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İSTANBUL TECHNICAL UNIVERSITY ★ INSTITUTE OF SCIENCE AND TECHNOLOGY

**MODEL-BASED ACTIVATED SLUDGE SYSTEMS ANALYSIS FOR
CARBON, NITROGEN AND PHOSPHORUS REMOVAL MECHANISMS**

**Ph.D. Thesis by
H. Güçlü İNSEL, M.Sc.**

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Supervisor (Chairman): Prof.Dr. Derin ORHON

**Co-Supervisor : Prof.Dr. Peter A. VANROLLEGHEM
(Ghent University)**

Members of the Examining Committee Prof.Dr. Nazik ARTAN (İTÜ.)

Prof.Dr. Seval SÖZEN (İTÜ.)

Prof.Dr. Emine UBAY ÇOKGÖR (İTÜ.)

Prof.Dr. Orhan YENİGÜN (BÜ.)

Prof.Dr. Ferhan ÇEÇEN (BÜ.)

[Handwritten signatures of Prof.Dr. Derin ORHON, Prof.Dr. Peter A. VANROLLEGHEM, Prof.Dr. Nazik ARTAN, Prof.Dr. Seval SÖZEN, Prof.Dr. Emine UBAY ÇOKGÖR, Prof.Dr. Orhan YENİGÜN, and Prof.Dr. Ferhan ÇEÇEN]

FOREWORD

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CONTENTS

	<u>Page</u>
ABBREVIATIONS	viii
LIST OF TABLES	ix
LIST OF FIGURES	xi
LIST OF SYMBOLS	xv
SUMMARY	xvii
ÖZET	xviii
1. GENERAL INTRODUCTION	1
1.1. Aim of the Thesis	1
1.2. Scope of the Thesis	3
1.3. Modelling of Activated Sludge Processes for Nutrient Removal	8
1.3.1. Modelling of biological nutrient removal	8
1.3.2. Activated sludge plant configurations for nutrient removal	17
1.3.2.1. Modified Lutzack Ettinger (MLE) and A/O system	17
1.3.2.2. Three stage Phoredox (A ² O) Process	18
1.3.2.3. Bardenpho (4-5 Stage) type plants	19
1.3.2.4. Step-feed process	20
1.3.2.5. University of Cape Town, UCT (Standard and Modified)	20
1.3.2.6. Virginia initiative plant, VIP	21
1.3.2.7. Johannesburg type plants	21
1.3.2.8. Oxidation ditch systems	22
1.3.2.9. Sequencing batch reactor, SBR	25
1.3.2.10. BCFS [®] process	26
1.3.2.11. Sharon [®] -Annamox [®] process	26
1.3.2.12. External Nitrification Biological Nutrient Removal Activated Sludge (ENBNRAS) Plants	27
1.4. A General Activated Sludge Model Calibration Methodology	31
1.5. Important Issues in Nutrient Removal Activated Sludge Modeling	43
1.5.1. General characteristics and operating parameters of activated sludge plants	43
1.5.2. Influent wastewater characteristics	45
1.5.3. Main processes in activated sludge models	48
1.5.3.1. Nitrification	48
1.5.3.2. Heterotrophic activity	50

	<u>Page</u>
2. IDENTIFICATION AND MODELLING OF AEROBIC HYDROLYSIS-APPLICATION OF OPTIMAL EXPERIMENTAL DESIGN	55
2.1. Introduction	55
2.2. Materials and Methods	58
2.2.1. Model and Wastewater Selection	58
2.2.2. Theoretical Identifiability	58
2.2.3. Practical Identifiability	60
2.2.4. Experimental Setup	61
2.3. Results and Discussion	62
2.3.1. Parameter Estimation and Sensitivity Analysis	62
2.3.2. Optimal Experimental Design (OED) Concept	67
2.4. Conclusions	69
3. IMPORTANT LIMITATIONS IN THE MODELING OF ACTIVATED SLUDGE BIASED CALIBRATION OF THE HYDROLYSIS PROCESS	70
3.1. Introduction	70
3.2. Relevance for Agro Industry	71
3.3. Respirometry as a Tool for Experimental Evaluation	72
3.4. Experimental Evaluation of Model Parameters	75
3.4.1. Experimental assessment of $\hat{\mu}_H$	76
3.4.2. Experimental assessment of b_H	77
3.4.3. Experimental assessment of X_H	78
3.4.4. Experimental assessment of k_h and K_X	79
3.5. Interpretation of the OUR Profiles	80
3.5.1. Relationship between endogenous decay and microbial growth	80
3.5.2. Assessment of the hydrolysis rates	84
3.6. Evaluation and Conclusion	86
4. IDENTIFIABILITY ANALYSIS FOR AEROBIC HYDROLYSIS KINETICS BASED ON SHORT TERM RESPIROMETRIC DATA	89
4.1. Introduction	89
4.2. Materials and Methods	91
4.2.1. Model and wastewater selection	91
4.2.1.1. Hydrolysis model and estimation of parameters	91
4.2.1.2. Practical identifiability methods	92
4.2.2. Experimental setup	95
4.3. Identifiability Results and Discussion	95
4.4. Conclusions	100

	<u>Page</u>
5. EFFECT OF TEMPERATURE ON THE NITROGEN REMOVAL PERFORMANCE OF A SEQUENCING BATCH REACTOR TREATING TANNERY WASTEWATER	102
5.1. Introduction	102
5.2. Materials and Methods	103
5.3. Results and Discussions	104
5.3.1. SBR Performance for nitrogen removal	104
5.3.2. Modeling nitrogen removal at steady state	106
5.3.3. Modelling nitrogen dynamics at low temperatures	107
5.4. Conclusions	111
6. EFFECT OF AERATION ON THE PERFORMANCE OF SMALL SEQUENCING BATCH REACTORS FOR ORGANIC CARBON AND NITROGEN REMOVAL	112
6.1. Introduction	112
6.2. Conceptual Basis for Oxygen Transfer Modeling	113
6.3. Materials and Methods	114
6.4. Results and Discussion	116
6.4.1. Calculation of volumetric oxygen transfer coefficient, $K_L a_f$	116
6.4.2. Model calibration and sensitivity analysis	117
6.4.3. Effect of aeration intensity on system performance	118
6.5. Conclusions	121
7. A CALIBRATION METHODOLOGY AND MODEL-BASED SYSTEMS ANALYSIS FOR SBRs REMOVING NUTRIENTS UNDER LIMITED AERATION CONDITIONS	123
7.1. Introduction	123
7.2. Materials and Methods	124
7.2.1. SBR Operation and process control	124
7.2.2. Wastewater characteristics	126
7.3. Results and Discussion	126
7.3.1. Measurement campaign results	126
7.3.2. Activated sludge model selection	128
7.3.3. Calibration methodology	129
7.3.4. System analysis	131
7.4. Conclusion	134

	<u>Page</u>
8. OPTIMAL BUT ROBUST N & P REMOVAL IN SBRs: A MODEL-BASED SYSTEMATIC STUDY OF OPERATION SCENARIOS	135
8.1. Introduction	135
8.2. Materials and Methods	136
8.2.1. Simulation platform	136
8.2.2. A systematic methodology for the optimization of SBR systems	136
8.3. Results and Discussion	138
8.3.1. Application of the systematic methodology to a lab-scale SBR	138
8.3.1.1. Objective of the optimization	138
8.3.1.2. Framework for the SBR optimization: degrees of freedoms and constraints	138
8.3.1.3 Model selection and calibration	139
8.3.1.4 Scenario analysis: formulation and simulation of grid of scenarios	139
8.3.2. Evaluation of the scenario analysis results	141
8.3.3. Effect of the oxygen set-point and length of the aerobic react phase	146
8.3.4. Effect of sludge age on the SBR performance and stability	147
8.3.4.1 Effect of sludge age on effluent quality	148
8.3.4.2 Effect of sludge age on the robustness of the SBR system	149
8.4. Conclusions	153
9. EVALUATION OF NUTRIENT REMOVAL PERFORMANCE FOR AN ORBAL PLANT USING ASM2d MODEL	155
9.1. Introduction	155
9.2. Materials and Methods	158
9.2.1. WWTP definition	158
9.2.2. Measurement campaign data and calibration	159
9.3. Results and Discussion	162
9.4. Conclusions	172
10. DYNAMIC MODEL CALIBRATION FOR AN INTERMITTENTLY AERATED CARROUSEL TYPE ACTIVATED SLUDGE PLANT: EVALUATION OF THE LONG TERM PREDICTION PERFORMANCE OF A CALIBRATED MODEL	174
10.1. Introduction	174
10.2. Materials and Methods	178
10.2.1. Wastewater treatment plant definition	178
10.2.2. Operation/Control strategy	178

	<u>Page</u>
10.2.3. Measurement campaigns	180
10.2.3.1. First measurement campaign (Insel et al., 2003b)	180
10.2.3.2. Second measurement campaign (MC2)	181
10.2.4. Calibration methodology	183
10.3. Results and Discussion	186
10.3.1 The results of the second measurement campaign (MC2)	186
10.3.1.1 Determination of degradable fraction of influent COD	186
10.3.1.2. Endogenous decay rate of the biomass	187
10.3.1.3. Average influent wastewater characterization (flux-based)	188
10.3.1.4. Diurnal changes in influent wastewater composition	191
10.3.2. The calibrated model	191
10.3.3. The calibrated model: validation with the second measurement campaign (MC2) data	193
10.3.4. Recalibration of the model	197
10.3.5. Model-based analysis of the nutrient removal in the Haaren WWTP	200
10.3.6 General discussion: the state and future perspective of model calibration	205
10.4. Conclusion and Perspectives	207
11. FINAL CONCLUSION AND PERSPECTIVES	208
REFERENCES	215
ANNEX	236
CURRICULUM VITAE	244

ABBREVIATIONS

ASM	: Activated Sludge Model
ATU	: Allyl Thio Urea (Nitrification inhibitor)
BNR	: Biological Nutrient Removal
BOD	: Biochemical Oxygen Demand
COD	: Chemical Oxygen Demand
COD_{tot}	: Total COD
Cond.	: Conductivity
CSTR	: Completely Stirred Reactor
DO	: Dissolved Oxygen
EBPR	: Enhanced Biological Phosphorus Removal
FIM	: Fisher Information Matrix
F/M (S₀/X₀)	: Food/Microorganism ratio
HRT	: Hydraulic Retention Time
IAF	: Intermittent Aeration Frequency
IR	: Internal Recycle
MC	: Measurement Campaign
meas	: Measurement
ML(V)SS	: Mixed Liquor (Volatile) Suspended Solid
NUR	: Nitrate Utilization Rate
NPR	: Nitrate Production Rate
NR	: Nitrified Recycle
OUR	: Oxygen Uptake Rate
OED	: Optimal Experimental Design
OR	: Oxygen Requirement
ORP	: Oxidation Reduction Potential
PAOs	: Phosphorus Accumulating Organisms
PUR	: Phosphate Utilization Rate
PST	: Primary Settling Tank
RAS	: Return Activated Sludge
RI	: Robustness Index
TOC	: Total Organic Carbon
STD	: Standard Deviation
SRT	: Sludge Retention Time
SRT_A	: Aerobic Sludge Retention Time
SND	: Simultaneous nitrification and denitrification
SSE	: Sum of Squared Errors
TKN	: Total Kjeldahl Nitrogen
TN	: Total Nitrogen
TP	: Total Phosphate
WWTP	: Wastewater Treatment Plant
VFA	: Volatile Fatty Acids

LIST OF TABLES

	Page
Table 1.1	Reactions of Sharon and Anammox processes
Table 1.2	Design and operating parameters for commonly used nitrogen and biological phosphorus-removal processes
Table 1.3	Reaction rate constants for nitrifying bacteria at 20 °C
Table 1.4	Variations of the hydrolysis constants
Table 2.1	Matrix representation of activated sludge model
Table 2.2	Identifiable parameter combinations for hydrolysis model
Table 2.3	Initial conditions for Experiments 1 and 2
Table 2.4	Estimated initial state variables and parameters and deduced sludge and wastewater characteristics
Table 2.5	Estimated initial states and parameters (multi-experimental fit)
Table 3.1	Typical characteristics of selected industrial effluents (Orhon <i>et al.</i> , 1999a)
Table 3.2	Matrix representation of an activated sludge model involving residual COD generation
Table 3.3	Wastewater characteristics adopted for the model simulations
Table 3.4	The effect of b_H on the estimation of other kinetic parameters
Table 3.5	The effect of $\hat{\mu}_H$ on the estimation of kinetic parameters for b_H : 0.2 d ⁻¹ (domestic wastewater)
Table 4.1	Matrix representation of aerobic hydrolysis model
Table 4.2	Parameter combinations for growth and hydrolysis
Table 4.3	Estimated parameters and correlation matrix for hydrolysis model
Table 4.4	Calculated collinearity indices and D-Criterion
Table 4.5	Eigenvalue decomposition of the parameter estimation covariance matrix
Table 5.1	Influent wastewater characterization
Table 5.2	Significant parameters of SBR performance
Table 5.3	Model coefficients characterizing plain-settled tannery wastewater
Table 5.4	COD fractionation of plain settled tannery wastewater
Table 7.1	ASM2dN based influent wastewater characterization
Table 7.2	Summary of the calibrated ASM2dN parameters
Table 8.1	The grid of scenarios to simulate the effect of key degrees of freedom on the SBR system
Table 8.2	Summary of the scenario analysis results: the best scenario in each category
Table 8.3	Sensitivity analysis and robustness index of the best scenarios
Table 9.1	Flux based average influent wastewater characterization
Table 9.2	Simulated steady state plant performance

Table 9.3	Parameters used in the calibration for ASM2d	<u>Page</u> 165
Table 10.1	BOD _U estimation results using BOD and simplified ASM1 models	187
	and degradable fraction (BOD _U /COD) of influent wastewater	
Table 10.2	Influent wastewater characterization and COD characterization	189
Table 10.3	Calibrated parameters for the first and re-calibration steps	198
Table A.1	Matrix representation of ASM2dN	236
Table B.1	Plant performance and average influent wastewater characteristics	239
Table B.2	The experimental results of the b _H experiment	243



LIST OF FIGURES

	Page
Figure 1.1	Schematic diagram for ASM1 (Henze <i>et al.</i> , 1987) components under (a) aerobic and (b) anoxic conditions 9
Figure 1.2	Schematic diagram for Wentzel <i>et al.</i> (1992) model under (a) anaerobic (b) anoxic and (c) aerobic conditions 11
Figure 1.3	Schematic diagram for ASM2/2d components under (a) anaerobic and (b) aerobic (ASM2/2d)/anoxic (ASM2d) conditions 12
Figure 1.4	Schematic diagram of Barker and Dold (1997) model for the components under (a) anaerobic and (b) aerobic/anoxic conditions 14
Figure 1.5	Schematic diagram of ASM3 for the components under (a) anoxic and (b) aerobic conditions 14
Figure 1.6	Anaerobic and aerobic metabolism of phosphorus accumulating organisms according to Smolders <i>et al.</i> (1994a; 1994b) 15
Figure 1.7	Predenitrification (MLE) or two stage Phoredox (A/O) system 18
Figure 1.8	Plant layout for A ² O 19
Figure 1.9	Layout for Bardenpho system 19
Figure 1.10	Step-Feed process 20
Figure 1.11	University of Cape Town, UCT 21
Figure 1.12	VIP process 22
Figure 1.13	Johannesburg type activated sludge 22
Figure 1.14	Simple oxidation ditch (Carrousel) systems 23
Figure 1.15	Pictures and flow scheme of Orbal [®] plant 24
Figure 1.16	Flow diagram for Bio-denitro process 24
Figure 1.17	Standard cycles of SBR 25
Figure 1.18	Schematic representation of BCFS [®] process 26
Figure 1.19	Coupling of Sharon-Anammox to main stream processes 27
Figure 1.20	The ENBNRAS system (Hu <i>et al.</i> , 2003a) 28
Figure 1.21	The BIOMATH model calibration protocol 33
Figure 1.22	Decision chart for hydraulic characterization (a) and hydraulic residence time distribution function, E(t') for different no. of tanks in series (b) 35
Figure 1.23	Decision chart on settling characterization 36
Figure 1.24	Parameter estimation routine (Wanner <i>et al.</i> , 1992) 39
Figure 1.25	Influent wastewater characterization for AS model 46
Figure 1.26	ASM2d based influent wastewater COD fractionation 47
Figure 1.27	Estimation of biodegradable COD fractions from respirograms 48
Figure 1.28	Respirometric batch test for nitrifiers 49
Figure 2.1	Simulated and measured OUR values for Experiment 1 (left), Experiment 2 (right) 63
Figure 2.2	Absolute-Relative (AR) sensitivity trajectories of the parameters for Growth (left) Hydrolysis (right) (Experiment 1) 66

