WP2 : Dynamical Modelling

2 models :

- EM1 : carbon removal (Mexico) :

  $S_C + S_O \rightarrow X$

- EM2 : carbon & nitrogen removal (denitrification/nitrification) :

  Anoxic phase : NO_3 reduction : $S_C + S_{NO3} \rightarrow X_h + S_{NO2}$

  NO_2 reduction : $S_C + S_{NO2} \rightarrow X_h + N_2$

  Ammonification : $S_N \rightarrow S_{NH}$

  Aerobic phase : NH_4 oxidation : $S_O + S_{NH} \rightarrow X_a + S_{NO2}$

  NO_2 oxidation : $S_O + S_{NO2} \rightarrow X_a + S_{NO3}$

  C-removal : $S_C + S_O \rightarrow X_h$

  Ammonification : $S_N \rightarrow S_{NH}$

Experimental protocol for parameter calibration :

- Datasets distributed in two (calibration set, validation set)
- Mathematical transformation : distribution of the parameters in 3 sets (transfer coefficients, yield coefficients, kinetic parameters) in order to provide independent calibration
- A priori identifiability analysis
- A posteriori statistical analysis of the calibration results

EM1 (Mexico)

$$\frac{dX}{dt} = \mu X - \frac{q_{in}}{V} X$$

$$\frac{dS_C}{dt} = -k_1 \mu X + \frac{q_{in}}{V}(S_{C,in} - S_C)$$

$$\frac{dS_O}{dt} = -k_2 \mu X - bX + \frac{q_{in}}{V}(S_{O,in} - S_O) + k_L a(S_{Os} - S_O)$$

$$\frac{dV}{dt} = q_{in}$$

Haldane kinetics : $\mu = \dfrac{\mu_0 S}{K_S + S + \dfrac{S^2}{K_I}}$

Parameter identification results

Parameter	Dimension	Value	Confidence interval
μ_0	h^{-1}	0.1916	0.00255
K_S	mg4CP/L	60	0.01499
K_I	mg4CP/L	3.753	0.00755
k_1	mg4CP/mgVSS	3.7	-
k_2	mgDO/mgVSS	1.0363	0.0578
b	h^{-1}	0.0059	0.0004
k_La	h^{-1}	16.8	0.1

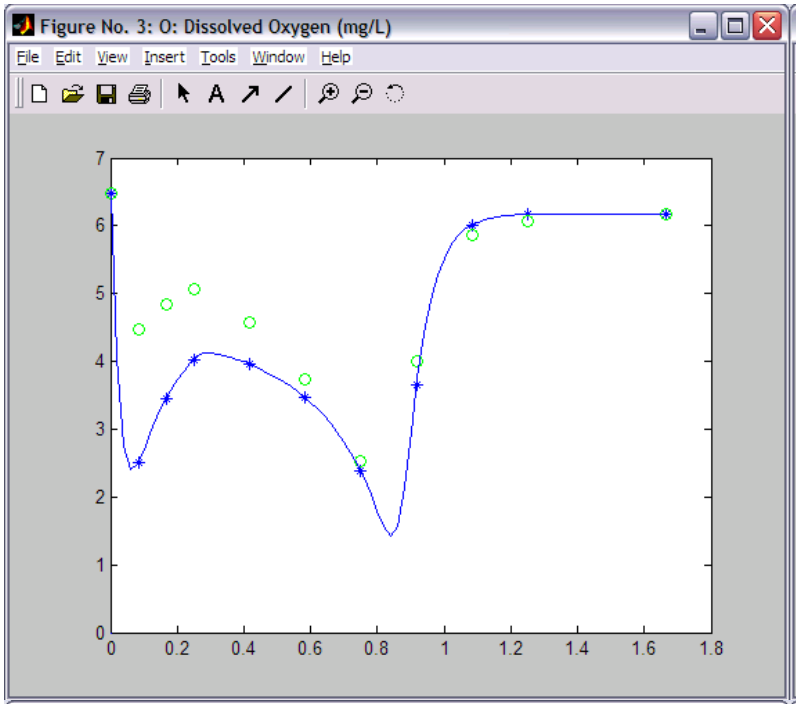


Figure No. 3: O: Dissolved Oxygen (mg/L)
File Edit View Insert Tools Window Help
0 1 2 3 4 5 6 7
0 0.2 0.4 0.6 0.8 1 1.2 1.4 1.6 1.8

