EOLI

WP 2 : Model Selection and Parameter Identification

Deliverable D2.3 : Validated Model

Manuel Betancur, Denis Dochain, Hadyan Fibrianto

1 Introduction

This deliverable provides a summary of the EOLI model(s) as they have been calibrated and validated on experimental data provided by WP1. Two different types of models are proposed to represent the dynamics of the two different types of processes evaluated in the framework of EOLI. The first model, referred as EM1, corresponds to the process run in Mexico. The second model represent the dynamics of the processes run at POLIMI, at the LBE and at the UU. Due to slight differences between the process dynamics, two submodels have been identified, i.e. EM2a for the POLIMI process, and EM2b for the LBE process. Herebelow only the reaction schemes, the mass balance equations (with the kinetic expresssions) and the parameter values are provided. Details about the identification procedures for the different models can be found in the related detailed reports.

2 Model EM1

The process operation consists of a fed-batch operation with one single aerobic growth reaction and an endogeneous respiration reaction :

$$\text{Growth} \quad : \quad S_C + S_O \longrightarrow X \tag{1}$$

$$\text{Endogeneous respiration} \quad : \quad S_O + X \longrightarrow X \tag{2}$$

where S_C, S_O and X represent the concentrations of organic matter, dissolved oxygen and biomass, respectively. The dynamics of the process are described by the following equations :

$$\frac{dX}{dt} = \mu X - \frac{q_{in}}{V} X \tag{3}$$

$$\frac{dS_C}{dt} = -k_1 \mu X + \frac{q_{in}}{V}(S_{C,in} - S_C) \tag{4}$$

$$\frac{dS_O}{dt} = -k_2 \mu X - bX + \frac{q_{in}}{V}(S_{O,in} - S_O) + K_L a(S_{Os} - S_O) \tag{5}$$

$$\frac{dV}{dt} = q_{in} \tag{6}$$

where μ, q_{in}, V, k_1, k_2, b, $S_{C,in}$, $S_{O,in}$, K_La and S_{Os} are the specific growth rate, the inlet flow rate, the volume, the yield coefficients (between X and S_C, and X and S_O), the endogeneous respiration kinetic constant, the inlet organic matter and dissolved oxygen concentrations, the trnsfer coefficient and the oxygen saturation concentration, respectively.

The specific growth rate is represented by the following Haldane model :

$$\mu = \frac{\mu_0 S_C}{K_S + S_C + \frac{S_C^2}{K_I}} \tag{7}$$

Different configurations have considered for the parameter calibration (e.g. with or without inlet dissolved oxygen, with or without oxygen sensor dynamics, with or without a modification in the early part of the Haldane kinetics). The following set of parameters (Table 1) correspond to $S_{O,in} = 0$, $S_{Os} = 6$ mg/L and no oxygen sensor dynamics (EM1-A3, in the report). k_1 has also been given from separate batch experiments.

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

Table 1: Parameter values for model EM1-A3

3 Model EM2a

The process operation consists of two successive batch steps : an anoxic phase followed by an aerobic phase. The model refers explicitely to these two phases. In EM2a, it is assumed that a two step denitrification takes place. The model is therefore based on the following reaction schemes :

1. Anoxic phase

$$\begin{aligned} NO_3 \text{ reduction} &: S_C + S_{NO_3} \longrightarrow X_h + S_{NO_2} && (8)\\ NO_2 \text{ reduction} &: S_C + S_{NO_2} \longrightarrow X_h + N_2 && (9)\\ \text{ammonification} &: S_N \longrightarrow S_{NH} && (10) \end{aligned}$$

2. Aerobic phase

$$\begin{aligned} NH_4 \text{ oxidation} &: S_O + S_{NH} \longrightarrow X_a + S_{NO_2} && (11)\\ NO_2 \text{ oxidation} &: S_O + S_{NO_2} \longrightarrow X_a + S_{NO_3} && (12)\\ \text{C} - \text{removal} &: S_C + S_O \longrightarrow X_h && (13)\\ \text{ammonification} &: S_N \longrightarrow S_{NH} && (14) \end{aligned}$$

In the above reactions, S_{NO_3}, S_{NO_2}, X_h, X_a, S_{NH}, S_N hold for the (concentrations of) nitrate, nitrite, the heterotroph and autotroph bacteria, the ammonia nitrogen and the soluble organic nitrogen, respectively. The dynamics are given by the following set of mass balance equations :