	<u>Page</u>
Figure 2.3	SSE contour plots for k_h and K_X experiment 1 (left) and experiment 2 (right)
Figure 2.4	SSE contour plots for K_X and X_{H0} (left) k_h and X_{H0} (right) for Experiment 1
Figure 2.5	Information content of experiments, experiment 1 (left) and experiment 2 (right)
Figure 3.1	Typical OUR profiles for domestic sewage and textile wastewaters
Figure 3.2	Sensitivity analysis for (a) growth and (b) hydrolysis processes on the OUR curve obtained for domestic sewage [$F/M = 1.35 \text{ gCOD(g cell COD)}^{-1}$]
Figure 3.3	Effect of b_H on OUR profile of acetate (left) domestic sewage (right)
Figure 3.4	Effect of $\hat{\mu}_H$ on the OUR profile of acetate (left) and domestic sewage (right)
Figure 3.5	Fitting the OUR profile for domestic sewage for b_H 0.1 and 0.25 d^{-1}
Figure 3.6	χ^2 contour plots for the estimation of k_h and K_X for $F/M = 1.35 \text{ g COD(gcellCOD)}^{-1}$
Figure 3.7	Simulation results for limiting k_h - K_X values for $\chi^2 = 128$ ($b_H=0.2 \text{ d}^{-1}$)
Figure 3.8	χ^2 contour plots for k_h - K_X values obtained with F/M ratios of 0.33 and 1.35 $\text{gCOD(gcellCOD)}^{-1}$
Figure 4.1	Data and model for batch respirograms for (a) domestic and (b)slaughter-house wastewaters
Figure 4.2	Absolute-Relative sensitivity simulations for model parameters and state variables for the domestic wastewater
Figure 4.3	Identifiability measures according to Brun <i>et al.</i> (2001) (a) domestic and (b) slaughter house wastewater
Figure 5.1	Steady state simulation for temperature at 20^0
Figure 5.2	Simulation for Temperature: 10^0C (initials states of 20^0C used)
Figure 5.3	Simulation for Temp: 10^0C (initials of 20^0C used)
Figure 5.4	Dynamic temperature effect on nitrogen fractions
Figure 5.5	Simulated autotrophic biomass concentration under low temperature
Figure 6.1	Simulation profiles for (a) nitrogen and (b) oxygen profiles
Figure 6.2	Absolute-relative sensitivity trajectories for (a)ammonia (b)nitrate
Figure 6.3	Simulations of (a) sensitivity trajectory for oxygen and (b) simulations of oxygen profiles for different K_{La} values
Figure 6.4	The simulations for (a) oxygen uptake rate, OUR and (b) nitrate utilization rate, NUR
Figure 6.5	Simulation of K_{La}^* effect on effluent nitrogen components
Figure 7.1	Schematic diagram of the SBR system
Figure 7.2	On-line measurements (left) ORP, conductivity and DO, pH (right)
Figure 7.3	Measurements (symbols) and simulations (lines) of the dissolved oxygen (left) and phosphate (right)

		Page
Figure 7.4	Measurements (symbols) and simulation (lines) of NH_4/NO_3 (left) soluble/particulate nitrogen (right)	129
Figure 7.5	Calibration methodology for the ASM2dN model	130
Figure 7.6	Nitrate production, P-release (left) and segments of phosphate utilization rate (right)	132
Figure 7.7	OUR and NUR contributions in a SBR cycle	132
Figure 7.8	The phosphate and oxygen utilization in one SBR cycle	133
Figure 8.1	A systematic methodology for the model-based optimization of SBR systems	137
Figure 8.2	Implementation of IAF with step-feed options to anoxic sub-phases. The arrow indicates the step feed instants. SBR with IAF 1 (A), IAF 2 (B) IAF 4 (C) and IAF 8 (D)	141
Figure 8.3	N and P-removal dynamics under the best scenario (BSC) obtained in IAF4 in comparison with the reference (REF) system	146
Figure 8.4	Trend of ammonium (A) and nitrate (B) as function of oxygen set-point under different lengths of aerobic react phase for the SBR operation with IAF4	147
Figure 8.5	SBR performance with respect to effluent TN (left-hand) and P concentrations (right-hand) as a function of sludge age under different oxygen set points: IAF2 (A) IAF4 (B) and IAF8 (C)	150
Figure 8.6	Stability/robustness of the SBR system with respect to TN (left-hand) and P removal (right-hand) as a function of sludge age under different oxygen set points: IAF2 (A) IAF4 (B) and IAF8 (C)	151
Figure 9.1	Pictures of biological reactor and vertical disc aerators	156
Figure 9.2	The plant layout for the simulated plant (left) and clarifier (right)	159
Figure 9.3	Implementation of plant layout in WEST	161
Figure 9.4	Influent flow rate (left), RAS and WAS flow rates (right)	162
Figure 9.5	Schematic representation of the calibration methodology	163
Figure 9.6	MLSS profiles in middle ring	163
Figure 9.7	$\text{NH}_4\text{-N}$ profile in outer and inner rings	167
Figure 9.8	Dissolved oxygen in middle and inner rings	169
Figure 9.9	Nitrate nitrogen profile in middle and inner rings	170
Figure 9.10	Phosphate profiles in middle and inner rings	170
Figure 9.11	Simulated biomass composition (middle ring)	171
Figure 9.12	Sludge blanket height, HS (left) and sludge concentration profile (right) in the clarifier (at day: 10)	172
Figure 10.1	Pictures and schematic diagram of activated sludge plant	179
Figure 10.2	Influent, effluent and RAS flowrates in the 1 st MC	181
Figure 10.3	Influent, effluent and sludge recycle flowrate in the 2 nd MC	182
Figure 10.4	Plant layout for simple steady state calibration (WEST)	184
Figure 10.5	Plant layout implemented in WEST software	185
Figure 10.6	The BOD_U results of the influent grab samples taken at 16/06/2003 and 17/06/2003 respectively and the model fits (left) BOD model (Eq10.1) (right) simplified ASM1 model	186
Figure 10.7	Endogenous respiration rate ($\text{OUR}_{\text{end}} - \diamond$) of biomass over 15 days and the model-fit to the data	188

	<u>Page</u>
Figure 10.8	Flux-based influent COD/TKN and COD/TP ratio (left) influent COD, TKN and TP concentrations (right) 190
Figure 10.9	Diurnal changes in COD/TKN and COD/TP load 191
Figure 10.10	Simulated and measured nitrogen (left) and dissolved oxygen (right) (Insel <i>et al.</i> , 2003b) 192
Figure 10.11	Simulated and measured MLSS (left) and effluent phosphate (right) (Insel <i>et al.</i> , 2003b) 193
Figure 10.12	Simulated phosphate (left) and dissolved oxygen (right) concentrations 195
Figure 10.13	Simulated and measured nitrogen components 196
Figure 10.14	Simulated and measured MLSS concentration in the carrousel 196
Figure 10.15	Simulated phosphate and dissolved oxygen concentrations 199
Figure 10.16	Simulated and measured nitrogen components (a) nitrate and (b) ammonium 199
Figure 10.17	Simulated and measured MLSS concentration in the carrousel 199
Figure 10.18	Simulations of the phosphorous release rate, PRR (right) and X_{PHA} (left) in the different sections of the selector 201
Figure 10.19	Simulation of S_A (VFA) concentrations in the selector and inlet of the carrousel 202
Figure 10.20	Simulations of the NUR in the selector (left) and the NUR and nitrate in the carrousel (right) 203
Figure 10.21	Simulations of the nitrification activity (as nitrate production rate, NPR) in the carrousel 204
Figure B.1	TP mass balance over the system 240
Figure B.2	The influent flowrate data 241
Figure B.3	Flow balance errors calculated for raw flow and filtered data 242
Figure B.4	Filtered (balanced) influent and effluent flow rates. 242

LIST OF SYMBOLS

Y_H	: Heterotrophic yield coefficient
Y_{NH}	: Net heterotrophic yield coefficient
$\hat{\mu}_H$	: Maximum heterotrophic growth rate
μ_{Amax}	: Maximum autotrophic growth rate
k_h	: maximum hydrolysis rate
K_S	: Half saturation constant for heterotrophic growth
k_h	: Maximum hydrolysis rate
K_x	: Half saturation constant for hydrolysis
K_O	: Oxygen half saturation constant for heterotrophs
K_{OA}	: Oxygen half saturation constant for autotrophs
S_s	: Readily biodegradable COD
X_s	: Slowly biodegradable COD
τ	: Transition term for start-up phenomena
S_{sini}	: Initial readily biodegradable COD
X_{sini}	: Initial slowly biodegradable COD
X_{Hini}	: Heterotrophic initial active biomass
C_S	: Biodegradable COD concentration (COD_{BD})
b_H	: Endogenous decay rate for heterotrophs
b_A	: Endogenous decay rate for autotrophs
f_E	: Inert fraction of endogenous biomass
σ	: Standard deviation
$Y(t_i, p)$	: Output sensitivity function with respect to the parameters
Q_i	: Measurement weighting matrix
χ^2	: Sum of Squared Error/Standard Deviation
λ_i	: Eigen Value
$s_{i,j}$	: Scaled sensitivity matrix
sc_i	: Scaling factor for measurements
$\partial y_i / \partial \theta_i$	: Sensitivity function of parameter, θ to model output, y
n	: Number of observations (i)
m	: Number of model parameters (j)
$Cov(\theta_N)$	: parameter estimation covariance matrix
γ	: Collinearity index
$\tilde{p}$	: Parameter Vector
$\tilde{S}$	: State Vector
r_o	: Respiration Rate
SBR	: Sequencing Batch Reactor
V_0	: Initial (stationary) volume of SBR
V_F	: Fill (stationary) volume of SBR
T_C	: Total cycle time of SBR
$T_F(T_{DN})$	: Fill/Anoxic period of SBR
T_S	: Settle period of SBR

T_D	: Draw period of SBR
T_A	: Aerobic cycle of SBR
T_{ANB}	: Anaerobic cycle of SBR
T	: Temperature
Q_{in}	: Influent Flowrate
S_O	: Dissolved oxygen concentration
S_{O-sp}	: Dissolved oxygen set-point concentration
$S_{O\infty f}$	: Dissolved oxygen saturation concentration under process condition
K_{La}	: Volumetric oxygen transfer coefficient
K_{La_f}	: Volumetric oxygen transfer coefficient under process condition
α	: Correction factor for process water K_{La_f} / clean water K_{La}
β	: Correction factor for process water $S_{O\infty f}$ / clean water $S_{O\infty f}^*$
θ_X	: Total Sludge Age
θ_{XA}	: Aerobic sludge age
θ_h	: Hydraulic retention time
θ	: Arrhenius coefficient (temperature correction)
N_X	: Nitrogen incorporated during heterotrophic growth
N_{Ox}	: Oxidized nitrogen
N_{DP}	: Denitrification potential
S_{NH}	: Ammonia nitrogen
S_{ND}	: Soluble organic nitrogen
S_{NO}	: Nitrate nitrogen
X_{ND}	: Particulate biodegradable nitrogen
S_{PO4}	: Ortho-phosphate
X_I	: Particulate Inert COD
S_I	: Soluble Inert COD
S_F	: Fermentable COD
S_A	: Acetate COD
S_H	: Rapidly hydrolyzable COD
X_H	: Active heterotrophic biomass
i_{NBM}	: Nitrogen fraction of biomass
$i_{NX?}$	: Nitrogen fraction of particulate COD, $X_?$
$i_{NS?}$	: Nitrogen fraction of soluble COD, $S_?$
$i_{PX?}$	: Phosphate fraction of particulate COD, $X_?$
$i_{PS?}$	: Phosphate fraction of soluble COD, $S_?$

MODEL-BASED ACTIVATED SLUDGE SYSTEMS ANALYSIS FOR CARBON, NITROGEN AND PHOSPHORUS REMOVAL MECHANISMS

SUMMARY

Increasing pollution potential of water sources in world brings along strict discharge standards together with necessity of efficient nutrient (nitrogen and phosphorus) removal from wastewaters. Compared to other treatment alternatives, the activated sludge technology is more convenient in terms of investment and operational costs. The discharge standards imposed should only be secured by appropriate design, operation and retrofit of activated sludge plants.

Activated sludge models have been widely used for the design, control and optimization of activated sludge plants operated for organic carbon and nutrient removal. However, appropriate use of those models essentially requires (1) precise influent-wastewater characterization (2) wise use of calibration methodology for activated sludge models and as a result: (3) interpretation of results obtained from modeling study.

In the first part of the study, a methodology was proposed for the determination of biodegradable and hydrolyzable organic matter based on respirometric measurements. In addition, practical problems in the identification of process kinetics and active heterotrophic biomass were addressed using respirometric data. Based on proposed method, influence of initial conditions of batch experiment on the identification of model components was investigated using Optimal Experimental Design (OED) techniques.

In the second part of the study, the nutrient removal mechanism was evaluated for Sequencing Batch Reactor systems treating domestic and leather tanning (common industrial branch in Turkey) wastewaters. The effect of environmental factors (i.e. temperature, aeration intensity) influencing the process performance for nutrient removal was investigated via system analysis with the aid of calibrated model. Finally, considering the reference model-based system analysis, available operation alternatives (i.e. aeration) were generated and the simulations results were evaluated in the view of simultaneous nutrient removal ability of SBRs together with robustness of system stability.

Last part of the study deals with the investigation of nutrient removal performance of two oxidation type full-scale activated sludge plants. The methodology of "Full Scale Activated Sludge Model Calibration Protocol" was partially applied in this study. The recalibration of model is required due to the mismatches of model results compared to two measurement-campaign data obtained from different period of time. In addition, the discrepancy between two modeling results was explained by the change of hydrolysis process kinetics.

AKTİF ÇAMUR SİSTEMLERİNDE KARBON, AZOT VE FOSFOR GİDERİMİ MEKANİZMALARININ MODEL DESTEKLİ ANALİZİ

ÖZET

Dünyadaki su kaynaklarının zamanla kirlenmesi, atıksu deşarj limitlerinin arttırılması ve atıksulardan nutrient (azot, fosfor) gideriminin gerekliliğini de beraberinde getirmiştir. Diğer nütrient giderimi alternatiflerinin yanında aktif çamur teknolojisi ekonomik olması sebebi ile dünyada yaygın olarak kullanılmaktadır. Öngörülen deşarj limitlerinin sağlanması da bu aktif çamur sistemlerinin şartlara uygun tasarımı, işletilmesi ve/veya optimizasyonu ile yerine getirilmektedir.

Aktif çamur modelleri artık aktif çamur tesislerinin tasarımı, kontrolü ve optimizasyon çalışmalarında yaygın olarak kullanılmaktadır. Ancak, bu modellerin doğru ve verimli olarak kullanılabilmesi için (1) kesin model bazlı-atıksu karakterizasyonu (2) arıtma tesislerine uygun modelleme yaklaşımı ve metodolojisinin uygulanması ve bunların sonucu olarak (3) elde edilen model sonuçlarının doğru olarak yorumlanması gerekmektedir.

Çalışmanın ilk aşamasında, endüstriyel ve evsel atıksulardaki hızlı ayrışan ve hidroliz olabilen organik maddelerin miktarının respirometrik ölçümlerle nonlinear yapıdaki modele bağlı çözüm yöntemi önerilmektedir. Bunun yanında ayrışma kinetiği ve aktif biyokütlenin bulunmasında karşılaşılan problemlere yer verilmiştir. Önerilen yöntemde, deneyin başlangıç koşullarının yine deneyin bilgi içeriğine etkisi optimal deney tasarımı (OED) yöntemiyle incelenmiştir.

Çalışmanın ikinci aşamasında, Türkiye’ de yaygınlık gösteren deri endüstrisi atıksuyu ve evsel nitelikli atıksular için pilot ölçekli Ardışık Kesikli Reaktörlerde (AKR), karbon, azot ve daha sonra fosfor giderimi mekanizmaları modelleme yardımı ile incelenmiştir. Azot ve fosfor giderimine etki eden faktörlerin (i.e. sıcaklık, havalandırma) nutrient giderimine etkisi araştırılarak arıtma performansı model destekli sistem analizi yardımı ile açıklanmıştır. Son aşamada, sistem analizi dikkate alınarak kalibre edilen model yardımı ile nutrient giderimi performansının artırılmasının havalandırmanın optimizasyonu ile de sağlanabileceği bulunmuştur.

Çalışmanın son aşamasında, oksidasyon tipi tam ölçekli aktif çamur tesislerinde nutrient giderimi performansı modelleme çalışması ile incelenmiştir. Çalışma kapsamında geliştirilen ‘Tam Ölçekli Arıtma Tesisleri için Model Kalibrasyon Metodolojisi’ nin kısmi uygulanması ile modelin belirli zaman aralıklarında tekrar kalibre edilmesi gerektiği ortaya konmuş ve kinetik değişkenlik gösteren hidroliz prosesinin sistem verimi üzerindeki önemi vurgulanmıştır.

1. GENERAL INTRODUCTION

1.1. Aim of the Thesis

Eutrophication limits the potential use of receiving waters due to algal blooms unless the input of nutrients is reduced and/or controlled at source. Uncontrolled discharge of organic carbon, nitrogen and phosphate, so called 'nutrients' originating from domestic and industrial sources cause inevitable eutrophication problems in receiving water bodies. To protect receiving water bodies from eutrophication, the EEC Directive 91/271 (CEC, 1991) enforces meeting strict discharge standards in terms of total nitrogen and phosphate in Europe.

The Biological Nutrient Removal (BNR) process is known to be the most convenient and economical alternative among other wastewater treatment methods to reduce the impact of nutrient (N, P) discharges. In this respect, the activated sludge technology has become more and more pronounced for meeting the strict nutrient and organic carbon discharge standards imposed. However, the most efficient way of sustainable nutrient removal must be achieved by optimal design and control of such activated sludge systems. From an engineering point of view, an appropriate design, operation and retrofit of activated sludge plants requires a better understanding of the complex biological reactions taking place in activated sludge systems. The degree of complexity increases in parallel to the vast progress in biotechnology. In addition to that, the performance of activated sludge systems is generally influenced by dynamic conditions (i.e. dynamic influent pollutant load; temperature) generally having an adverse impact on the effluent quality. Thus, the evaluation of those complex biological reactions together with dynamic factors requires computer aided model solutions to provide better insight in process dynamics and robust design and/or upgrade options for activated sludge plants.

Until recently, the activated sludge models have become convenient and popular tools for design, operation and upgrade of activated sludge systems for organic carbon and nutrient

removal. In reality, from a practical point of view, the model simulations enable to visualize a number of process scenarios under various conditions in a short period of time compared to a trial and error methodology. However, these activated sludge models strictly require (a) accurate model-based influent wastewater characterization (e.g. COD fractionation) and (b) dynamic model calibration to make the model mimic the actual behavior of the system. To optimize the removal of organic carbon, nitrogen and phosphorus in activated sludge plants, detailed model-based evaluations are useful since the process efficiency mainly depends upon the dynamics of the influent wastewater characteristics, the environmental factors and the operating conditions *etc.*

The experimental data obtained from lab-scale setups, pilot-scale setups and full-scale plants provide ample information on process stoichiometry and kinetics to be used in activated sludge model itself. However, the nonlinear structure and the high degree of complexity make it often difficult to end up with mathematically meaningful results.