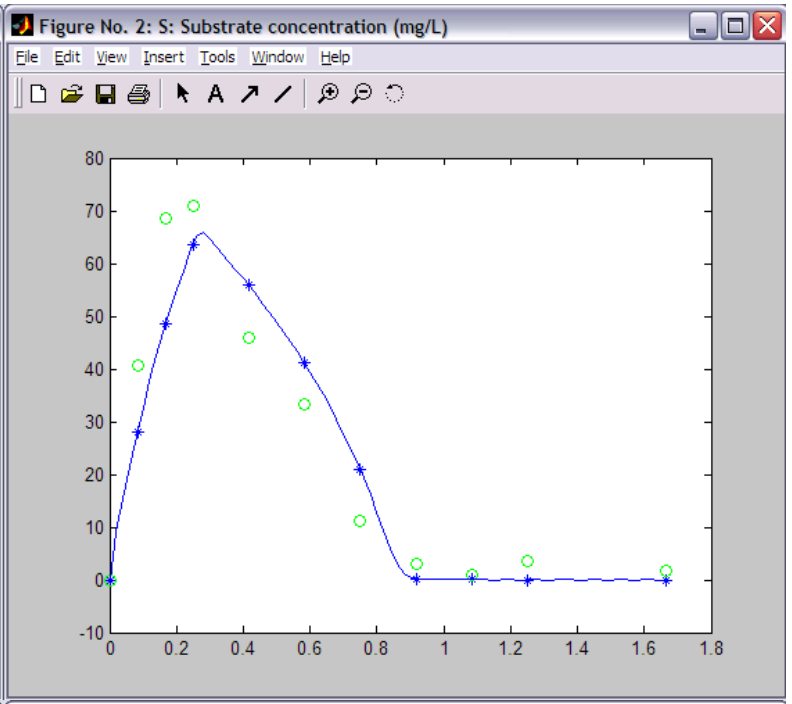


Figure No. 2: S: Substrate concentration (mg/L)
File Edit View Insert Tools Window Help
-10 0 10 20 30 40 50 60 70 80
0 0.2 0.4 0.6 0.8 1 1.2 1.4 1.6 1.8

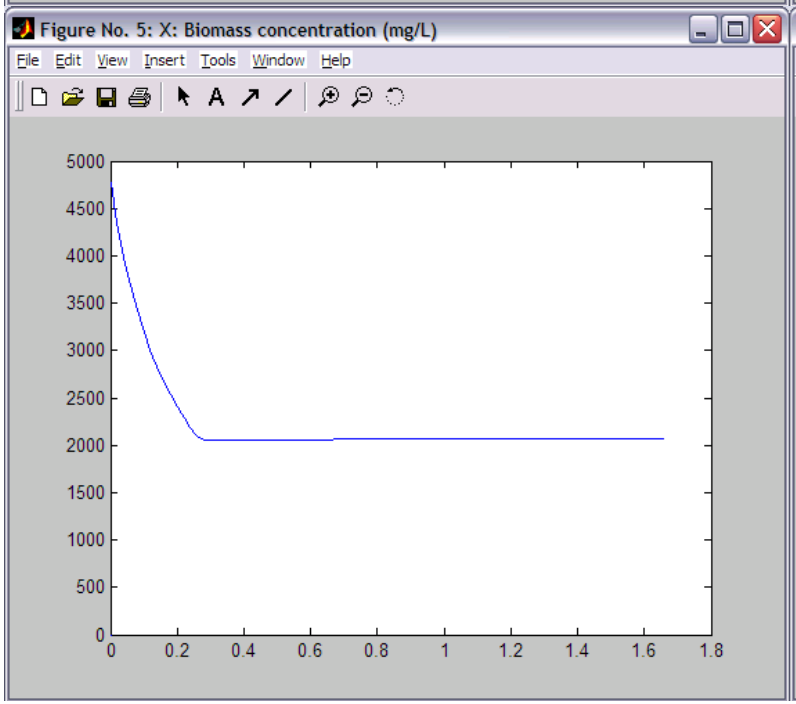


Figure No. 5: X: Biomass concentration (mg/L)
File Edit View Insert Tools Window Help
0 500 1000 1500 2000 2500 3000 3500 4000 4500 5000
0 0.2 0.4 0.6 0.8 1 1.2 1.4 1.6 1.8

