorganism yield coefficient | 0.0342 | g COD /g COD | (3) |
| $Y_{SRB,h}$ | microorganism yield coefficient | 0.0366 | g COD /g COD | (3) |
| $Y_{IRB}$ | microorganism yield coefficient | 0.035 | g COD /g COD | (4) |

| | | | | |
|---|---|---|---|---|
| $K_{h2s,bu}$ | Inhibition constant by $H_2S$ on $X_{bu}$ | 276 | g S $m^{-3}$ | (3) |
| $K_{h2s,pro}$ | Inhibition constant by $H_2S$ on $X_{pro}$ | 276 | g S $m^{-3}$ | (3) |
| $K_{h2s,irb}$ | Inhibition constant by $H_2S$ on *IRB* | 340 | g S $m^{-3}$ | (4) |
| $K_{h2s,srb,bu}$ | Inhibition constant by $H_2S$ on $X_{SRB,bu}$ | 256 | g S $m^{-3}$ | (3) |
| $K_{h2s,srb,pro}$ | Inhibition constant by $H_2S$ on $X_{SRB,pro}$ | 256 | g S $m^{-3}$ | (3) |
| $K_{h2s,srb,ac}$ | Inhibition constant by $H_2S$ on $X_{SRB,ac}$ | 244 | g S $m^{-3}$ | (3) |
| $K_{h2s,srb,h}$ | Inhibition constant by $H_2S$ on $X_{SRB,h}$ | 213 | g S $m^{-3}$ | (3) |
| $C_{ac}$ | carbon content of acetate | 0.0313 | mol $g^{-1}$ COD | (2) |
| $C_{bio}$ | carbon content of biomass | 0.0313 | mol $g^{-1}$ COD | (2) |
| $C_{bu}$ | carbon content of butyrate | 0.0250 | mol $g^{-1}$ COD | (2) |
| $C_{pro}$ | carbon content of propionate | 0.0268 | mol $g^{-1}$ COD | (2) |
| $C_{su}$ | carbon content of sugar | 0.0313 | mol $g^{-1}$ COD | (2) |
| $C_{xc}$ | carbon content of decay | 0.0279 | mol $g^{-1}$ COD | (2) |
| $N_{bio}$ | Nitrogen content of biomass | 0.00625 | mol N $g^{-1}$ COD | (2) |
| $N_{xc}$ | Nitrogen content of decay | 0.002 | mol N $g^{-1}$ COD | (2) |
| Source: (1) Gujer et al., 1999; (2) Bastone et al., 2002; (3) Fedorovich et al., 2003; (4) estimated in this work using experimental data; and (5) Somasundaram et al., 2009. | | | | |

**Additional Reference:**


Gujer, W., Henze, M., Mino, T. and Loosdrecht, M.v., 1999. Activated sludge model no. 3. Water Science and Technology. 39(1), 183-193.

Batstone, D.J., Keller, J., Angelidaki, I., Kalyuzhnyi, S.V., Pavlostathis, S.G., Rozzi, A., Sanders, W.T.M., Siegrist, H. and Vavilin, V.A., 2002. The IWA Anaerobic Digestion Model No 1(ADM 1). Water Science & Technology. 45(10), 65-73.

Fedorovich, V., Lens, P. and Kalyuzhnyi, S., 2003. Extension of Enaerobic Digestion Model No. 1 with processes of sulfate reduction. Applied biochemistry and biotechnology. 109(1-3), 33-45.

Somasundaram, V.; Philip, L.; Bhallamudi, S. M., Experimental and mathematical modeling studies on Cr (VI) reduction by CRB, SRB and IRB, individually and in combination. J. Hazard. Mater. 2009, 172, (2), 606-617.