In the first part of this thesis, the generation of a mathematical approach was developed for the model-based influent COD characterization (i.e. readily and slowly biodegradable substrate) and the estimation of extant model parameters using batch respirometric data obtained with real wastewaters. Then, the reliability of generated solutions was tested by applying different identifiability analysis methods. Finally, the effect of initial experiment conditions on the estimation of model parameters was formulized to visualize the information content of the experiment.

The second part deals with the dynamic modelling of pilot-scale SBR systems. First, the organic carbon and nitrogen removal processes have been interpreted with the aid of a calibrated model. The effects of environmental and operational conditions in the SBR were evaluated with respect to nitrogen removal process in an industrial application. Second, a stepwise model calibration methodology, a model-based process analysis and a robust optimization methodology approach were proposed for an SBR system removing carbon, nitrogen and phosphorus simultaneously.

In the third part, the removal efficiencies of nitrogen and phosphorus for two full-scale treatment plants were evaluated with the aid of a modelling effort. A proposed model calibration methodology, 'BIOMATH Protocol' was partially applied here. Finally, the

success of activated sludge models were questioned in the view of necessity for recalibration, the influent wastewater characterization together with operational strategies.

1.2. Scope of the Thesis

This thesis is composed of 11 Chapters, including general conclusions and perspectives. The general scope and content of each chapter is summarized as follows:

Chapter 1: General Introduction

Until now, different model structures have been proposed to explain the biological reactions with respect to carbon, nitrogen and phosphorus removal processes. A general purpose model calibration methodology (BIOMATH Protocol) to be used in full-scale calibration exercises is proposed. In addition, the effect of certain processes in accordance with the influent wastewater characteristics on plant performance and modelling is briefly discussed.

Chapter 2: Identification and modelling of aerobic hydrolysis-application of optimal experimental design

In this chapter, the surface-saturation-type hydrolysis kinetics was investigated based on respirometric measurements within the context of the theoretical and the practical identifiability of mathematical models. The identifiable parameters of a selected model were derived from batch respirograms. In addition, the information contents of the experiments were evaluated on the basis of the Optimal Experimental Design (OED) methodology by setting the initial conditions (i.e. initial biomass concentration) of the batch respirometric experiment.

Chapter 3: Important limitations in the modelling of activated sludge- biased calibration of the hydrolysis process

The merit of activated sludge models depends on the accuracy and reliability of the information they contain on the wastewater to be treated and the biochemical mechanisms involved. In most advanced calibration studies, respirometry i.e. the measurement of the oxygen utilization rate, (OUR), provides the majority of the required experimental database. However, currently used procedures still involve a number of basic and practical

problems. Model evaluation of the OUR-data may generate a distorted image of the processes involved. Hydrolysis is the most important, yet the most vulnerable process as far as the experimental assessment of accurate kinetic parameters is concerned. This study intends to provide an overview of the major experimental limitations in the modelling of activated sludge, with emphasis on the appropriate experimental design for the assessment of the hydrolysis rate.

Chapter 4: Identifiability analysis for aerobic hydrolysis kinetics based on short-term respirometric data

Short-term respirometric tests allow estimating the model parameters and COD fractions. In this study concerning the surface saturation type hydrolysis model, two different respirograms were analyzed with the aid of different practical identifiability tests. They yielded corroborating and complementary results. The initial experimental conditions and the shape of the respirogram play an important role in the identification of parameter subsets. In parallel to the findings of Chapter 2 and 3, the practical identifiability study revealed that 8 out of 11 kinetic parameters and initial state variables were found to be identifiable from respirometric data.

Chapter 5: Effect of temperature on the nitrogen removal performance of a sequencing batch reactor treating tannery wastewater

The effect of temperature on the nitrogen removal performance of a sequencing batch reactor was evaluated for tannery wastewater. The study involved the operation of a pilot-scale sequencing batch reactor installed on site to treat the plain-settled effluent. The nitrogen balance of the system was observed for a wide temperature range between 9 to 30°C. The results are evaluated by means of model calibration using nitrate and ammonia nitrogen concentration profiles obtained during cyclic operation. The fates of the major nitrogen parameters are also interpreted on the basis of the fundamental stoichiometry for nitrification and denitrification.

Chapter 6: Effect of aeration on the performance of small sequencing batch reactors for organic carbon and nitrogen removal

Aeration plays a dominant role in the removal of organic carbon and nitrogen simultaneously. The volumetric oxygen transfer coefficient, K_La can be calculated based

on biological oxygen requirements using process stoichiometry. After model calibration, the distribution of the oxygen requirement along the aeration phase was illustrated using oxygen uptake rate simulations. According to model results, the oxygen limitation at the start of the aeration phase caused simultaneous nitrification denitrification (SND). In addition, the effect of oxygen half saturation constants were stressed using sensitivity trajectories. Finally, the effect of different process K_{La} selections on nitrogen removal efficiency of SBRs was discussed.

Chapter 7: A calibration methodology and model-based systems analysis for SBRs removing nutrients under limited aeration conditions

A methodology was proposed for the model calibration of nutrient removing lab-scale SBRs under limited aeration. Based on in-process measurements and influent wastewater characterization, the ASM2d model was modified (ASM2dN) by adding an organic nitrogen module linked to the hydrolysis mechanism. After calibration the simulation results showed that enhanced biological nutrient removal occurred during the fill-period and under reduced aeration that achieves so-called ‘Simultaneous Nutrient Removal’. A model-based systems analysis was performed in terms of the contributions of the different processes to overall oxygen, nitrogen and phosphate utilization. In addition, simultaneously occurring biological reactions in SBR phases were compared.

Chapter 8: Optimal but robust N and P removal in SBRs: A model-based systematic study of operation scenarios

In the first part of this chapter, a systematic approach to determine the optimal operation strategy for nitrogen (N) and phosphorus (P) removal of sequencing batch reactors (SBRs) has been developed and applied successfully to a lab-scale SBR. The developed methodology is based on using a grid of possible scenarios to simulate the effect of the key degrees of freedom in the SBR system. The grid of scenarios is simulated using a calibrated ASM2dN model developed and calibrated in Chapter 7. Effluent quality in combination with a robustness index for each of the scenarios is used to select the best scenario. With the best scenario, it is possible to improve/increase the current performance of the SBR system by around 54% and 74% for N and P removal respectively. In the second part of this chapter, the effect of the oxygen set-point and sludge age on the

performance and robustness of the SBR system are analysed using a model-based approach. Robustness of the system as a function of sludge age and oxygen set-point was observed to have a trend completely opposite to the trend of effluent quality. Also, improving effluent quality decreases the stability of the SBR performance. This means that under optimal operating conditions, the system is forced to operate close to its limits, thereby making the system fragile against external variations/disturbances.

Chapter 9: Evaluation of nutrient removal performance for an ORBAL plant using the ASM2d model

An Orbal plant achieving biological nutrient removal was modeled using nitrate, oxygen, ammonium-nitrogen and phosphate measurements for calibration. It was found that the oxygen and nitrate concentration in the outer and middle-ring is the bottleneck for modelling enhanced biological phosphorus removal (EBPR) whilst the system is under diurnal variation in the influent load. The simulation results showed that the overall system performances for total Kjeldahl-Nitrogen and phosphate removal are around 77% and 94%, respectively.

Chapter 10: Dynamic model calibration for an intermittently aerated carousel type activated sludge plant: evaluation of the long-term prediction performance of a calibrated model

To gain a better insight and increase the confidence in full-scale application of activated sludge models (ASMs), it is very important to have an idea about the life-time of a calibrated model to adequately predict dynamic behavior of complex wastewater treatment plants (WWTP). In other words, how long and to what extent does a calibrated model remain valid to adequately represent a WWTP? To address this question, a mathematical model (ASM2d) was calibrated for a municipal wastewater treatment plant (Haaren WWTP, The Netherlands) using measurement campaign data (MC1) collected 3 years ago. The calibrated ASM2d model was then used to predict the current dynamic performance using a new measurement campaign (MC2) data. The BIOMATH protocol (Chapter 1) was used in each case to ascertain a standard/systematic calibration procedure. The calibrated model was observed to remain largely valid over this long-term and was as such able to successfully predict the dynamics of MLSS and $\text{NO}_3\text{-N}$ in the treatment plant

measured 3 years after the calibration period. On the other hand, $\text{PO}_4\text{-P}$ and $\text{NH}_4\text{-N}$ trends in the treatment plant could be better predicted by adjusting a few relevant parameters without compromising the good model-fits on the measured MLSS and $\text{NO}_3\text{-N}$ trends. The results obtained in this study particularly suggest that the life cycle of a calibrated model is compatible with the life cycle of a WWTP (in this case, the Haaren WWTP). This is expected to stimulate confidence in mechanistic modelling of WWTPs and the use of calibrated models for further applications, e.g. optimization, upgrade or design of WWTP. However, a detailed characterization of the influent wastewater (i.e. model input) was observed to be the key to a successful model calibration, i.e. it directly determines the quality of the model outputs. Since in both measurement campaigns summer conditions prevailed, the model response (i.e. its prediction performance) should also be checked for different seasons, i.e. winter, spring and autumn.

Chapter 11: Final Conclusions and Perspectives

A full-scale model calibration requires accurate characterization of influent wastewater in terms of COD fractionation. Short-term respirometric tests are the most convenient tools providing rapid and important information on COD fractionation and model parameters indicating the activity of biomass in the system. Another aspect is the necessity of model calibration procedure for modeling the activated sludge plants using the full scale data. Various design and operating strategies of activated sludge plants (ie. aeration, reactor type and hydraulics) together with influent wastewater characteristics trigger certain processes and yield different interactions between those processes (ie simultaneous nutrient removal). Thus, model based evaluation of the activated sludge process performance with the aid of a 'model calibration procedure' should be considered as a site-specific matter. To improve the model calibration success and stability, more research should be devoted to the development of data collection systems together with the application of Optimal Experimental Design (OED) techniques.

1.3. Modelling of Activated Sludge Processes for Nutrient Removal

1.3.1. Modelling of biological nutrient removal

The nitrogen and phosphate originating from domestic and industrial discharges cause eutrophication problems in receiving water bodies. Generally, the eutrophication problem limits the potential use of receiving water due to diurnal algal activity unless the input of nutrients is reduced and/or controlled based on legislation. To protect water bodies from eutrophication, in Europe, the EEC Directive 91/271 (CEC, 1991) enforces discharge standards with respect to total nitrogen and phosphate within sensitive areas. A cost-effective and sustainable nutrient discharge reduction into receiving waters can be guaranteed by appropriate utilization of the activated sludge process that has already been successfully applied for biological nutrient removal. Sustainable nutrient removal in an efficient way can be achieved by optimal design and control of activated sludge systems built for nutrient (N, P) removal. From an engineering point of view, depending upon environmental disturbances, an appropriate design and operation of activated sludge plants requires better understanding of the complex biological properties of activated sludge systems.

In the last decades, activated sludge models have become widely used tools for understanding and predicting the complex behavior of activated sludge plants. However, external factors (ie. environmental conditions, operating conditions), interactions between complicated and still rather unknown biological reactions make it difficult to comprehend the expected response of the system under certain conditions. A better understanding of biological processes can be provided by means of devoted research and developments in parallel to advancing technologies in biotechnology. Thus, important discoveries in physical and biological processes in biotechnology promoted the increasing trend in the complexity of activated sludge modelling. In this chapter, the principal model developments in activated sludge modelling for nutrient (N, P) removal are discussed on the basis of model structures and requirements.

In the 1980s, the research group of the University of Cape Town first proposed a general model for the activated sludge process (Dold *et al.*, 1980). This model deals with carbon removal from domestic wastewaters under aerobic conditions. One year later, the Dold

et al. (1980) model was extended and the denitrification process was incorporated by Van Haandel *et al.* (1981). The readily biodegradable COD is directly utilized by heterotrophic biomass. The slowly biodegradable COD fraction (X_S) is subjected to 4 subsequent reactions given as follows (a) X_S is enmeshed in the flocs (b) adsorbed in heterotrophic biomass (c) hydrolyzed to hydrolysis products via surface saturation kinetics and finally (d) utilized by heterotrophs, X_H .

Considering carbon and nitrogen removal, the ASM1 was developed by IAWPRC Task Group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment (Henze *et al.*, 1987). A schematic diagram for transformations of ASM1 components is illustrated in Figure 1.1. Under aerobic conditions, the readily biodegradable COD (S_S) is directly utilized by heterotrophs (X_H). Inert microbial product (X_P) is generated during lysis of X_H with fraction f_p . On the other hand, the remaining fraction of $(1-f_p)$ is transformed into slowly biodegradable substrate (X_S). In anoxic conditions nitrate is utilized as a final electron acceptor. The death regeneration concept was adopted in both ASM1 and Dold *et al.* (1980).

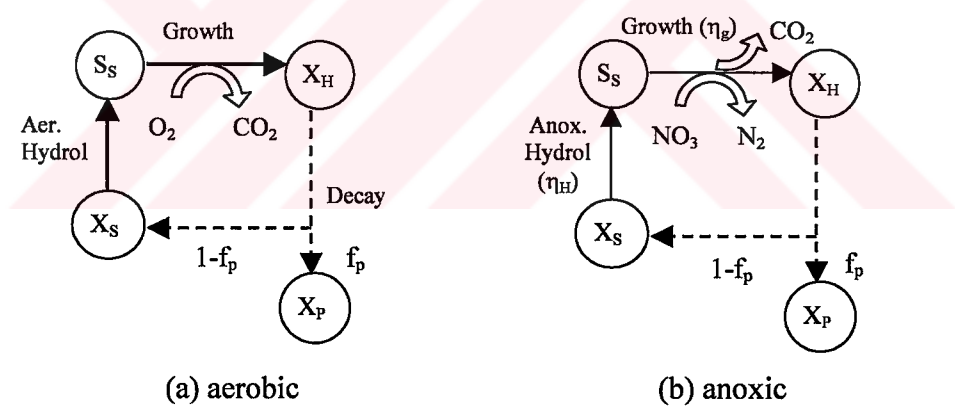


Figure 1.1 Schematic diagram for ASM1 components under (a) aerobic and (b) anoxic conditions (Henze *et al.*, 1987)

In ASM1, single step slowly biodegradable COD degradation follows a surface saturation type reaction. The slowly biodegradable COD is hydrolyzed to readily biodegradable COD that can be utilized by the ordinary heterotrophs. On the other hand, according to Dold *et al.* (1980), the hydrolysis reaction is handled by two consecutive reactions and the products are finally consumed by the heterotrophic biomass. In the

ASM1 and Dold models, the nitrogen components were introduced with the aid of a 'nitrogen module'. The biodegradable particulate organic nitrogen (X_{ND}) is first hydrolyzed to soluble organic nitrogen (S_{ND}) and the reaction rate is controlled by a surface saturation type reaction in parallel to hydrolysis process (see Chapter 7). Soluble biodegradable nitrogen (S_{ND}) is ammonified to ammonia nitrogen by ordinary heterotrophs by a first order type reaction.

Biological nitrogen and phosphorus was then combined in the model of Wentzel *et al.* (1992) (Figure 1.2). The reactions related to the phosphorus accumulating organisms (Poly-P or X_{PAOS}) were introduced by extending the model of Dold *et al.* (1980). According to this model, hydrolyzable material is first enmeshed within the flocs (S_{enn}) and adsorbed as S_{ads} onto the active sites of heterotrophic biomass for utilization under aerobic or anoxic conditions (Figure 1.2.b and Figure 1.2.c). The anoxic growth rate is corrected by a factor of $\eta:0.60$ (Wentzel *et al.*, 1992) instead of 0.33 according to Dold *et al.* (1980) to reflect the increased denitrification rates during hydrolysis and endogenous decay level.

The available readily biodegradable substrate (S_{bsc}) is fermented to short chain volatile fatty acids, VFA and stored as polyhydroxybutyrate (S_{PHB}) by Poly-P microorganisms (Z_{BG}) under anaerobic conditions. The heterotrophic biomass can utilize nitrate as a nutrient when ammonia nitrogen is not available. Under anoxic conditions, Poly-P organisms are able to store VFA but cannot grow on S_{PHB} . Moreover, Poly-P organisms additionally cleave phosphate into the bulk for their maintenance under both anaerobic and anoxic conditions.

The decay of cells generates unbiodegradable soluble (S_{US}) and inert particulate matter (Z_E). It is pertinent to note that the phosphate uptake and growth of Poly-P processes are controlled only via a single reaction running on S_{PHB} according to the model of Wentzel *et al.* (1992). Another important feature of this model is that the Poly-P organisms are not able to use nitrate for anoxic phosphate uptake (Clayton *et al.*, 1991; Kuba *et al.*, 1993). The activity loss of Poly-P organisms under aerobic conditions is modeled with the endogenous decay approach. Hence, oxygen is utilized during the decay of bacterial cells.