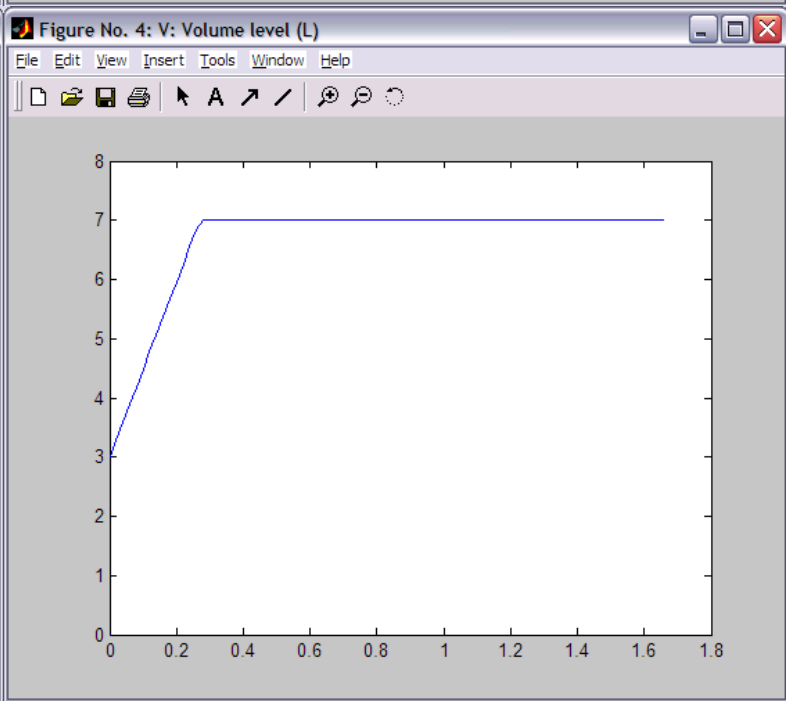


Figure No. 4: V: Volume level (L)
File Edit View Insert Tools Window Help
0 1 2 3 4 5 6 7 8
0 0.2 0.4 0.6 0.8 1 1.2 1.4 1.6 1.8

EM2a (POLIMI)

a) Anoxic phase

$$\frac{dX_h}{dt} = \mu_{h1} X_h$$

$$\frac{dS_C}{dt} = -k_1 \mu_{h1} X_h - k_2 \mu_{h2} X_h$$

$$\frac{dS_{NO_3}}{dt} = -k_3 \mu_{h1} X_h$$

$$\frac{dS_{NO_2}}{dt} = k_4 \mu_{h1} X_h - k_5 \mu_{h2} X_h$$

$$\frac{dS_{NH}}{dt} = k_6 r_N$$

$$\frac{dS_N}{dt} = -r_N$$

b) Aerobic phase

$$\frac{dX_h}{dt} = \mu_h X_h$$

$$\frac{dX_a}{dt} = \mu_{a1} X_a + \mu_{a2} X_a$$

$$\frac{dS_C}{dt} = -k_7 \mu_h X_h$$

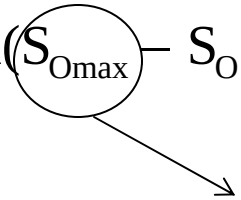
$$\frac{dS_O}{dt} = -k_8 \mu_h X_h - k_9 \mu_{a1} X_a - k_{10} \mu_{a2} X_a + k_L a(S_{Omax} - S_O)$$

$$\frac{dS_{NO_3}}{dt} = k_{11} \mu_{a2} X_a$$

$$\frac{dS_{NO_2}}{dt} = k_{13} \mu_{a1} X_a - k_{12} \mu_{a2} X_a$$

$$\frac{dS_{NH}}{dt} = k_6 r_N - k_{14} \mu_{a1} X_a$$

$$\frac{dS_N}{dt} = -r_N$$



includes endogeneous respiration

Kinetix expressions

$$\mu_{h1} = \mu_{h1\max} \frac{S_C}{K_{Ch1} + S_C - S_{Cmin}} \frac{S_{NO_3}}{K_{NO_3h} + S_{NO_3}}$$

$$\mu_{h2} = \mu_{h2\max} \frac{S_C}{K_{Ch2} + S_C - S_{Cmin}} \frac{S_{NO_2}}{K_{NO_2h} + S_{NO_2}}$$

$$\mu_{h} = \mu_{h\max} \frac{S_C}{K_{Ch} + S_C - S_{Cmin}} \frac{S_O}{K_{Oh} + S_O}$$

$$\mu_{a1} = \mu_{a1\max} \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_O}{K_{Oa1} + S_O}$$