1. Anoxic phase

$$\frac{dX_h}{dt} = \mu_{h1}X_h + \mu_{h2}X_h \quad (15)$$
$$\frac{dS_C}{dt} = -k_1\mu_{h1}X_h - k_2\mu_{h2}X_h \quad (16)$$
$$\frac{dS_{NO_3}}{dt} = -k_3\mu_{h1}X_h \quad (17)$$
$$\frac{dS_{NO_2}}{dt} = k_4\mu_{h1}X_h - k_5\mu_{h2}X_h \quad (18)$$
$$\frac{dS_{NH}}{dt} = k_6 r_N \quad (19)$$
$$\frac{dS_N}{dt} = -r_N \quad (20)$$

2. Aerobic phase

$$\frac{dX_h}{dt} = \mu_h X_h \quad (21)$$
$$\frac{dX_a}{dt} = \mu_{a1}X_a + \mu_{a2}X_a \quad (22)$$
$$\frac{dS_C}{dt} = -k_7\mu_h X_h \quad (23)$$
$$\frac{dS_O}{dt} = -k_8\mu_h X_h - k_9\mu_{a1}X_a - k_{10}\mu_{a2}X_a + k_L a(S_{Omax} - S_O) \quad (24)$$
$$\frac{dS_{NO_3}}{dt} = k_{11}\mu_{a2}X_a \quad (25)$$
$$\frac{dS_{NO_2}}{dt} = k_{13}\mu_{a1}X_a - k_{12}\mu_{a2}X_a \quad (26)$$
$$\frac{dS_{NH}}{dt} = k_6 r_N - k_{14}\mu_{a1}X_a \quad (27)$$
$$\frac{dS_N}{dt} = -r_N \quad (28)$$

In the oxygen balance equation, the term S_{Omax} accounts for the endogeneous respiration via the following relationship :

$$S_{Omax} = S_{Os} - \frac{r_e}{k_L a} \quad (29)$$

where r_e holds for the endogeneous respiration rate (assumed to be (almost) constant).

In the above equations, the yield coefficients k_i (i = 1 to 5, 7 to 14) are related to the standard IWA notations as follows :

$$k_1 = \frac{1}{Y_{h1}},\ k_3 = \frac{1 - Y_{h1}}{1.17Y_{h1}},\ k_2 = \frac{1}{Y_{h2}},\ k_4 = k_5 = \frac{1 - Y_{h2}}{1.71Y_{h2}},\ k_7 = \frac{1}{Y_h},\ k_8 = \frac{1 - Y_h}{Y_h} \quad (30)$$
$$k_9 = \frac{3.43 - Y_{a1}}{Y_{a1}},\ k_{13} = k_{14} = \frac{1}{Y_{a1}},\ k_{10} = \frac{1.14 - Y_{a2}}{Y_{a2}},\ k_{11} = k_{12} = \frac{1}{Y_{a2}} \quad (31)$$

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_{NO_3h}	mgN/L	44.65	7.87
μ_{h2max}	min^{-1}	0.0015	0.0007
K_{Ch2}	$mgCOD/L$	21.17	16.05
K_{NO_2h}	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 x 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 x 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 x 10^{-10}
K_{NO_2a}	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

Table 2: Parameter values for model EM2a for POLIMI data

The kinetic expressions are the following :

$$\mu_{h1} = \mu_{h1max}\frac{S_C - S_{Cmin}}{K_{Ch1} + S_C - S_{Cmin}}\frac{S_{NO_3}}{K_{NO_3h} + S_{NO_3}} \quad (32)$$

$$\mu_{h2} = \mu_{h2max}\frac{S_C - S_{Cmin}}{K_{Ch1} + S_C - S_{Cmin}}\frac{S_{NO_2}}{K_{NO_2h} + S_C - S_{NO_2}} \quad (33)$$

$$\mu_h = \mu_{hmax}\frac{S_C - S_{Cmin}}{K_{Ch} + S_C - S_{Cmin}}\frac{S_O}{K_{Oh} + S_O} \quad (34)$$

$$\mu_{a1} = \mu_{a1max}\frac{S_{NH}}{K_{NH} + S_{NH}}\frac{S_O}{K_{Oa1} + S_O} \quad (35)$$

$$\mu_{a2} = \mu_{a2max}\frac{S_{NO_2}}{K_{NO_2a} + S_{NO_2}}\frac{S_O}{K_{Oa2} + S_O} \quad (36)$$

$$r_N = \mu_0(S_N - S_{Nmin}) \quad (37)$$

In the above kinetic expressions, the terms S_{Cmin} and S_{Nmin} account for the non-biodegradable part of the compounds S_C and S_N. The identification procedure resulted in the set of parameter

values from the POLIMI data given in Table 2.