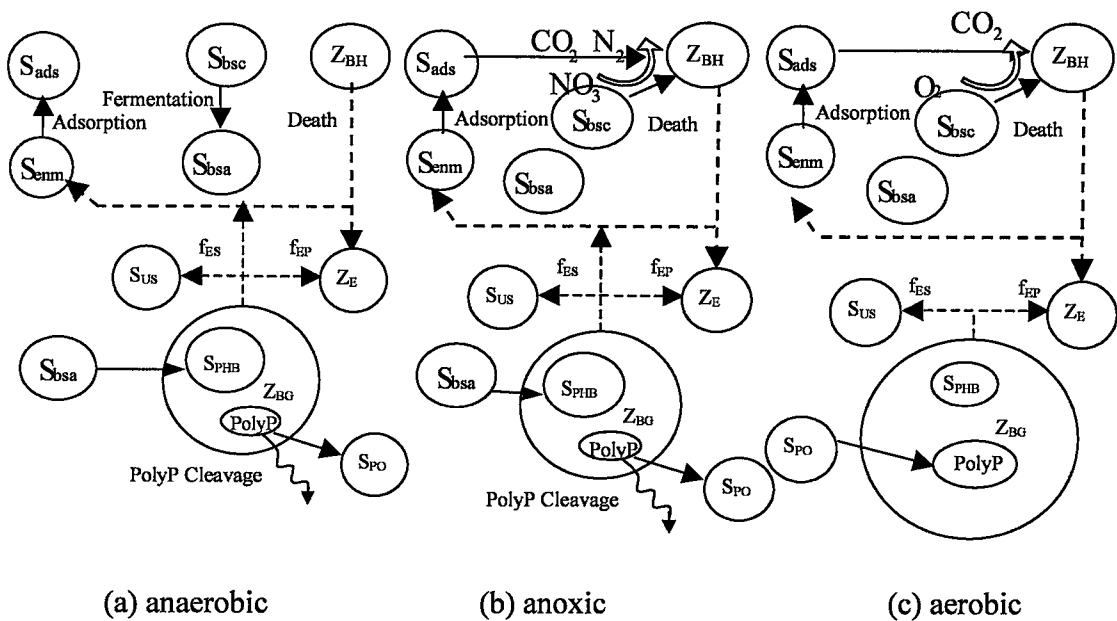


Figure 1.2 Schematic diagram of the Wentzel *et al.* (1992) model under (a) anaerobic, (b) anoxic and (c) aerobic conditions

The IWA Task Group extended ASM1 to ASM2 by keeping the original death regeneration concept and incorporating the enhanced biological phosphorus removal (EBPR) process (Henze *et al.*, 1995a). According to the proposed model, the phosphorus accumulating organisms (X_{PAOS}) store acetate (S_A) as polyhydroxyalkanoate (X_{PHA}) at the expense of VFA. The phosphate storage takes place under aerobic conditions. Similar to the Wentzel *et al.* (1992) model, the readily biodegradable COD in the influent wastewater is subdivided into two fractions as the fermentable COD (S_F) and acetate COD (S_A). Different from the Wentzel model, the heterotrophs are able to consume VFA (S_A) under aerobic and anoxic conditions. The hydrolysis process is controlled by a single surface saturation type equation together with the reduction factors of η_{HNO_3} (default: 0.6) and η_{fe} (default: 0.1) pertaining to the anoxic and anaerobic conditions, respectively. Under anaerobic conditions, the slowly biodegradable COD (X_S) is hydrolyzed to fermentable COD (S_F) by ordinary heterotrophs (Figure 1.3).

In ASM2 the nitrogen components are incorporated into the COD components with $i_{N?}$ fractions. For instance, particulate organic nitrogen (X_{ND}) is introduced as i_{NXS} fraction of the slowly biodegradable COD (X_S). The inert soluble (S_I) and particulate COD (X_I) are generated via hydrolysis and decay processes with f_{SI} and f_{XI} inert fractions,

respectively (see Figure 1.3). Under aerobic conditions, the growth of X_{PAOs} and phosphate uptake processes utilize a single internal substrate pool (X_{PHA}) and they are independently controlled by two different surface saturation type process rates (see Eq1.1 and Eq1.2).

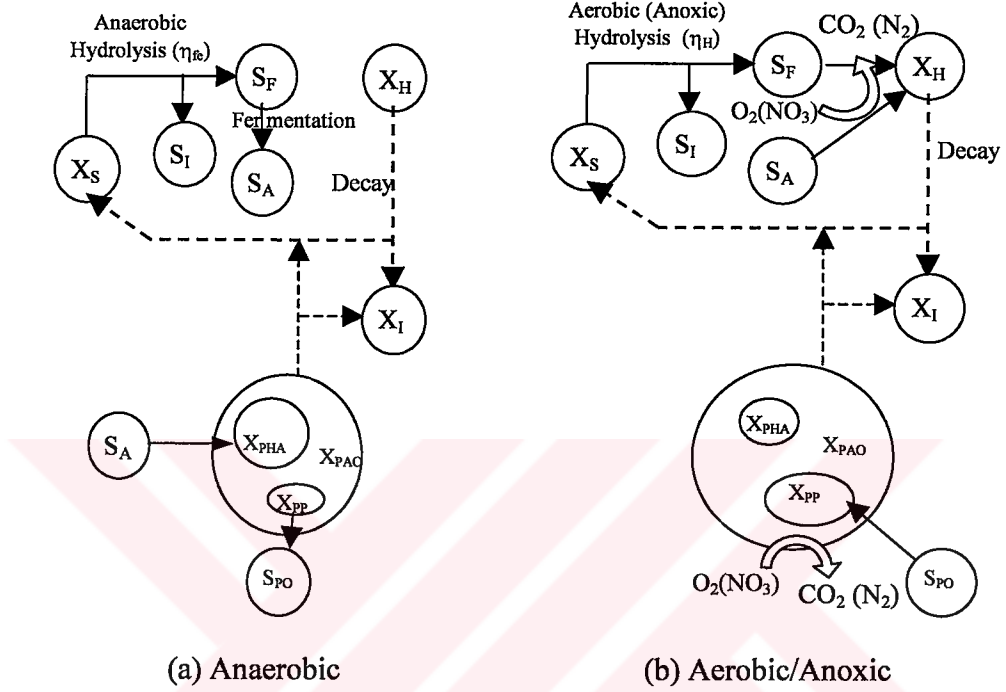


Figure 1.3 Schematic diagram for ASM2/2d (Henze *et al.*, 2000) components under (a) anaerobic and (b) aerobic (ASM2/2d)/anoxic (ASM2d) conditions

Basically, compared to the luxury phosphate uptake; the growth of X_{PAOs} can run under limited phosphate (S_{PO4}) levels. This can be adjusted by manipulating the half saturation constant for phosphate uptake (K_{PS}) and the half saturation phosphate concentration as nutrient (K_P) as given in equation 1.1 and 1.2 ($K_{PS} > K_P$):

$$\text{P Storage} \rightarrow q_{pp} \cdot \frac{S_{PO4}}{K_{PS} + S_{PO4}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot \frac{K_{MAX} - X_{PP}/X_{PAO}}{K_{IPP} + K_{MAX} - X_{PP}/X_{PAO}} \cdot X_{PAO} \quad (1.1)$$

$$\text{Growth} \rightarrow \hat{\mu}_{PAO} \cdot \frac{S_{PO4}}{K_P + S_{PO4}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \cdot X_{PAO} \quad (1.2)$$

where q_{pp} : Rate constant for storage of X_{PP} [$gX_{PP} / gX_{PAO} d$]; μ_{PAO} : Maximum growth rate for PAO [$1/d$]; K_{IPP} : Inhibition coefficient for poly-P storage [gX_{PP} / gX_{PAO}]; K_{PHA} :

Saturation coefficient for PHA [gX_{PHA} / gX_{PAO}] and K_{MAX} : Maximum ratio of X_{PP}/X_{PAO} [gX_{PP} / gX_{PAO}]. Later, the anoxic phosphate uptake was included in ASM2 and that was extended to ASM2d (Henze *et al.*, 2000). Accordingly, a fraction of X_{PAOS} ($\eta_{NO3} = 0.6$) achieves anoxic phosphate uptake (Kerrn-Jespersen and Henze, 1993; Mino *et al.*, 1995a; Murnleitner *et al.*, 1997). Another difference between ASM2 and ASM2d is that the anaerobic hydrolysis reduction factor (η_{fe}) is increased from 0.1 to 0.4 in order to increase the VFA generation via hydrolysis, in turn, leading to better EBPR. In ASM2d, the heterotrophic yields under anoxic and aerobic conditions are set to the same value of $Y_H = 0.63$ gcellCOD/gCOD. Another model was proposed by Barker and Dold (1997) based on the combination of ASM1 and the EBPR model of Wentzel *et al.* (1988; 1989a) with the addition of processes. A schematic representation of the model components for the Barker and Dold model is illustrated in Figure 1.4. Additional processes are: (1) the COD loss and (2) denitrification with anoxic P-uptake by phosphorus accumulating organisms (Z_P). COD loss is also included since the COD recovery based on a mass balance is frequently less than 100%. According to the model, the COD loss is expected during anaerobic and aerobic hydrolysis, fermentation and acetate uptake by Poly-P organisms (Barker and Dold, 1995). In the literature, this is attributed to the fact that the anaerobic growth process has much lower yield values (Ekama and Wentzel, 1999). The death-regeneration concept is adopted for ordinary heterotrophic biomass, represented by Z_{BH} . Conversely, Poly-P organisms consume oxygen during their decay.

The decay process regarding the Poly-P organisms (Z_P) together with storage compounds (S_{PHB} and Poly-P) are separately formulated with 13 reactions depending upon electron acceptor conditions. The biodegradable COD is fermented to VFAs (S_{bsa}) via heterotrophic biomass activity. Then, S_{bsa} is taken up by Poly-P organisms (Z_P) and stored as S_{PHB} to be used for cell synthesis (growth) and P-uptake under aerobic or anoxic conditions. The reactions concerning P uptake are controlled by a single reaction as aerobic or anoxic growth of poly-P organisms.

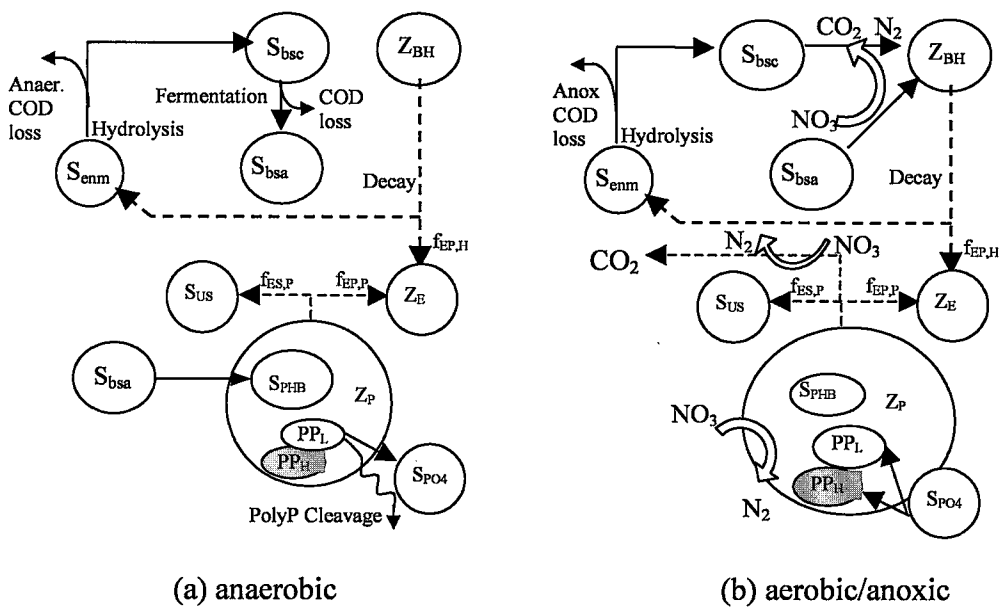


Figure 1.4 Schematic diagram of the Barker and Dold (1997) model

In addition, similar to the ASM2d model, the rates of phosphate uptake and growth of Poly-P are influenced if bulk phosphate becomes limiting. In order to do so, within Poly-P organisms, the phosphate components having high and low molecular weights are included in state variables as P_{PP-L0} and P_{PP-HI} , respectively. In case of low phosphate levels in the bulk liquid, P necessary for growth is stored as P_{PP-L0} as a nutrient. Otherwise, sequestered phosphate is stored as P_{PP-L0} and P_{PP-HI} with the stoichiometry of f_{PP} and $1-f_{PP}$, respectively.

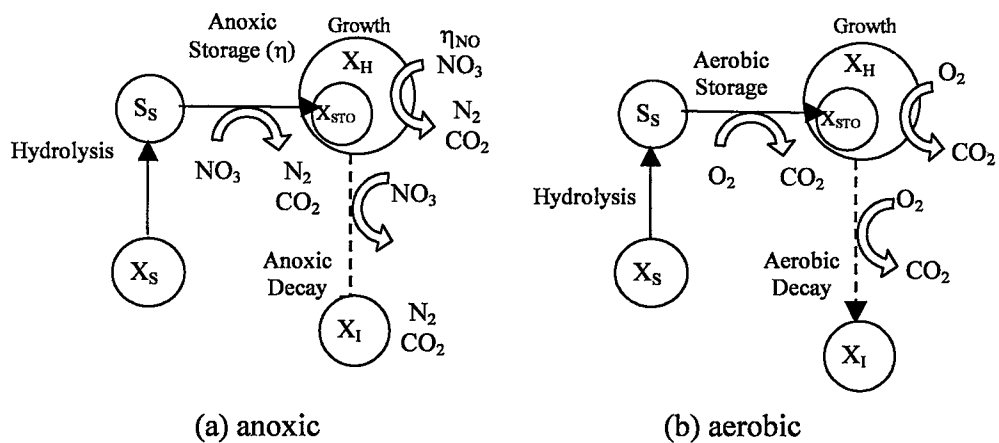


Figure 1.5 Schematic diagram of ASM3 (Henze *et al.*, 2000) for the components under (a) anoxic and (b) aerobic conditions

The heterotrophic biomass, including non-poly-P and poly-P organisms, is able to use nitrate as a nutrient when ammonia nitrogen is limited. The maximum rate constant for anoxic phosphate uptake is governed by a lower value than that under aerobic condition. The endogenous decay based ASM3 model was built on the basis of the storage concept of readily biodegradable substrate (Gujer *et al.*, 1999; Henze *et al.*, 2000). A schematic diagram of ASM3 is given in Figure 1.5. First, the readily biodegradable COD is stored as intracellular polymers (X_{STO}). Then, it can be utilized for heterotrophic growth. In addition, in the model structure only organic carbon and nitrogen removal processes are considered. The nitrogen components are incorporated within the COD components and the processes regarding the autotrophic biomass are directly adopted from ASM1.

The hydrolysis process rate in ASM3 is considered not to be influenced by the electron acceptor conditions (i.e. anaerobic, anoxic or aerobic). The reaction rate for hydrolysis characterized by surface saturation type kinetics, is reduced via increasing the hydrolysis half saturation constant ($K_X=1.0$ gcellCOD/gCOD). Except for autotrophic growth, all processes running under anoxic conditions have reduced process rates (η_{NO_3}).

The EAWAG (Swiss Federal Institute for Environmental Science and Technology) Bio-P model was built by combining the storage concept of ASM3 with the EBPR module of ASM2d (Siegrist *et al.*, 2002; Rieger *et al.*, 2001). According to the model, the fermentation process is omitted and the readily biodegradable COD (S_S) is directly generated through the hydrolysis of slowly biodegradable COD (X_S).

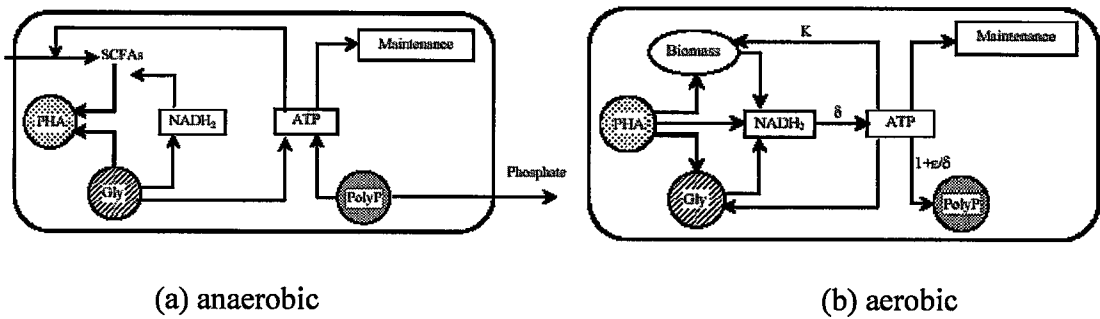


Figure 1.6 Anaerobic and aerobic metabolism of phosphorus accumulating organisms according to Smolders *et al.* (1994a; 1994b); (a) anaerobic and (b) aerobic conditions

Smolders *et al.* (1995) developed the first structured metabolic model for an enhanced culture performing EBPR. The model was developed for an SBR system operated in anaerobic/aerobic mode at the expense of (non-limiting) external substrate. Basically, the first reaction in the anaerobic phase is the acetate (Short Chain Fatty Acids, SCFAs) uptake. Energy (ATP) is provided from Poly-P degradation and Glycogen (Gly) usage. Reducing force (NADH_2) to be used during the conversion of Acetyl-CoA to PHA is derived from the Glycogen (Gly) pool. The amount of released phosphate is function of external pH since more energy is required due to the difference of internal and external pH (Smolders, 1995). A second reaction is related to the supply of maintenance energy for the cell, which is provided by the breakdown of Poly-P pool via hydrolysis (see Figure 1.6.a). The reducing power, NADH_2 , and ATP can be produced via the TCA cycle or via degradation of glycogen via EMP-pathway (Smolders *et al.* 1994b).

Under aerobic conditions, new biomass is synthesized; the external phosphate is taken up; the glycogen pool is replenished and aerobic maintenance of PAO is provided. The PHA degradation (via TCA cycle) generates NADH_2 and ATP is produced. Subsequently, the phosphate is taken up and stored as Poly-P. As a result, new cells are produced and the glycogen pool of the cell is replenished (Figure 1.6.b). The PHA pool is also used for aerobic maintenance energy. Later on, Filipe and Daigger (1998) revised the model of Smolders (1995). Basically, the new concept of (i) glycogen limitation is added for acetate uptake, (ii) maximum glycogen limitation is incorporated and finally (iii) the power function that relates to aerobic P uptake in relation to PHA is modified into a surface saturation type reaction.