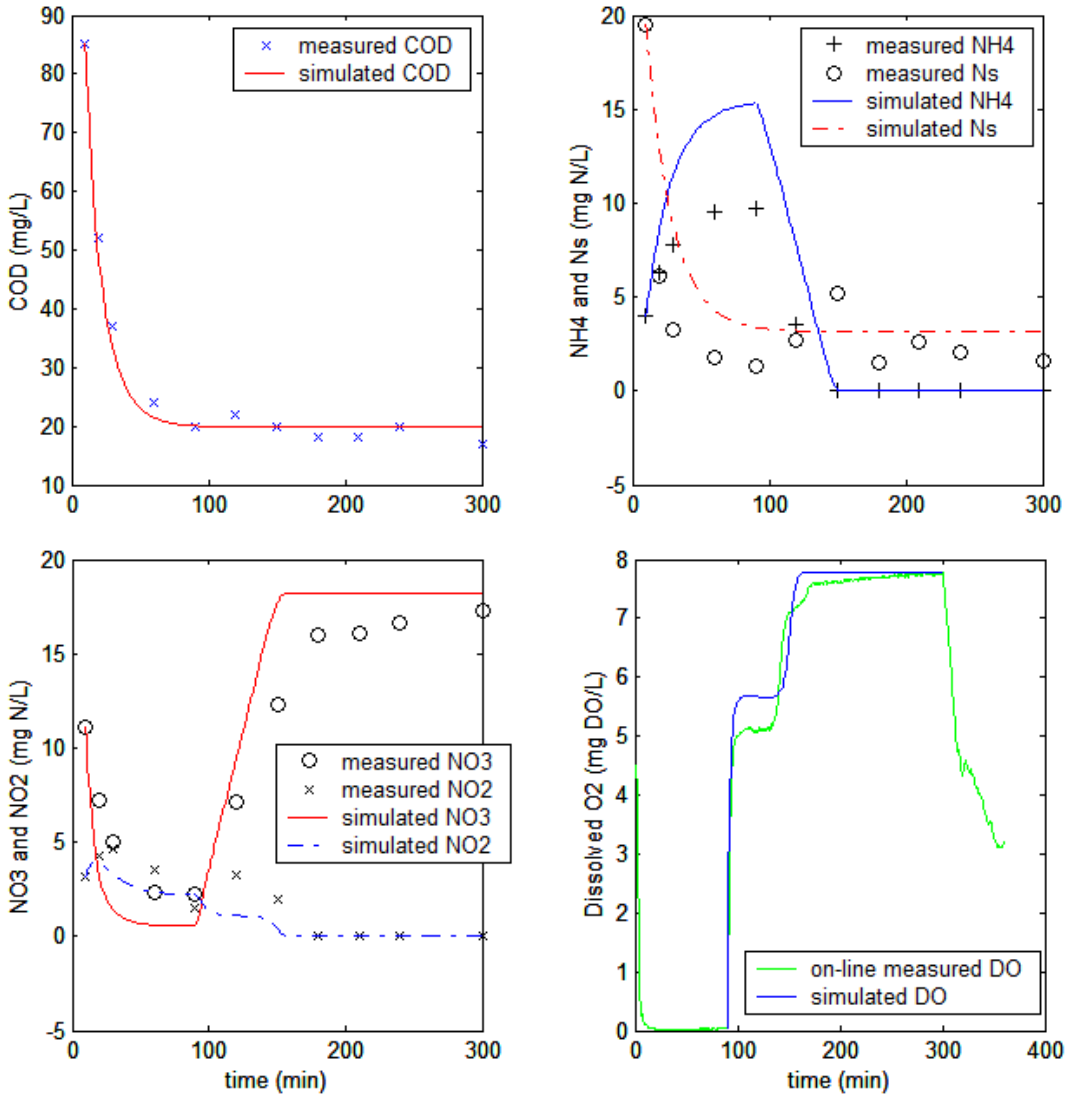
$$\mu_{a2} = \mu_{a2\max} \frac{S_{NO_2}}{K_{NO_2a} + S_{NO_2}} \frac{S_O}{K_{Oa2} + S_O}$$