4 Model EM2b

The main difference with EM2a is that only one denitrification step and one step nitrification are considered in the anoxic and aerobic phases, respectively. Therefore the reaction scheme considered here is the following.

1. Anoxic phase

$$\begin{aligned} \text{denitrification} &: S_C + S_{NO} \longrightarrow X_h + N_2 && (38)\\ \text{ammonification} &: S_N \longrightarrow S_{NH} && (39) \end{aligned}$$

2. Aerobic phase

$$\begin{aligned} \text{nitrification} &: S_O + S_{NH} \longrightarrow X_a + S_{NO} && (40)\\ \text{C} - \text{removal} &: S_C + S_O \longrightarrow X_h && (41)\\ \text{ammonification} &: S_N \longrightarrow S_{NH} && (42) \end{aligned}$$

The dynamics are given by the following set of mass balance equations :

1. Anoxic phase

$$\begin{aligned} \frac{dX_h}{dt} &= \mu_{hN} X_h && (43)\\ \frac{dS_C}{dt} &= -k_1 \mu_{hN} X_h && (44)\\ \frac{dS_{NO}}{dt} &= -k_2 \mu_{hN} X_h && (45)\\ \frac{dS_{NH}}{dt} &= k_3 r_N && (46)\\ \frac{dS_N}{dt} &= -r_N && (47) \end{aligned}$$

2. Aerobic phase

$$\begin{aligned} \frac{dX_h}{dt} &= \mu_h X_h && (48)\\ \frac{dX_a}{dt} &= \mu_a X_a && (49)\\ \frac{dS_C}{dt} &= -k_4 \mu_h X_h && (50)\\ \frac{dS_O}{dt} &= -k_5 \mu_h X_h - k_6 \mu_a X_a + k_L a (S_{Omax} - S_O) && (51)\\ \frac{dS_{NO}}{dt} &= k_7 \mu_a X_a && (52)\\ \frac{dS_{NH}}{dt} &= k_3 r_N - k_8 \mu_a X_a && (53)\\ \frac{dS_N}{dt} &= -r_N && (54) \end{aligned}$$

In the above equations, the yield coefficients k_i (i = 1, 2, 4 to 8) are related to the standard IWA notations as follows :

$$k_1 = \frac{1}{Y_{hN}},\ k_2 = \frac{1 - Y_{hN}}{2.86 Y_{hN}},\ k_4 = \frac{1}{Y_h},\ k_5 = \frac{1 - Y_h}{Y_h},\ k_6 = \frac{\beta_1}{Y_a},\ k_7 = \frac{\beta_2}{Y_a},\ k_8 = \frac{1}{Y_a} \quad (55)$$

The kinetic expressions are the following :

$$\mu_{hN} = \mu_{hNmax} \frac{S_C - S_{Cmin}}{K_{C1} + S_C - S_{Cmin}} \frac{S_{NO}}{K_{NO} + S_{NO}} \quad (56)$$

$$r_N = \mu_0 (S_N - S_{Nmin}) \quad (57)$$

$$\mu_h = \mu_{hmax} \frac{S_C - S_{Cmin}}{K_{Ch} + S_C - S_{Cmin}} \frac{S_O}{K_{Oh} + S_O} \quad (58)$$

$$\mu_a = \mu_{amax} \frac{S_{NH}}{K_{NHa} + S_{NH}} \frac{S_O}{K_{Oa} + S_O} \quad (59)$$

The identified parameter values from the LBE data are given in Table 3.

Parameter	Dimension	Value	Confidence interval
Y_{hN}	$mgVSS/mgCOD$	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 x 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

Table 3: Parameter values for model EM2b for LBE data