Besides the dominance of aerobic PAOs in EBPR systems, many studies have also been devoted to characterize the denitrifying capability of PAOs in mixed and enhanced cultures (Mino *et al.*, 1995a; Kuba *et al.*, 1993; 1996; Barker and Dold; 1997; Henze *et al.*, 1999). Although experimental evidence supports the existence of two different types of microorganisms (Kern-Jespersen and Henze, 1993; Meinhold *et al.*, 1999), to provide model simplicity, only one type of microorganisms with different stoichiometry/kinetics for the anoxic-P uptake processes was incorporated in the activated sludge models (Henze *et al.*, 1999; Barker and Dold, 1997; Murnleitner *et al.*, 1997; Filipe and Daigger, 1999). To mimic the real performance of an activated sludge

plant, the combination of the metabolic model of Murnleitner *et al.* (1997) together with ASM2d (i.e. hydrolysis processes) were studied by Brdjanovic (1998a). Considering the EBPR for real wastewaters, other processes describing the trade-off between particulate and soluble organic carbon (i.e. hydrolysis and fermentation) is required. Further research is still being devoted to combine those models, which have different structures.

Another aspect in EBPR is the occurrence of glycogen accumulating organisms GAOs, which do not contribute to the luxury phosphate uptake. Laboratory and full-scale experimental studies revealed unexpected increases in effluent phosphorus concentrations with considerable VFA uptake under anaerobic conditions (Cech and Hartman, 1993; Satoh *et al.* 1994). In literature, the reasons of GAO occurrence are attributed to many factors such as low influent P/COD, high temperature, propionate in the influent, low pH, etc. From a modelling point of view, Carucci *et al.* (1999a) proposed an anaerobic yield (Y_H) including both anaerobic growth and storage by non-PAOs (GAOs). The simulation runs indicated that competition under anaerobic conditions of ordinary heterotrophs with PAOs significantly alters the effluent phosphate concentration of the system. Based on the pioneering work of Mino *et al.* (1995a); the processes related to GAOs were added to ASM2d to mimic the competition of PAOs and GAOs (Manga *et al.*, 2001; Yagci *et al.* 2004).

1.3.2 Activated sludge plant configurations for nutrient removal

In this section, the treatment plant configurations designed for nutrient removal have been summarized, briefly. Starting from widely accepted carbon and nitrogen removal systems, the EBPR systems together with recent developments in activated sludge processes are given below.

1.3.2.1 Modified Lutzack Ettinger (MLE) and A/O system

The first treatment plant configuration for nitrogen removal is the predenitrification type plant, also known as Modified Lutzack and Ettinger layout (Barnard, 1973). The activated sludge plant is divided into two main sections including the aerobic and anoxic zones (see Figure 1.7). These zones can be (1) created by appropriate adjustments in the aeration facility along a plug-flow reactor or (2) separated via arranging the reactors in

series, physically. For municipal wastewater, high internal nitrified recycle (NR) from the aerobic through the pre-anoxic reactor ($3-5 Q_{\text{influent}}$) is required to acquire efficient nitrogen removal (Kayser, 1999). The dissolved oxygen carry over from the aerobic to the anoxic zone should be minimized since some biodegradable organic carbon is aerobically removed in the first reactor (Orhon and Artan, 1994). In practice, the anoxic zone can be divided into 3-4 stages in series. The MLE process is a very adaptable configuration to be utilized for retrofitting activated sludge plants from carbon to nitrogen removal (Metcalf and Eddy, 2003).

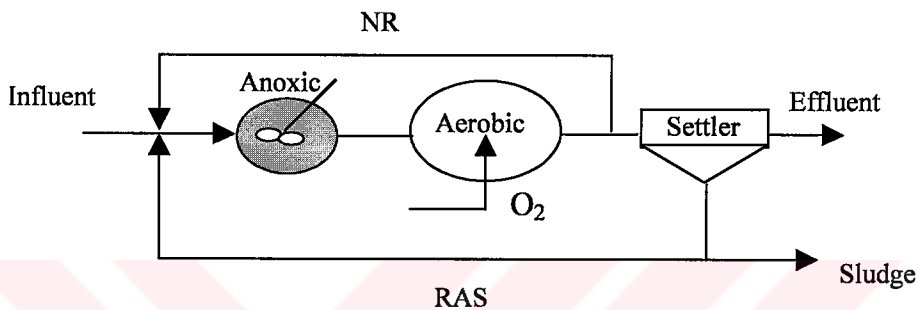


Figure 1.7 Predenitrification (MLE) or two stage Phoredox (A/O) system

Enhanced biological phosphorus removal can be achieved with A/O type systems, widely known as Phoredox systems. This type of plant consists of anaerobic (A) reactor prior to the aerobic reactor (O) operated similar to predenitrification type plants. However, the nitrification is hindered by operating the plant under very low sludge ages (2 to 4 days).

Without any internal recycle stream, the first reactor becomes anaerobic since no nitrate is generated in the aerobic reactor (Barnard, 1974). The enhanced biological phosphorus removal, EBPR is promoted via uptake of volatile fatty acids in anaerobic reactor. The system is not operated for denitrification since there are no anoxic zones in the system layout.

1.3.2.2 Three stage Phoredox (A²O) process

The difference of A²O and the AO process is the presence of an additional anoxic reactor between the anaerobic and aerobic reactor. This layout is the modification of the AO system designed for denitrification together with EBPR. The anoxic zone reduces

the nitrate load coming to the anaerobic compartment. The hydraulic retention time for the anoxic reactor is selected approximately around 1 hour (Metcalf and Eddy, 2003).

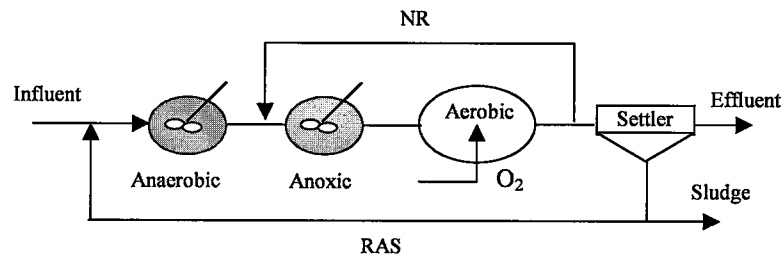


Figure 1.8 Plant layout for A²O

1.3.2.3 Bardenpho (4-5 Stage) type plants

The Bardenpho (4-stage) process combines the two processes of pre-anoxic and post-anoxic systems for nitrogen removal. An internal recycle is added to divert the nitrified mixed liquor to the first anoxic compartment. The retention time of the post-anoxic stage is about the same or larger than that of pre-anoxic zone. It was reported that the nitrate was reduced from 5-7 mgN/l to less than 3 mgN/l in the secondary anoxic and aerobic zone (Metcalf and Eddy, 2003). A plant layout for a 4-stage Bardenpho is given in Figure 1.9.

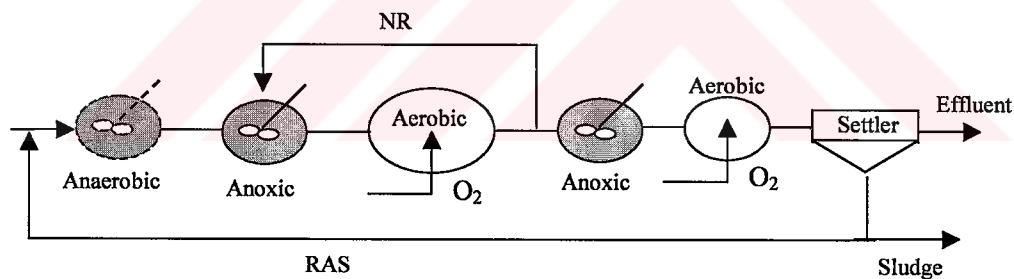


Figure 1.9 Layout for Bardenpho system

The process can be modified into a 5-stage Bardenpho by introducing an anaerobic compartment to promote acetate uptake for enhanced biological phosphorus removal. Different from the A²O layout depicted in Figure 1.8, the second anoxic stage removes the additional nitrate using the endogenous carbon source. The final aerobic stage is required for nitrogen gas stripping for a possible failure of activated sludge settling.

1.3.2.4 Step-Feed process

The reactor configuration of the step-feed is arranged with the anoxic and aerobic reactors in series where the return activated sludge, RAS, is diverted into the first anoxic zone. The influent wastewater is distributed to the two denitrification zones achieving nitrogen removal (see Figure 1.10). The final flow portion diverted to the last anoxic/aerobic zone is critical since the nitrate is produced in the aerobic reactor and will otherwise not be removed. Thus, this will determine the effluent nitrate concentration. With the Step-Feed process configuration, EBPR can be achieved by appropriate arrangement of first reactor(s) as an anaerobic selector.

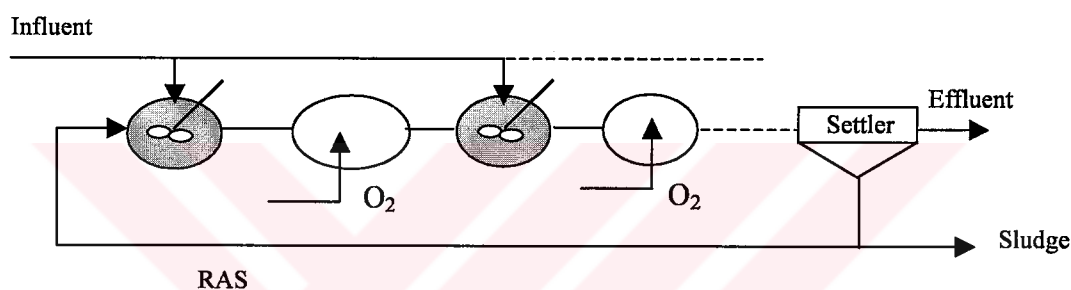


Figure 1.10 Step-Feed process

1.3.2.5 University of Cape Town, UCT (Standard and Modified)

The UCT process was developed by the research group of the University of Cape Town (South Africa) for EBPR from weak wastewaters. The objective was to minimize the amount of nitrate in the anaerobic reactor, which is critical for EBPR. In order to do so, the nitrate from the settler is recycled to the anoxic reactor ($2 \cdot Q_{\text{influent}}$). An additional denitrified recycle, DNR (see Figure 1.11) is introduced from the anoxic to the anaerobic compartment. Since the mixed liquor is at a lower biomass concentration, the retention time for anaerobic reactor should be longer than that of the Phoredox systems. The retention time is generally in the range of 1-2 hours for the anaerobic reactor. In the Modified UCT process, the anoxic reactor is separated into 2 anoxic compartments. The first and second compartments receive the return activated sludge RAS and nitrified recycle, respectively.

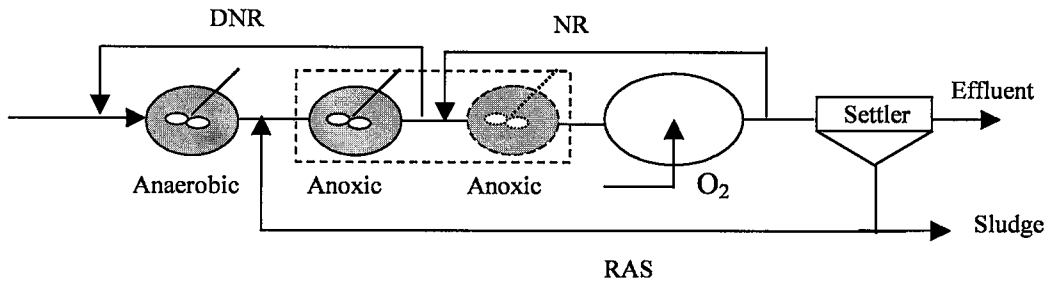


Figure 1.11 University of Cape Town, UCT

1.3.2.6 Virginia initiative plant, VIP

The VIP process was developed by Daigger *et al.* (1988) (see Figure 1.12). The distinctive feature of VIP from A²O and UCT plants is that the all zones are staged consisting at least 2 CSTRs in series. As shown in Figure 1.12, the nitrified recycle (NR) and return activated sludge (RAS) are connected to the first compartment of the anoxic reactor. The plug flow regime of the anoxic reactor provides better denitrification. As a result, the nitrate load recycled to the anaerobic reactor is reduced. The VIP process can be operated in high rate and extended aeration mode. The sludge retention time SRT and hydraulic retention time, HRT for anaerobic and anoxic compartments are generally in the range of 1.5-3 days and 1.0-1.5 hours, respectively (Metcalf and Eddy, 2003).

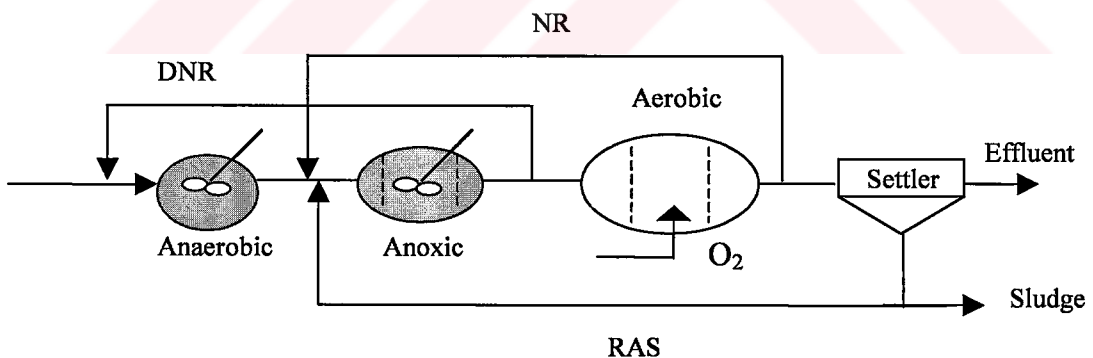


Figure 1.12 VIP process

1.3.2.7 Johannesburg type plants

Another alternative is the Johannesburg type activated sludge plant. In comparison to UCT and MUCT, the RAS is diverted to a pre-anoxic reactor where the nitrate is denitrified by endogenous activity of biomass (Figure 1.13). The appropriate selection of

sufficient reactor configuration and volume allows a reduced nitrate load in the anaerobic reactor. In the anaerobic reactor, higher MLSS concentration can be maintained compared to the UCT process.

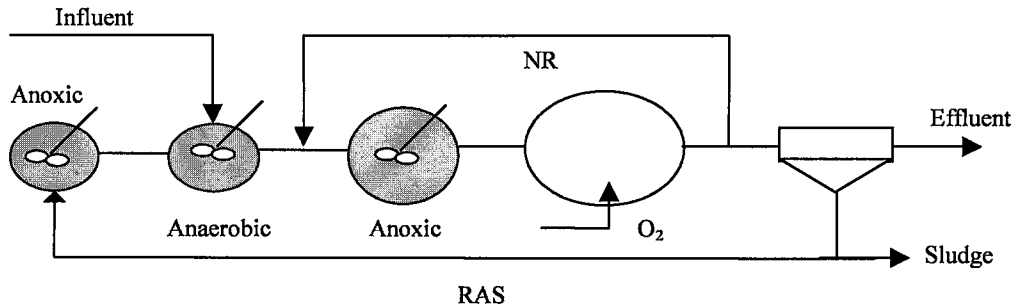


Figure 1.13. Johannesburg type activated sludge

1.3.2.8 Oxidation ditch systems

Oxidation ditch plants are designed to be operated in extended aeration mode (high SRT) with the aid of a closed loop bioreactor having high internal recycle rates (Grady *et al.*, 1999; Randall *et al.*, 1992). The internal recycle rate is adjusted by maintaining the mixed liquor velocity around 0.25-0.3 m/sec along the channel, keeping the system in suspension (Metcalf and Eddy, 2003). The aeration is provided via installing horizontal rotating brush aerators, a vertically arranged disc aerators at certain points of the reactor. As shown in Figure 1.14, the aerobic and anoxic zones in the channel are generated by means of the aerator and control of the control aeration itself (U.S. EPA, 1992). In oxidation ditch systems, high internal recycle ratios turn the system into completely mixed bioreactors having only a DO gradient. The low DO concentration triggers simultaneous nitrification and denitrification (SND) in the reactor. In case of insufficient mixing, additional vertical mixers may be required to keep the mixed liquor in suspension. The implementation of an anaerobic selector prior to the oxidation ditch (carrousel reactor) is required to achieve EBPR (U.S. EPA, 1992).

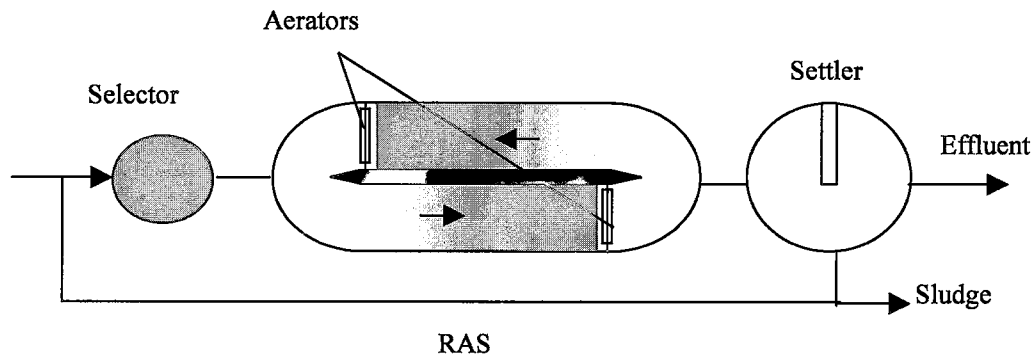


Figure 1.14. Simple oxidation ditch (Carrousel) systems

An Orbal[®] plant is a type of oxidation ditch activated sludge plant, which claims to achieve simultaneous nitrification and denitrification, SND in a single reactor offering reduced aeration costs. Generally, three or four concentrically arranged channels that can be regarded as CSTRs are recommended, as shown in Figure 1.15 (Drews *et al.*, 1972). The SND in the outer loop that receives the influent wastewater provides an overall denitrification performance of 80%. The system is operated under moderate sludge ages in order to suppress the growth of microorganisms causing bulking and settling problems (Daigger and Littleton, 2000). The outer loop is designed to be the largest channel used for simultaneous nitrification-denitrification and it combines the advantages of completely mixed and plug flow reactors in one bioreactor (Smith, 1996). Step-feed RAS and influent wastewater can be applied for effluent nutrient optimization (Applegate *et al.*, 1980).