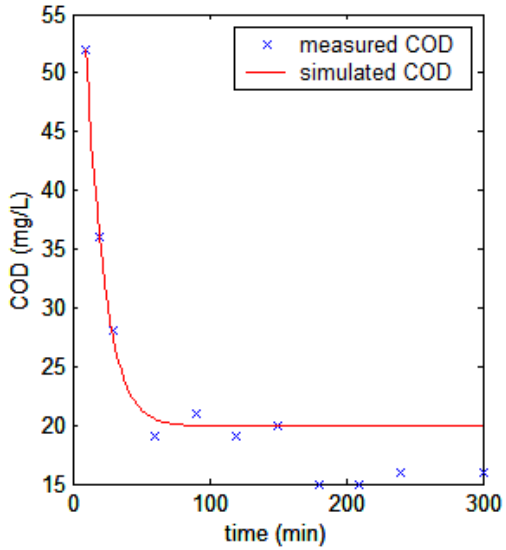
$$r_N = \mu_0 (S_N - S_{Nmin})$$

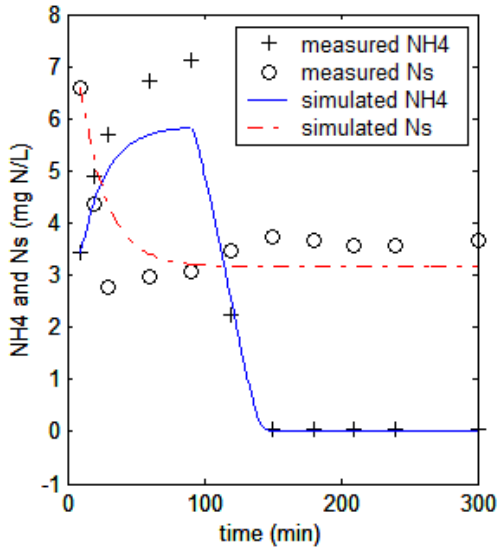
Non-Biodegradable part

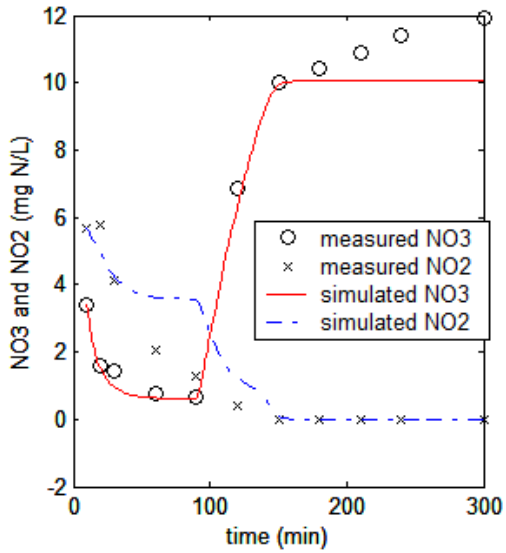
Parameter	Dimension	Value	Confidence interval
Y_{h1}	mgVSS/mgCOD	0.616	0.152
Y_{h2}	mgVSS/mgCOD	0.788	0.129
k_6	mgN/mgN	0.706	0.143
μ_{h1max}	min^{-1}	0.012	0.003
K_{Ch1}	mgCOD/L	57.45	21.15
K_{NO3h}	mgN/L	44.65	7.87
μ_{h2max}	min^{-1}	0.0015	0.0007
K_{Ch2}	mgCOD/L	21.17	16.05
K_{NO2h}	mgN/L	4.99	4.22
μ_0	min^{-1}	0.0529	0.0011
k_La	min^{-1}	0.252	0.079
S_{Omax}	mg/L	7.38	0.36
Y_h	mgVSS/mgCOD	0.75	0.067
Y_{a1}	mgVSS/mgN	1.69	0.37
Y_{a2}	mgVSS/mgN	0.187	0.09
μ_{hmax}	min^{-1}	0.0122	1.5×10^{-10}
K_{Ch}	mgCOD/L	18.96	7.42
K_{Oh}	mgDO/L	40	10.34
μ_{a1max}	min^{-1}	0.0235	1.74×10^{-10}
K_{NH}	mgN/L	0.479	0.208
K_{Oa1}	mgDO/L	29.9	9.47
μ_{a2max}	min^{-1}	0.0117	1.5×10^{-10}
K_{NO2a}	mgN/L	4.963	2.742
K_{Oa2}	mgDO/L	24.9	7.75
S_{Cmin}	mgCOD/L	19.92	1.4
S_{Nmin}	mgN/L	3.16	0.44

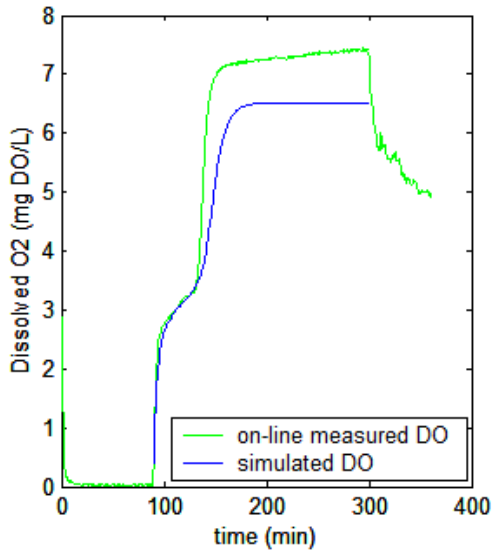
Validation data (POLIMI)




measured COD
simulated COD
COD (mg/L)
time (min)


measured NH4
measured Ns
simulated NH4
simulated Ns
NH4 and Ns (mg N/L)
time (min)


measured NO3
measured NO2
simulated NO3
simulated NO2
NO3 and NO2 (mg N/L)
time (min)


on-line measured DO
simulated DO
Dissolved O2 (mg DO/L)
time (min)

EM2b (LBE)

- absorption : 50% deduced from the initial data

a) Anoxic phase

$$\frac{dX_h}{dt} = \mu_{hN} X_h$$

$$\frac{dS_C}{dt} = -k_1 \mu_{hN} X_h$$

$$\frac{dS_{NO}}{dt} = -k_2 \mu_{hN} X_h$$

$$\frac{dS_{NH}}{dt} = k_6 r_N$$

$$\frac{dS_N}{dt} = -r_N$$

b) Aerobic phase

$$\frac{dX_h}{dt} = \mu_h X_h$$

$$\frac{dX_a}{dt} = \mu_a X_a$$

$$\frac{dS_C}{dt} = -k_4 \mu_h X_h$$

$$\frac{dS_O}{dt} = -k_5 \mu_h X_h - k_6 \mu_a X_a + k_L a(S_{Omax} - S_O)$$

$$\frac{dS_{NO}}{dt} = k_7 \mu_a X_a$$

$$\frac{dS_{NH}}{dt} = k_6 r_N - k_8 \mu_a X_a$$

$$\frac{dS_N}{dt} = -r_N$$

Kinetic expressions

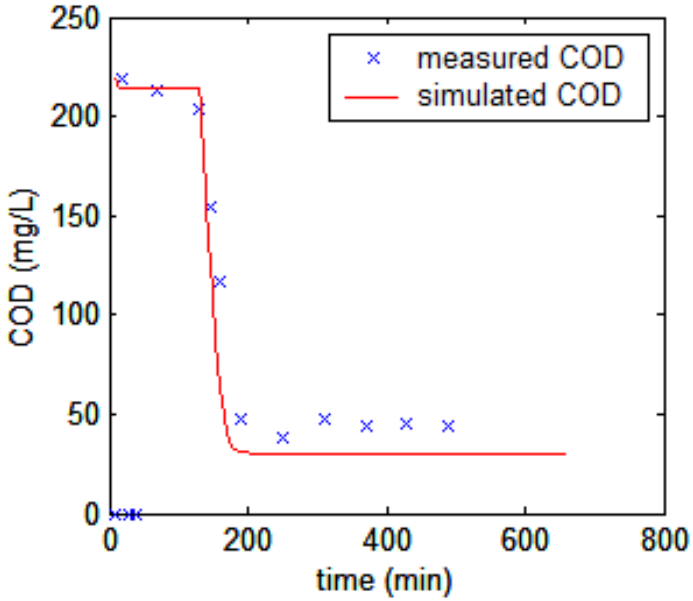
$$\mu_{hN} = \mu_{hN\,\max} \frac{S_C}{K_{C1} + S_C - S_{Cmin}} \frac{S_{NO}}{K_{NO} + S_{NO}}$$

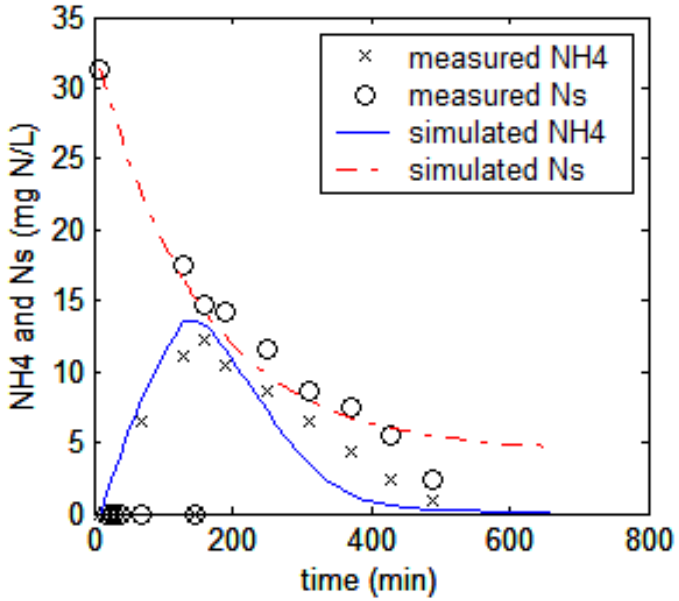
$$\mu_h = \mu_{h\,\max} \frac{S_C}{K_{Ch} + S_C - S_{Cmin}} \frac{S_O}{K_{Oh} + S_O}$$

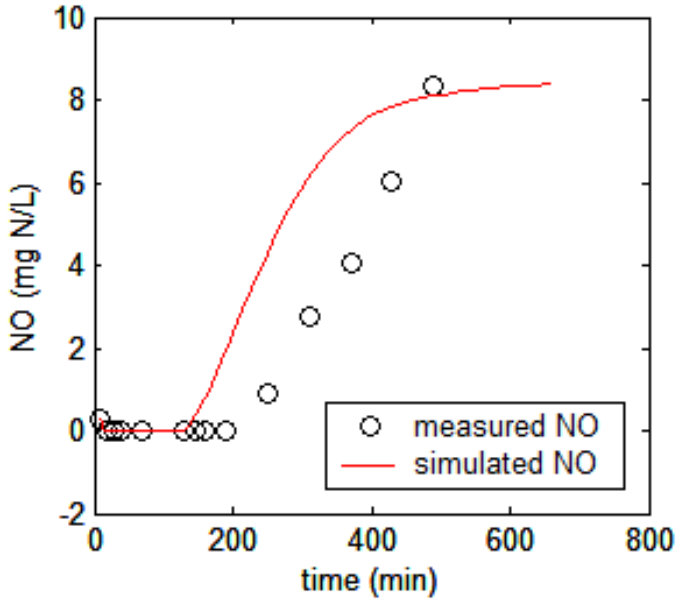
$$\mu_a = \mu_{a\,\max} \frac{S_{NH}}{K_{NHa} + S_{NH}} \frac{S_O}{K_{Oa} + S_O}$$