A completely mixed reactor can be operated in intermittent aeration (IA) mode to achieve nitrification and denitrification in the same reactor volume. Another example is the intermittent feeding of oxidation ditches arranged in series with timer control implementation to achieve nutrient removal known as Bio-denitro and Bio-denipho (Bundgaard *et al.*, 1989) type plants. Similar to operation diagram shown in Figure 1.16, the two parallel inter-connected tanks are alternatingly fed with wastewater and RAS mixture by switching on and off aeration.

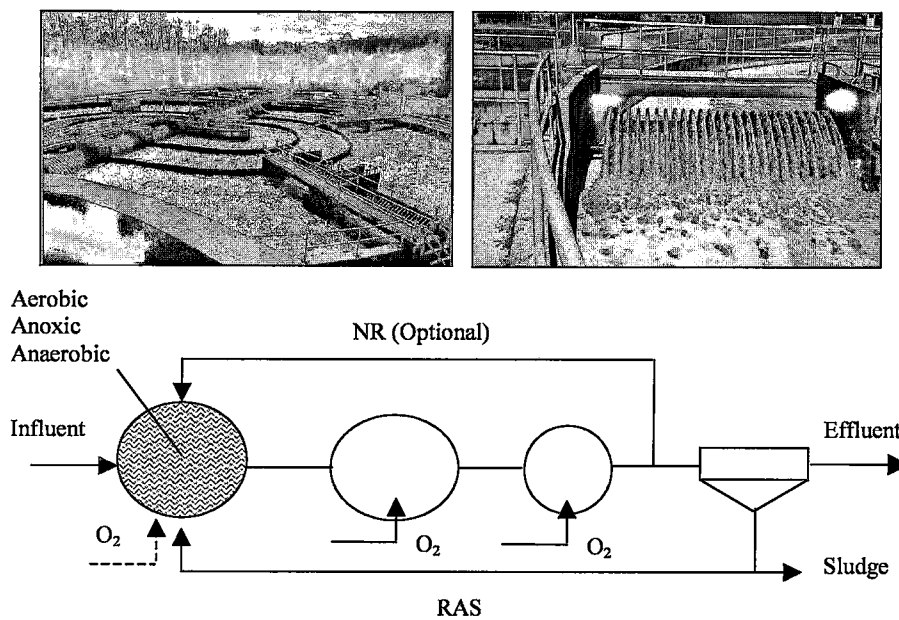


Figure 1.15 Pictures and flow scheme of the Orbal® plant

The alternating aeration (and dissolved oxygen levels) is usually supplied with timer controller. Each tank is equipped with aerator installations, mixing devices and the valves for diverting flows through the reactors. Different from Bio-denitro, the Bio-denipho plants accomodate anaerobic reactors prior to the main biological reactors.

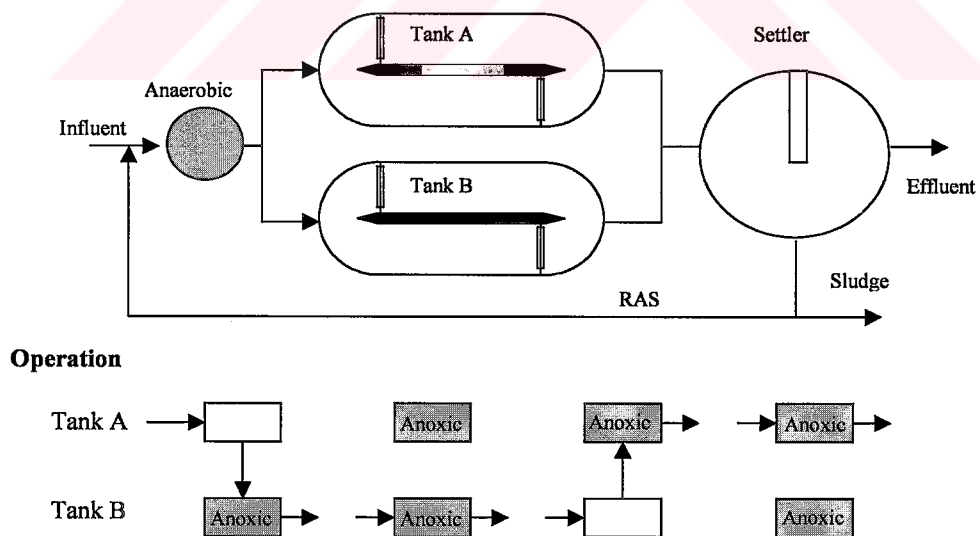


Figure 1.16 Flow diagram for Bio-denipho process

1.3.2.9 Sequencing Batch Reactor (SBR)

In general, SBR systems are viable alternatives to treat the wastewater of small communities (Wilderer *et al.*, 2001). The cycles of SBR are illustrated in Figure 1.17. The sequence of processes in SBRs is time dependent and the sum of phase durations makes a complete process cycle (T_C) repeated progressively. In general, the durations can be the (2) Fill/Mix period, (2) aeration period, (3) settling period (4) decant period and (5) the idle period. Compared to other process scheme, it allows greater flexibility in the operation via manipulating the feeding patterns (feeding to aeration period), cycle time adjustments, alternating aeration etc. to reach lower effluent nutrient levels. In that way, the operation strategy can be easily optimized depending upon wastewater characteristics and environmental conditions. With the appropriate selection of feeding pattern, anaerobic and anoxic periods can easily be created for biological nutrient removal (Artan *et al.*, 2001; Wilderer *et al.*, 2001). The SBR system also allows automatic process control (i.e. dissolved oxygen, DO control) for the optimization of effluent nutrient. The operation mode can be switched from one to another allowing the system to resemble any of the above-mentioned plant layouts. For instance, a SBR can be operated in predenitrification (MLE) mode by combining an anoxic fill and a successive aerobic period. Alternatively, it can be operated in simultaneous nitrification and denitrification (SND) mode by implementing dissolved oxygen set-point control in parallel to a continuous feeding pattern (see Chapter 7-8).

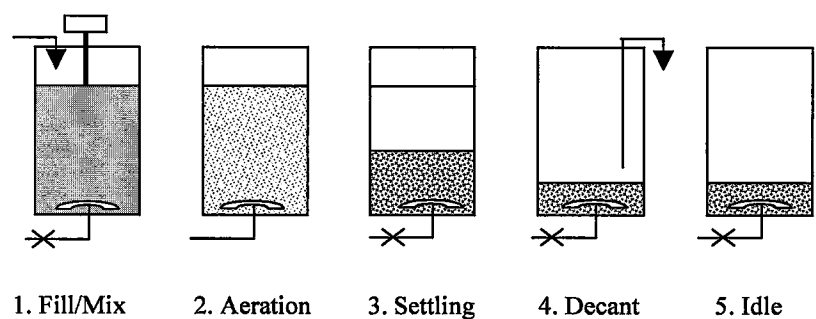


Figure 1.17 Standard phases of SBR

1.3.2.10. BCFS[®] process

The BCFS[®] process (Biological-chemical phosphorus and nitrogen removal) process is based upon the modified UCT process and has been developed to achieve low nutrient effluent concentrations at relatively low COD/N and COD/P ratios in the influent (van Loosdrecht *et al.*, 1998). The BCFS[®] process consists of five compartments (see Figure 1.18), a P-stripper from the anaerobic compartment and three internal recirculation (IR) flows. A contact tank is added to remove slowly biodegradable COD (X_S) with nitrate, which is conveyed via return sludge (RAS). A mixed tank is additionally introduced to promote simultaneous nitrification and denitrification ($DO \approx 0.5$ mg/l) if necessary. In the BCFS[®] process, longer sludge retention times are favorable for removal of nitrogen.

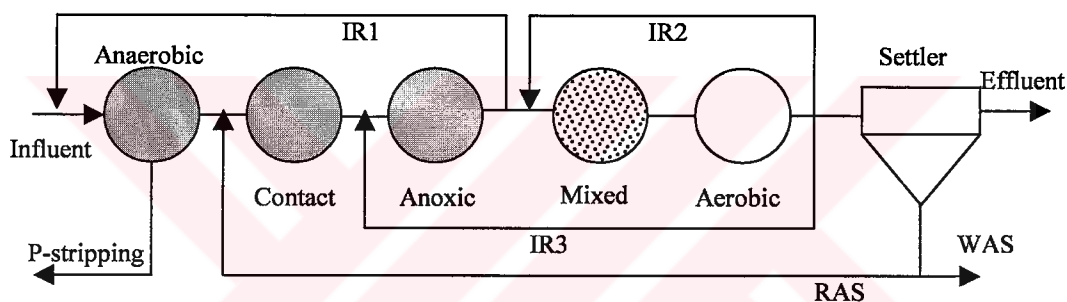


Figure 1.18 Schematic representation of BCFS[®] process

1.3.2.11 Sharon[®]/Anammox[®] process

In the Sharon (Single reactor system for High Ammonium Removal Over Nitrite) process, ammonium is converted to nitrite under aerobic conditions at low sludge age and high temperatures (≈ 1 day sludge age, 35°C) by ammonium-oxidizing bacteria (Hellings *et al.*, 1998; Jetten *et al.*, 1999). As a result of the short retention time and high temperature, the nitrite-oxidizers are washed out (STOWA, 2001) from the system and only nitrite is formed as an end product.

Table 1.1 Reactions of Sharon and Anammox processes

Sharon:	$0.5 \text{ NH}_4^+ + 0.75 \text{ O}_2 \rightarrow 0.5 \text{ NO}_2^- + 0.5 \text{ H}_2\text{O} + \text{H}^+$
Anammox:	$0.5 \text{ NH}_4^+ + 0.5 \text{ NO}_2^- \rightarrow 0.5 \text{ N}_2 + \text{H}_2\text{O}$
Overall process:	$\text{NH}_4^+ + 0.75 \text{ O}_2 \rightarrow 0.5 \text{ N}_2 + 1.5 \text{ H}_2\text{O} + \text{H}^+$

The Sharon reactor is operated such that ammonium is only partially converted to nitrite to promote the growth of ammonia-oxidizers. In the Anammox (ANaerobic AMMonia OXidation) process, the ammonia is oxidized if nitrite is available (STOWA, 2001). Finally, a combined Sharon-Anammox process was developed by van Dongen *et al.* (2001). The process stoichiometry is given in Table 1.1. The Sharon-Anammox Process can be an alternative to remove nitrogen if a sludge digester is available. For this process, a scheme is illustrated in Figure 1.19. One-stage ammonium removal process can also be achieved in a biofilm reactor with simultaneous nitrification and Anammox, so called ‘CANON (Completely Autotrophic N-removal Over Nitrite)’ process (Strous *et al.*, 2000).

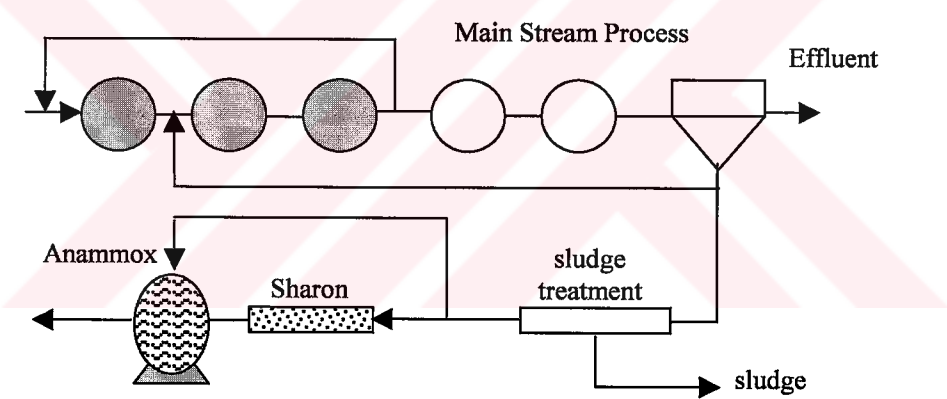


Figure 1.19 Coupling of Sharon-Anammox to main-stream processes

1.3.2.12 External nitrification biological nutrient removal activated sludge (ENBNRAS) plants

The idea of external nitrification biological nutrient removal activated sludge plant was first suggested by Bortone *et al.* (1996). The nitrification is externally provided by fixed film bioreactor with an internal settling tank. Ekama and Wentzel (1999) stated the difficulties of long sludge age requirements and low F/M bulking problems in BNR activated sludge plants. In order to cope with these problems, a few studies were devoted to coupling an external nitrification process coupled to biological nutrient removal

activated sludge systems, so called “ENBNRAS” systems (Bortone *et al.*, 1996; Hu *et al.*, 2001; 2003a). The schematic diagram of the plant layout is given in Figure 1.20. The sludge age of the system can be reduced from 20-25 days to 8-10 days by encouraging anoxic phosphate uptake in the main anoxic tank. Lab-scale investigations of Hu *et al.* (2003a) showed that high nitrogen removal was achieved (80-90%) with a relatively low DSVI (<100 ml/g) under low influent COD/TKN ratio (~7).

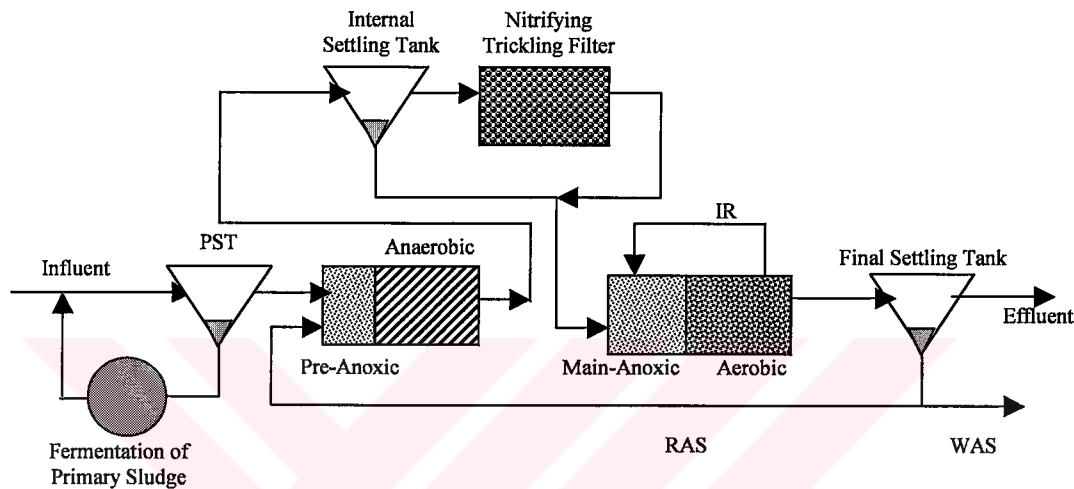


Figure 1.20 The ENBNRAS system (Hu *et al.*, 2003a)

The design and operating parameters for commonly used nitrogen and biological phosphorus-removal processes are given in Table 1.2. According to the table, sludge retention time (SRT) covers a wide range for the processes of nitrogen and phosphorus removal. If only phosphorus removal is considered (e.g. A/O, A²/O processes), lower SRT values are selected in order to suppress nitrification since the nitrate consumes required VFA for EBPR. The mixed liquor suspended solid (MLSS) concentration to be maintained in biological reactor is generally around 2-4 mg/l for nutrient removal processes. Selection of higher hydraulic retention times (HRT) for oxidation ditch type plants (Biodenitro, Orbal) and SBRs are preferred for process design, which provides greater flexibility. For phosphorus removal, in parallel to reduced SRTs, lower HRTs are sufficient for A/O and A²/O processes to maintain desired MLSS in biological reactor. For nitrogen and phosphorus removal, SBRs are more flexible in terms of HRT selection. Broader return activated sludge (RAS) range of 25%-100% corresponds to

A/O and A²/O processes because of the fact that the nitrate load through the anarobic compartment should be reduced for better EBPR efficiency. Mostly, a minimum RAS value of 50% (sludge thickening factor) is preferred in order not to sludge blanket build up in the final clarifier. The Bardenpho, UCT and VIP processes require high internal recycle rates since the process train is composed of multi-staged reactors. In the operation, higher internal recycle rates are necessitated from aerobic to anoxic, anoxic to anaerobic reactors for those processes. In oxidation ditches, higher internal recycles are maintained in closed loop bioreactor with the aid of mixers. Thus, no internal recycle is required in oxidation ditches. Internal recycle alternative is kept optional for Orbal type plants for the improvement of nitrogen removal (see Chapter 9).



Table 1.2 Design and operating parameters for commonly used nitrogen and biological phosphorus-removal processes (Metcalf and Eddy, 2003)

Activated Sludge	SRT*	MLSS	HRT**(h)				RAS	Internal Recycle
Process	day	g/L	Total	Anaerobic zone	Anoxic Zone	Aerobic Zone	% of Influent	% of Influent
<i>Nitrogen Removal</i>								
MLE	7-20	3-4	5-15		1-3	4-12	50-100	100-200
SBR	10-30	3-5	20-30		Variable	Variable	-	-
Bardenpho (4-stage)	10-20	3-4	8-20		1-3 (1 st stage) 2-4 (3 st stage)	4-12 (2 nd stage) 0.5-1 (4 th stage)	50-100	200-400
Oxidation Ditch	20-30	2-4	18-30		Variable	Variable	50-100	
Biodenitro™	20-40	3-4	20-30		Variable	Variable	50-100	
Orbal	10-30	2-4	10-20		6-10	3-6 (1 st stage) 2-3 (2 nd stage)	50-100	Optional
<i>Phosphorus Removal</i>								
A/O	2-5	3-4		0.5-1.5	-	1-3	25-100	
A ² /O	5-25	3-4		0.5-1.5	0.5-1	4-8	25-100	100-400
UCT	10-25	3-4		1-2	2-4	4-12	80-100	200-400 (anoxic) 100-300 (aerobic)
VIP	5-10	2-4		1-2	1-2	4-6	80-100	100-200 (anoxic) 100-300 (aerobic)
Bardenpho (5-stage)	10-20	3-4		0.5-1.5	1-3 (1 st stage) 2-4 (2 nd stage)	4-12 (1 st stage) 0.5-1 (2 nd stage)	50-100	200-400
SBR	20-40	3-4		1.5-3.0	1-3	2-4		

* Sludge Retention Time (temperature dependent); ** Hydraulic Retention Time

1.4 A General Activated Sludge Model Calibration Methodology

The BIOMATH protocol (Vanrolleghem *et al.*, 2003) for the calibration of activated sludge models is composed of four main stages and 12 modules (see Figure 1.21). The first stage is the definition of the target(s) of the modelling exercise followed by decision making on the necessary information to be obtained from the activated sludge (AS) plant such that the target of the modelling study can be reached. Some of the modules (1-11) can be skipped depending on the general evaluation whether the targets are reached. The second stage is the collection of detailed information on the activated sludge plant. The mass transfer (hydraulic and oxygen transfer), biological, settling and the influent characterizations are included in this step. In addition, the experimental or lab-scale work is incorporated with usage of the Optimal Experimental Design (OED) methodology. By averaging the influent and operational characteristics, steady state modelling is performed for the mass transfer, settler and the biological model (e.g. ASMs). The third step includes the complete calibration of the activated sludge model using the dynamic influent data, and incorporating the parameter values obtained from lab scale experiments or full-scale data. At the last stage, decisions will be made upon eventual re-iteration of a number of the modules.