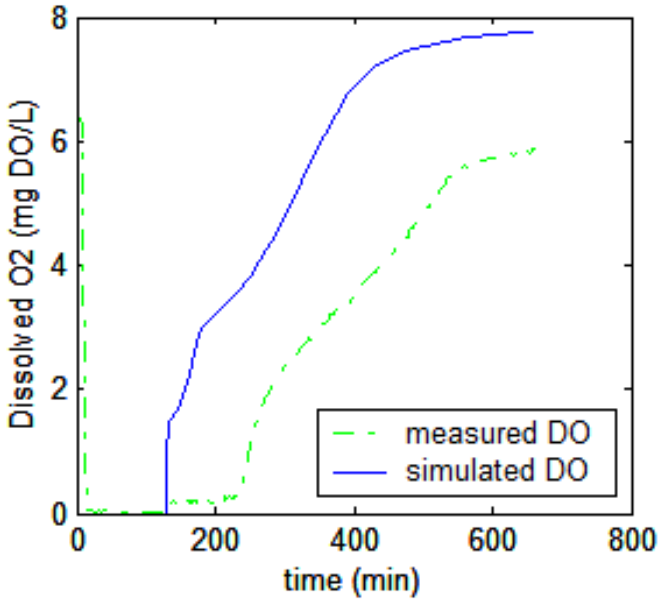
$$r_N = \mu_0 (S_N - S_{Nmin})$$

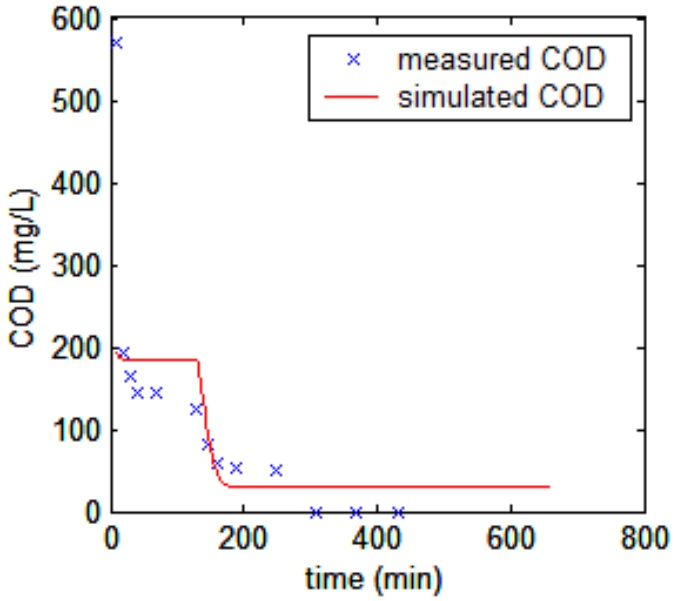
Parameter	Dimension	Value	Confidence interval
Y_h	mgVSS/mgCOD	0.828	0.069
k_3	mgN/mgN	0.905	0.014
μ_{hNmax}	min^{-1}	0.016	0.004
K_{C1}	mgCOD/L	144.45	4.16
K_{NO}	mgN/L	20.47	0.85
μ_0	min^{-1}	0.0067	0.0023
k_La	min^{-1}	0.3	0.031
S_{Omax}	mg/L	7.86	0.59
Y_h	mgVSS/mgCOD	0.81	0.17
Y_a	mgVSS/mgN	1.705	2×10^{-5}
β_1		11.62	3.42
β_2		0.35	0.076
μ_{hmax}	min^{-1}	0.0029	0.0019
K_{Ch}	mgCOD/L	133.35	5.71
K_{Oh}	mgDO/L	39.68	3.61
μ_{amax}	min^{-1}	0.021	0.0019
K_{NHa}	mgN/L	31.91	5.17
K_{Oa}	mgDO/L	60.72	5.43
S_{Cmin}	mgCOD/L	30.42	7.42
S_{Nmin}	mgN/L	4.38	0.88