The proposed protocol for the modelling of the treatment plant is refined on the basis of a previous protocol developed by Petersen (2000). As illustrated in Petersen *et al.*, (2002) the details of the modules underlying each step are shown in Figure 1.21, and they are summarized below.

Stage-1. Definition of a target for modelling

In the first step, the main objectives have to be defined for the modelling of continuous systems, sequencing batch reactors (SBR), alternating activated sludge plants etc. The decision is usually based on the time and/or budget necessary/available for the modelling task. Some of the stages can be omitted depending upon the objectives (see Figure 1). The main objectives for a modelling case can be:

- Optimization and upgrading of an existing activated sludge plant
- Meeting the effluent criteria

- Cost reduction in the operation
- Reuse of effluent wastewater
- Development of control strategies
- Design of the treatment plant or the combination of those.

Stage 2. Plant survey/data analysis and process characterization

A general description of the treatment plant to be used in the model calibration can be compiled from the operation database/log files of the activated sludge treatment plant itself, the design documents and/or personal communication with the plant operators. The design data consist of the physical characteristics such as volumes, a number of compartments, pumping capacities, a number of aerators and connections installed. The operational data is mainly the actual working volumes, the flow rates, energy consumption, the distributions of sludge/wastewater over the compartments and specific design parameters for certain treatment plant alternatives.

The *design data* consist of the general plant layout and configuration, compartments/process units, volumes/areas/depths, water and sludge lines, installed capacities, pumps, aerators, P&I diagrams, hydraulic layout. On the other hand, the *operational data* concern the flow rates for influent, sludge recycles, sludge wastage and internal recirculation; sludge/wastewater distributions over parallel lines, step feed *etc.*; location, type and implementation of control strategies. The most important issue is the (available) *measured data* comprising the conventional characterization of influent and effluent (e.g. COD, TKN, PO₄, TP, NO₃, NH₄, TSS, pH, T (°C)); on-line measurements from the treatment plant (dissolved oxygen, NO₃, SVI, ML(V)SS, PO₄, NH₄, pH, Temperature, sludge blanket height in the clarifier, TSS concentration in the return sludge and effluent, P and N content of sludge, sludge age and daily sludge production, VSS/SS ratio of the sludge).

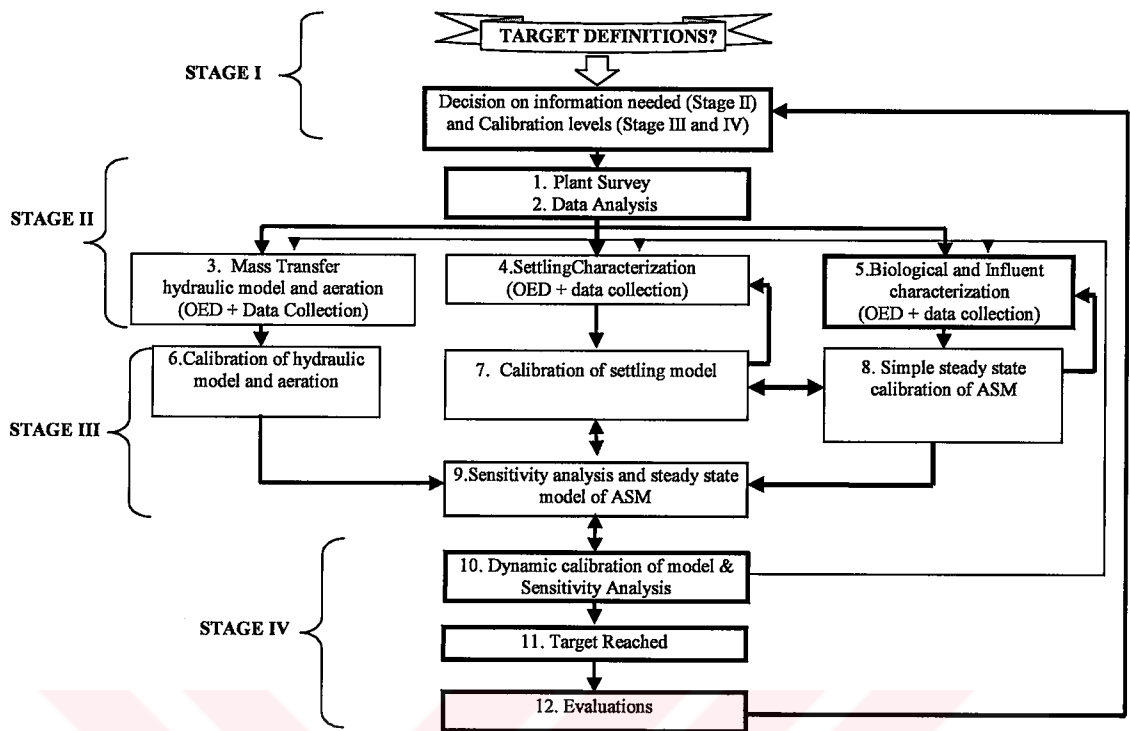


Figure 1.21 The BIOMATH model calibration protocol

The information collected in this step is of great importance for the understanding of the capacity and the behavior of the system. So, the design, the operational data and the measured data should be evaluated and processed for understanding of the entire process. For data quality assessment, outlier detection is applied here and interpolation of data can be done whenever it is appropriate and possible. Mass balances regarding the flow rate and the sludge (considering the N and P content) are crucial for the model calibration; particularly for the accurate estimation of the system sludge age (Barker and Dold, 1995; Nowak *et al.*, 1999). From a modelling point of view, it should be noted that the sludge age is the most sensitive parameter with respect to all model outputs.

In addition, some other factors that exert a critical influence on the system performance such as pH, temperature changes, industrial discharges, addition of auxiliary chemicals, energy consumption and generation of daily and monthly operational and maintenance costs etc., should be evaluated in this step.

Stage 2.1. Mass transfer characterization

In the mass transfer characterization; two main aspects have to be considered. The first one is the determination of the oxygen transfer efficiency (K_{La}) in all reactors (e.g. surface aerators, compressed air). The second aspect is the hydraulic characterization of the treatment plant.

Oxygen transfer characterization: Regarding the determination of the K_{La} for aeration, first, the influences of operational and biological factors on the oxygen transfer have to be considered (i.e. temperature, salt content). The volumetric mass transfer coefficient, (K_{La}) should be estimated under process conditions. A variety of methods have been developed over the last 2 decades (Boyle and Campbell, 1984; Capella *et al.*, 1999; Gillot, *et al.* 1997; Mueller and Boyle, 1988). Daily power consumptions of the aerators and/or the information provided from the manufacturers may give hints about the oxygen transfer coefficient of the aeration system.

Hydraulic characterization: The second aspect concerns the question whether hydraulic characterization is needed or not. The reactor configuration and the modelling objectives will have an influence on the selection of the degree of accuracy required from the hydraulic characterization. Importantly, complex hydraulics may affect the best sampling location to obtain representative measurements for the calibration. In case it is difficult to understand the hydraulics of the plant from experience, the plant layout and the survey of the plant (e.g. higher volumes and dispersions), a detailed hydraulic characterization is essential.

A “tracer test” can be performed in order to obtain information about the mixing characteristics allowing for determination of the number of tanks in series (see Figure 1.22-right). It should be noted here that the transient hydraulic behavior of the treatment system due to flow changes, on/off controls of the pumps-aeration etc. can also be important factors (De Clercq *et al.*, 1999). Alternatively, dispersion models (or terms) can be incorporated in the models for the hydraulic characterization (Stamou, 1997). The tracer experiment may also provide more information about the dead volumes and/or recycles in the reactors. If a detailed hydraulic characterization is not required, possible assumptions can be made on the number of tanks-in-series based on the

configuration/dimensions of the compartments or by using empirical equations (Chambers, 1992).

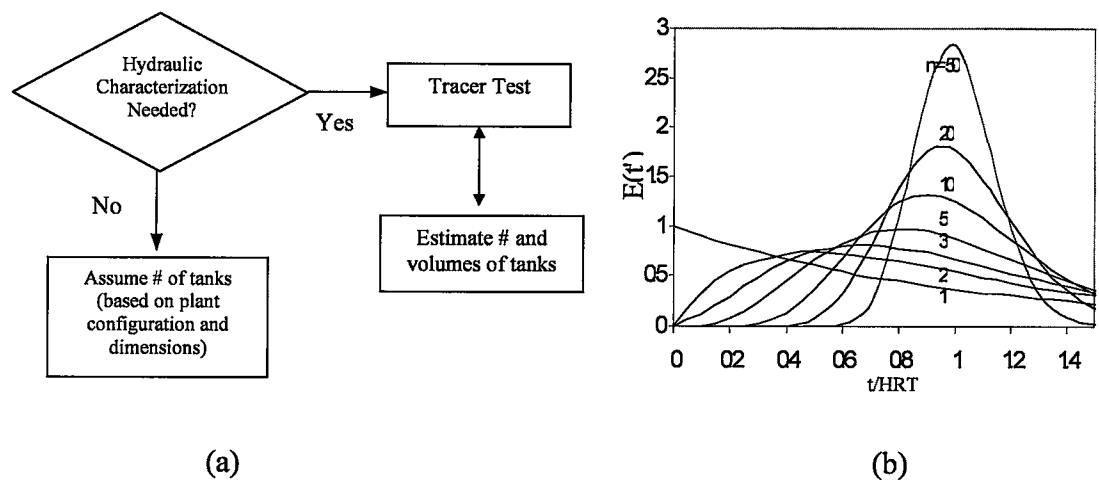


Figure 1.22 Decision chart for hydraulic characterization (a) and hydraulic residence time distribution function, $E(t')$ for different numbers of tanks in series (b)

Stage 2.2. Settling Characterization

A detailed settling characterization is necessary if the settling performance and the reactions during settling influence the overall system behavior (e.g. effluent COD, N and P). In addition, the target(s) might be the optimization of settling or may be the amendment of effluent suspended solid removal. From a modelling point of view, the investigation could be focused on either settling in the primary and/or final clarifier. If a detailed settling characterization is necessary, settling experiments (Daigger and Roper, 1985; Ekama and Marais, 1986a) and/or other relevant measurements such as SVI have to be carried out before selecting the settling model.

In addition, reactions such as denitrification and phosphorus release in the settler may have to be considered (Henze *et al.*, 1993; Koch *et al.*, 1999; Wouters-Wasiak *et al.*, 1996). This can be checked by calculating the mass balance over nitrate-phosphate or by site observations such as the occurrence of nitrogen gas bubbles entrapped in the flocs (Henze *et al.*, 1993).

If the solid separation in the settler is working well, no detailed settling characterization is necessary (see Figure 1.23). So, a point settler model can be used to describe the

separation of the suspended solid flux from the main stream. If a considerable amount of sludge is maintained in the settler, a virtual reactor can be defined next to the point settler. The residence time in the settler can then be modeled by placing a CSTR with a volume equal to the sludge-blanket volume of the settler in series with the settler. The smoothing effect of the secondary clarifier on the effluent quality with respect to COD, total nitrogen and phosphorus etc. should be accounted for.

As mentioned above, if a specific analysis of the plant is required and if the settler affects the performance of the plant critically, then a more detailed model for the settler should be used. This can be done via one-, two- or three-dimensional settling models. Of course, the complexity of the model should meet the requirements. For operation and control of a WWTP a one-dimensional model is advised. The most commonly used one-dimensional model is the settling model presented in Takács *et al.* (1991), but alternatives (both simpler and more complex) exist (Krebs *et al.*, 2000).

Selection of the appropriate model is based on the measurement of concentration profiles or sludge-blanket-height time profiles (De Clercq *et al.*, 2003). The model, which fits the measured concentration profiles or the sludge blanket heights best, should be selected. The reactions should be included in the settler model if they significantly affect the performance. The decision flow diagram for the settling characterization is illustrated in Figure 1.23.

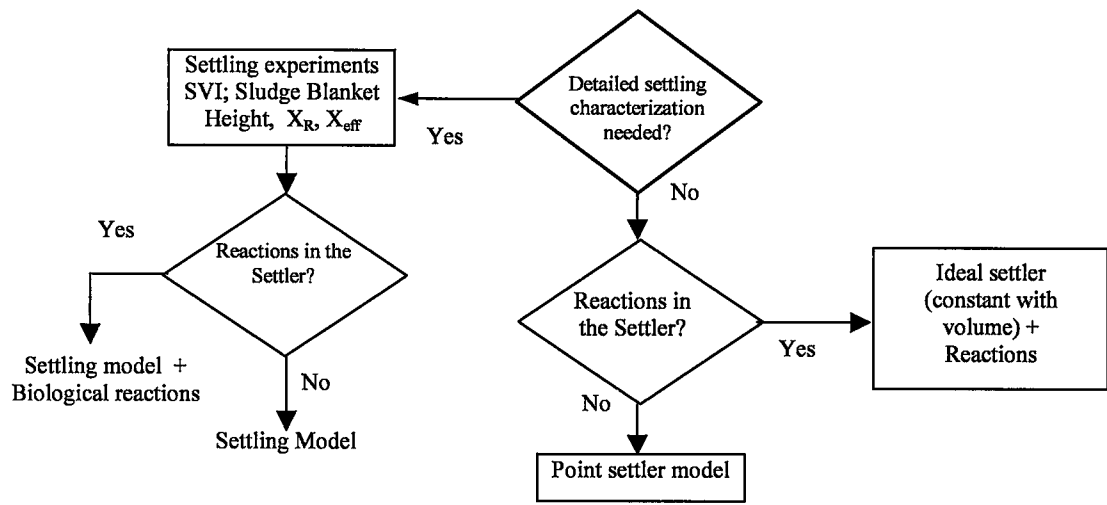


Figure 1.23 Decision chart on settling characterization

The primary clarifiers ahead of the biological reactors also have a vital importance since there might be activation and/or interactions between physico-chemical and biological reactions. For instance, in addition to biological reactions, the COD removal can be expressed as a physico-chemical reaction such as flocculation and solubilization of the particulate COD fractions into soluble fractions. A large amount of COD (up to 50%) can be removed by gravity settling (Orhon *et al.*, 2002). The biomass in wastewater leads to biological processes such as fermentation, acidification and ammonification due to heterotrophic activity and depend on the environmental conditions in the primary clarifier (Gernaey *et al.*, 2001). The settling and biological reactions should be incorporated in the model if the effect of the primary clarifier on the overall process performance is evident. The effect of the primary clarifier can be evaluated by performing some relevant on-site experimental analyses such as filtered/unfiltered COD, $\text{NH}_4\text{-N}$, TP, pH and VFA analysis etc. in the influent and the effluent streams of a primary clarifier.

Stage 2.3. Biological Characterization

Activated Sludge Models (ASM1, ASM2-ASM2d, ASM3) proposed by the IWA (formerly IAWPRC, then IAWQ) task group on Mathematical Modelling for Design and Operation of Biological Wastewater Treatment are the most commonly applied mathematical models for the modelling of the biological compartments of wastewater treatment plants. The ASM family models has been successfully applied to full-scale treatment plants and shown to be a good compromise between the complexity of the activated sludge processes and prediction of the plant behavior under dynamic conditions. Therefore, in the proposed BIOMATH protocol, the calibration methodology focuses on the ASM family models.

Model selection for the modelling of the biological activity is dependent on: (a) biological processes/activity (e.g. COD removal, N & P removal) occurring in the treatment plant and (b) on the purpose of the model application. Model selection should be based on the targets of the modelling in order to optimize the calibration efforts in accordance with the modelling objectives. Appropriate modifications or extensions of

the proposed models can also be considered (i.e. build-up of nitrite during nitrification or denitrification or the fate of specific chemicals).

The determination of all model components is an expensive and time-consuming process. Therefore, whenever possible it is suggested that the default values reported in previous applications should be assigned to the model parameters (Henze *et al.*, 2000). In this context, a sensitivity analysis allows, based on the target of the modelling exercise, to discriminate between the relatively less sensitive and the most sensitive parameters (De Pauw *et al.*, 2004; Weijers and Vanrolleghem, 1997). This information should be used in the calibration protocol and is expected to minimize the calibration efforts and therefore optimize the overall calibration procedure towards the objectives of the modelling. For instance the most important (sensitive) parameters for the prediction of MLSS in the system are mainly the particulate inert materials concentration (or COD) in the influent (X_I), the heterotrophic biomass yield coefficient (Y_H), the heterotrophic biomass decay coefficient (b_H) and the sludge retention time (Nowak *et al.*, 1999).