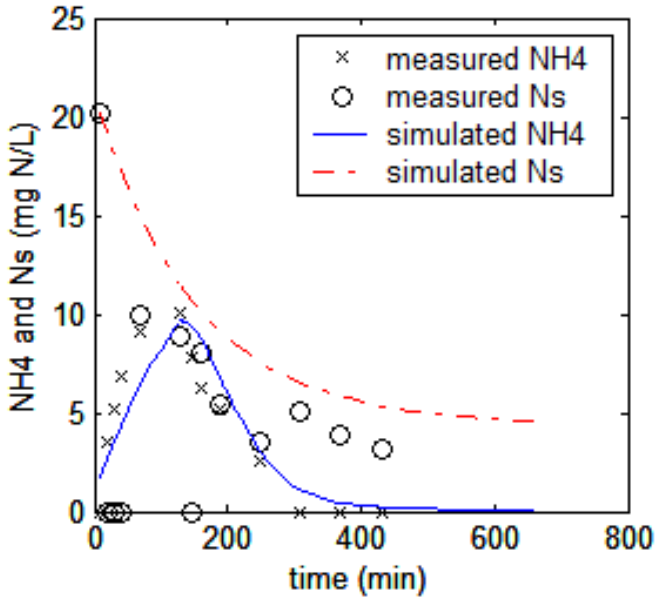

measured COD
simulated COD
COD (mg/L)
time (min)
0
50
100
150
200
250
0
200
400
600
800

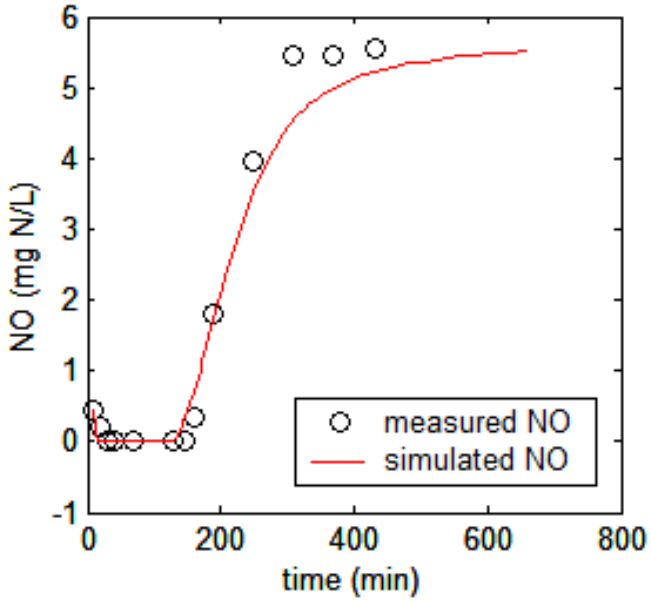

measured NH4
measured Ns
simulated NH4
simulated Ns
NH4 and Ns (mg N/L)
time (min)
0
5
10
15
20
25
30
35
0
200
400
600
800

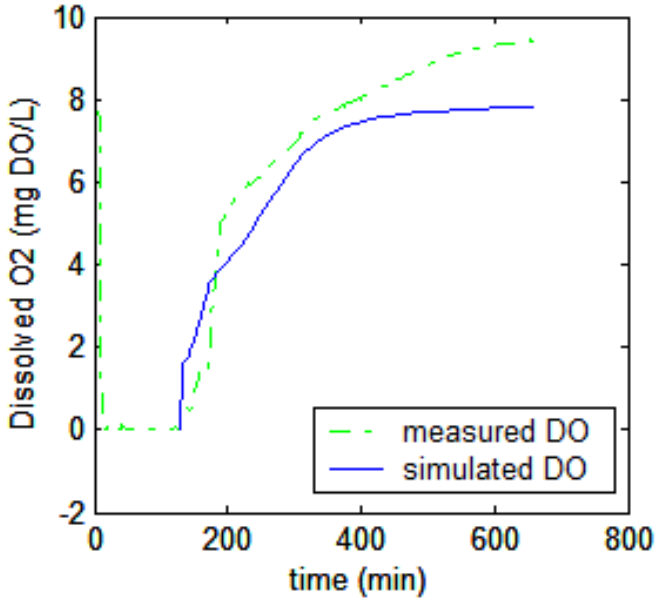

measured NO
simulated NO
NO (mg N/L)
time (min)
-2
0
2
4
6
8
10
0
200
400
600
800


measured DO
simulated DO
Dissolved O2 (mg DO/L)
time (min)
0
2
4
6
8
0
200
400
600
800


measured COD
simulated COD
COD (mg/L)
time (min)
0
100
200
300
400
500
600
0
200
400
600
800


measured NH4
measured Ns
simulated NH4
simulated Ns
NH4 and Ns (mg N/L)
time (min)
0
5
10
15
20
25
0
200
400
600
800


measured NO
simulated NO
NO (mg N/L)
time (min)
-1
0
1
2
3
4
5
6
0
200
400
600
800


measured DO
simulated DO
Dissolved O2 (mg DO/L)
time (min)
-2
0
2
4
6
8
10
0
200
400
600
800