Optimal Experimental Design (OED): Calibration of a mathematical model asks for at least the determination of a couple of parameters that can be selected among all model parameters by analyzing the sensitivity functions of the parameters with respect to the model component explicitly specified in the target of the modelling exercise (e.g. minimum nitrate concentration in the effluent). Another approach for the selection of the parameter subset for the calibration is to apply the collinearity index (Brun *et al.*, 2002; Reichert and Vanrolleghem, 2001). In the context of calibration of the Activated Sludge Models, several lab-scale experiments and full-scale measurement campaigns are usually needed (Henze *et al.*, 1987; Carucci *et al.*, 1999; Coen *et al.*, 1997; Petersen *et al.*, 2001b, 2003) which are expensive and time consuming. The OED concept should be incorporated into the experimental work of the calibration to maximize the information content of each of the experiments (Dochain and Vanrolleghem, 2001). This approach therefore is expected to minimize time and cost aspects of the laboratory work. Optimal experimental design methodology can be applied for lab-scale experimental set-ups or even for full-scale systems. However, OED applications to full-scale systems need a high level of a priori information and expert knowledge.

Estimation of Activated Sludge Model parameters: The ASM1 introduced by Henze *et al.* (1987) essentially describes a single-stage activated sludge system performing simultaneous COD oxidation, nitrification and denitrification processes. A detailed description and explanation of the model processes and components can be found in the technical report of the IWA task group. Application of the ASM1 to a specific treatment plant, i.e. simulation of an activated sludge system based on ASM1, requires the calibration of the ASM1 model to the system under study. That requires the calibration of the stoichiometric and kinetic parameters and characterization of wastewater and biomass of the system in accordance with the ASM1 model. This overall process is called calibration of the ASM1 model.

Parameter estimation consists of determining the ‘optimal’ values of the parameters of a selected model with the aid of measured data (Petersen *et al.*, 2003). Initially, the model structure, of which parameter(s) need to be estimated, initial concentration of the components and experimental data are necessary. According to Figure 1.24, the initial values of the parameters (or combinations) and initial conditions have to be defined. By application of this routine, the parameter estimation is terminated when the objective function reaches a minimum with certain accuracy. Numerical techniques for parameter estimation can be found in Dochain and Vanrolleghem (2001).

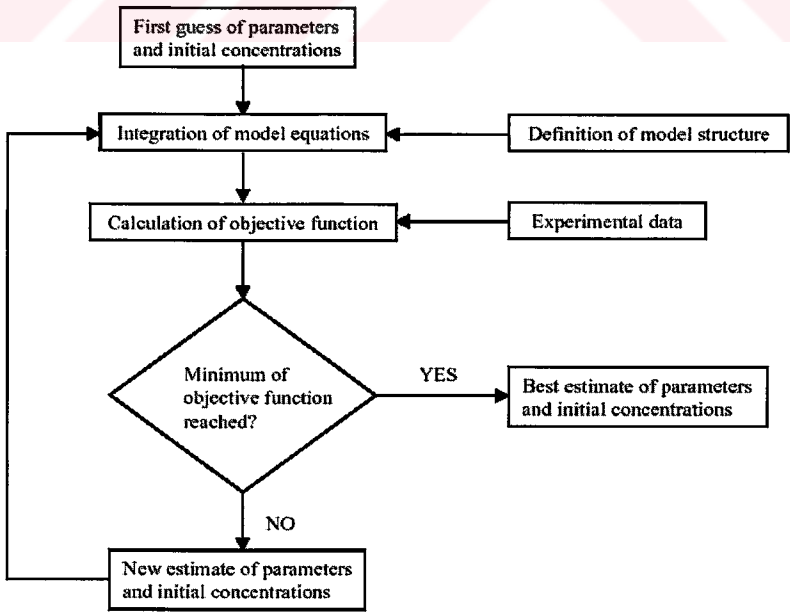


Figure 1.24 Parameter estimation routine (Wanner *et al.*, 1992)

The selection of estimation methods for biomass activity, process stoichiometry and kinetics are based on dedicated lab-scale experimental methods devoted to ASM model parameters and wastewater characteristics. However, it is important to stress that not all those experiments should be performed. Only the experiments aiming at providing data to identify the relevant parameters shown to be influential in the sensitivity analysis should be carried out. In other words, the experiments that have to be performed will be dependent on the system under study as well as on the target of the modelling study. In this context, the proposed model calibration procedure is not fixed but it should be considered as dynamic depending on each specific case study. Some of the dedicated lab-experiments (i.e. respirometry) designed for wastewater characterization, process stoichiometry and kinetics will be discussed in the following chapters.

Stage-3. Steady state calibration of the selected model

In this phase, the different reactors in the treatment plant are represented by an ideal perfectly mixed tank as a simple treatment plant configuration (Figure 1.20-Module 8). The data of the full-scale wastewater treatment plant are averaged, assuming that this average represents the steady state, and the model is calibrated to fit to average effluent concentration and sludge wastage data. The calibration of the activated sludge model and the settler are linked to each other in order to describe the final effluent quality. At this stage, the interaction between the steady state calibration and the settler model calibration is taken into consideration. Another advantage is the characterization of wastewater components that can be adjusted by changing model parameters (i.e. Y_H , b_H etc.) during calibration using the full-scale data. The mass balance of the sludge and the sludge production of the activated sludge plant should be fitted to the actual measurements. In addition, the actual sludge age could also be controlled or determined by calculating the phosphate mass-balance over the system.

After the combination of the sub-models, a steady state calibration of the overall activated sludge plant is carried out with the collected data in Stage II (and/or using available long term data). The steady state calibration is done for each of the sub-models, i.e. the calibration of the mass transfer model, the settling model and the biological model. Depending on the objectives and/or conditions of the treatment plant,

these sub-models can be omitted or considered as a sub-model in the general steady state calibration task (Module 9). In the steady state calibration of the model the controllers (aeration, return and internal recycle rates etc.) are incorporated in the model. The main idea is to estimate the appropriate biomass composition, biomass distribution over the reactor(s) or settler(s). It should be noted here that the biomass composition obtained from the steady state calibration is used in the dynamic model calibration as the initial biomass composition.

Influent wastewater characterization is essential for the simulation of the activated sludge plant. Therefore, the wastewater characterization has to be performed carefully. After that the sub-models should be selected based upon the objectives of the modelling study. Then, the overall steady state simulation of the model is carried out using the default parameters and the flux based average influent characterization of the wastewater.

The steady-state simulation (calibration) results can be compared on the basis of averaged effluent COD, N and P concentrations, oxygen consumption and sludge production. If the simulated steady state performance is in good agreement with the data collected in Stage II or with the long-term data, the dynamic calibration of the general model can be performed.

Stage-4. Dynamic calibration and evaluation of the results

In Stage IV, the dynamic calibration of the activated sludge model is aimed at. Before proceeding into more details of the dynamic calibration, the sludge production must be modeled and must be in good agreement with the real situation (this is expected to be achieved in Stage III). As an initial guess, the biomass composition resulting from the steady state calibration as described in Stage III is taken. The dynamic calibration of the model necessitates the availability of dynamic influent concentration data profiles. A larger amount of data and optimized sampling both provide sufficient information on the understanding of the system behavior and allow a precise estimation of parameters, which should be considered in Stage II. Now, the decision has to be made on the parameters to be estimated (i.e. kinetic or stoichiometric constants for the biological model).

The sensitivity analysis is necessary and uses the dynamic influent data and the parameters obtained in Stage III. The output variables again have to be selected upon the objectives of the modelling study or the availability and the quality of the data. For instance, if the effluent nitrate concentration is measured or the objective is the optimization of the effluent nitrate concentration, the sensitivity analysis of the parameters should be carried out with respect to effluent nitrate. In this way, one may conclude which parameters are more influential to the available effluent nitrate data. Then, the calibration of the model can be done by fine-tuning the parameters on the basis of fitting the model to dynamic data obtained from the measurement campaign. After the dynamic calibration, if the standard deviations are still quite high for the most sensitive parameters, additional lab experiments could be performed. In this respect, one should refer to Stage II and Stage III for the experimental study. The calibration can be performed manually or using the optimizer (or parameter estimation) module available in the various wastewater treatment plant simulators. The first approach is expert-knowledge driven and requires a sound insight into the system. Whereas the latter approach requires a priori information about model structure and quality of the available information obtained from the measurement campaign. In other words, it usually requires system identification (structural and/or practical) (Weijers and Vanrolleghem, 1997; Reichert and Vanrolleghem, 2001; Brun *et al.*, 2002) where the parameter sub-sets that can be estimated under available measurement campaign data are determined. From practical application point of view, this optimization approach is usually not preferred due to the over-parameterized nature of the ASM models with respect to availability of the dynamic data (Reichert and Vanrolleghem, 2001). It is therefore not surprising to see that almost all of the calibration studies dealing with ASMs are done manually.

Following the calibration of the AS model, a final evaluation should be performed within the context of the objectives to be reached. The success of the calibrated model should be judged. If it is found that the calibrated activated sludge model does not mimic the dynamic behavior of the system, solutions have to be investigated by re-evaluation of the plant data, the sub-models or even the targets defined in the first step. Additionally, it can be proposed that the existing model needs to be modified or that an alternative activated sludge model is used in the calibration.

1.5 Important Issues in Nutrient Removal Activated Sludge Modeling

In this section, effects of important issues in the modelling of carbon and nutrient removal systems were briefly discussed. These are mainly (i) the characteristics and operating parameters of activated sludge plants (ii) influent wastewater characteristics and (iii) principal processes associated in the structure of general activated sludge models.

1.5.1 General characteristics and operating parameters of activated sludge plants

Hydraulics: The hydraulics, type of reactor configurations are important factors and should be well-defined in order to mimic the real layout of the system. As an example, the plug-flow regime of a reactor influences the oxygen distribution along the channel and may trigger the denitrification by creating spatial anoxic zones along the reactor. In addition to that, the internal flow rate determination is of great importance since the nitrified recycle will carry oxygen and nitrate over the anaerobic and/or anoxic reactors which directly effects the total nitrogen and phosphate removal capacity of the system. The oxidation ditch can be a good example since the internal recycle rate in the channel is much higher than that of influent flowrate. Theoretically, if the internal recycle rate is changed, the travel time of mixed liquor from one aerator to another will be changed accordingly. So, the mixed liquor will be subjected more frequently to air on/off period if the internal recycle rate is increased. Practically, it means that the cycle-time (T_C) is decreased by increasing the internal recycle which causes considerable change in the nitrate in the reactor. Hence, additional measurements should be performed for the determination of internal recycles, influent flowrate and sludge feeding-wastage patterns and sampling points (De Clercq *et al.*, 1999).

Sludge Retention Time (SRT): The most difficult and crucial point in the modelling is the accurate determination of the actual total SRT. The total SRT -known as the most sensitive operating parameter- directly affects the solid balance on the system as well as the active biomass concentration (WERF, 1999). From a modelling point of view, a minor change (or error) in the SRT can be compensated by the endogenous decay rates (b_H) and/or yield coefficients (Y_H) to close the solids balance over the system. In addition, the reaction rates governed by Monod expressions are the result of active

biomass concentrations which are highly dependent on the SRT-value. The use of solid and total phosphate balance calculations over the system facilitate the estimation of the actual sludge age of the system. In reality, the activity of biomass is lowered because of elevated protozoan activity, the formation of inert materials *etc.* at higher sludge ages (van Loosdrecht and Henze, 1999).

Air (oxygen) Transfer: In activated sludge models, the oxygen transfer is expressed by the volumetric oxygen transfer coefficient K_{La} under process conditions (WEF, 1996). The oxygen oxygen concentration in a CSTR tank can be formulized as follows:

$$\frac{dS_O}{dt} = K_{La_f}(S_{O_{\infty f}} - S_O) - (OUR_{nitrifiers} + OUR_{heterotrophs}) \quad (1.3)$$

where K_{La_f} is the volumetric oxygen transfer coefficient under process condition; $S_{O_{\infty f}}$ is the oxygen saturation concentration under process condition, S_O is the actual oxygen concentration in the tank; OURs are the oxygen uptake rates for nitrification and heterotrophic biomass, respectively. The determination of oxygen (air) input into the system is an important issue since it switches on and off the nitrification, carbon oxidation and denitrification processes depending upon oxygen half saturation constants (K_O). Based on Monod expressions, the lower the K_O values, the higher the oxygen consumption rates.

Consequently, this can be taken advantage of to activate the simultaneous nutrient removal process with appropriate aeration control providing limited oxygen levels (Naidoo *et al.*, 2002; Ritmann and Langeland, 1985; Insel *et al.*, 2004; Munch *et al.*, 1996). From a modelling point of view, the effect of K_{La_f} on nutrient removal can be compensated by manipulating the oxygen half saturation constants for heterotrophs (K_O) and autotrophs (K_{OA}). The reaction rates can then be adjusted via reducing those parameters with an underestimated K_{La_f} . Hence, the K_{La_f} should be measured under process conditions. Measured (online/offline) oxygen data may be useful to estimate the magnitude of the process K_{La} . The power consumption and air flow rate give information to estimate the aeration intensity.

Sludge Settling: The performance and operation of final settling tanks is of great importance since (1) it can maintain a mass fraction of mixed liquor depending upon operating conditions (i.e. RAS, surface loading, retention time) (2) the effluent quality can be deteriorated by resuspension, bulking and rising of the sludge blanket and (3) additional nitrate removal due to denitrification can take place (Henze *et al.*, 1993) together with possible secondary phosphate release (Wouters-Wasiak *et al.*, 1996). The dynamics and contribution of final settling tanks to overall system efficiency should be well-defined and incorporated in the modelling task. On the other hand, primary settling tanks (PST) influence the distribution of particulate and soluble COD components prior to the biological reactor. However, depending upon retention time and sludge blanket in the PST, the hydrolysis and fermentation process can be activated. As a result, a probable increase in VFA potential can be observed due to heterotrophic activity.

Process control: Automatic control technologies have become fashionable tools to provide process stability for nutrient removal (i.e. Supervisory Control and Data Acquisition-SCADA systems). The aeration, return and internal cycles together with RAS, sludge wastages, chemical dosing *etc.* in continuous and batchwise systems became important controlled variables (actuators) for system optimization (Copp *et al.*, 2002; Olsson and Jeppsson, 1994). In that way, the control algorithms may alter the performance of the system by influencing the composition of the mixed liquor. As a result, for accurate modelling, it is essential to implement the control algorithms in the simulators.

1.5.2 Influent wastewater characteristics

Nutrient removal performance of activated sludge process depends upon the influent wastewater characterization in terms of biodegradable COD, COD/TKN and COD/TP ratios (Randall *et al.*, 1992). Practical experiences show that the removal of 1.0 mg NO₃-N and 1.0 mg PO₄-P requires 6.0 mg biodegradable-COD and 10 mg VFA-COD, respectively (Grady *et al.*, 1999). Hence, an accurate (model-based) influent wastewater characterization is a sensitive process in the modelling task since it directly influences the response of model output and importance of certain processes. In addition to that, model simplification could be an option if some components are not available in the

influent wastewater. For instance, there is no need to include the fermentation process if there is no influent fermentable COD available. Because, according to ASM models, the hydrolysis is the rate-limiting step for sewage treatment.

The conventional wastewater characterization is the determination of total/filtered COD, Total Kjeldahl Nitrogen (TKN), total phosphate (TP) and total suspended solids (TSS) *etc.* with the aid of Standard Methods (APHA, 1998). However, due to the increasing model complexity in parallel to vast biotechnological developments, more detailed model-based wastewater characterization is essential. In most studies, the conventional wastewater characterization is translated into the model input, which can be regarded as another sub-modelling process (see Figure 1.25). In this process, dedicated physical, analytical methods (i.e. STOWA procedure: Roeleveld and van Loosdrecht; 2002) together with widely accepted respirometric tests are used to determine the model inputs in terms of biodegradable/inert COD, nitrogen and phosphate fractionations and active biomass in the influent (Vanrolleghem *et al.*, 1999; Sperandio and Paul, 2000; Sollfrank and Gujer, 1991; Ekama *et al.*, 1986b). In the view of full-scale modelling, the influent wastewater and biomass characterization were widely reviewed by Petersen *et al.* (2003)

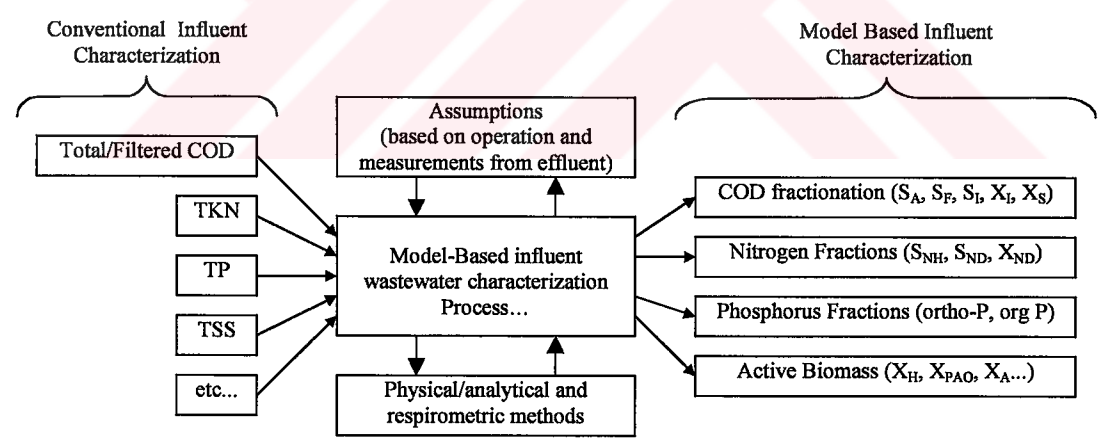


Figure 1.25 Influent wastewater characterization for activated sludge model

In Figure 1.26, an ASM2d based COD fractionation is given (Henze *et al.*, 1995c). Shortly, the biodegradable COD is composed of acetate (VFA) COD (S_A), fermentable COD (S_F) and slowly biodegradable COD, (X_S). The X_S is hydrolyzed to S_F under

anaerobic, anoxic and aerobic conditions. Then, the S_F is fermented to the acetate COD (S_A) via heterotrophic activity under anaerobic conditions.

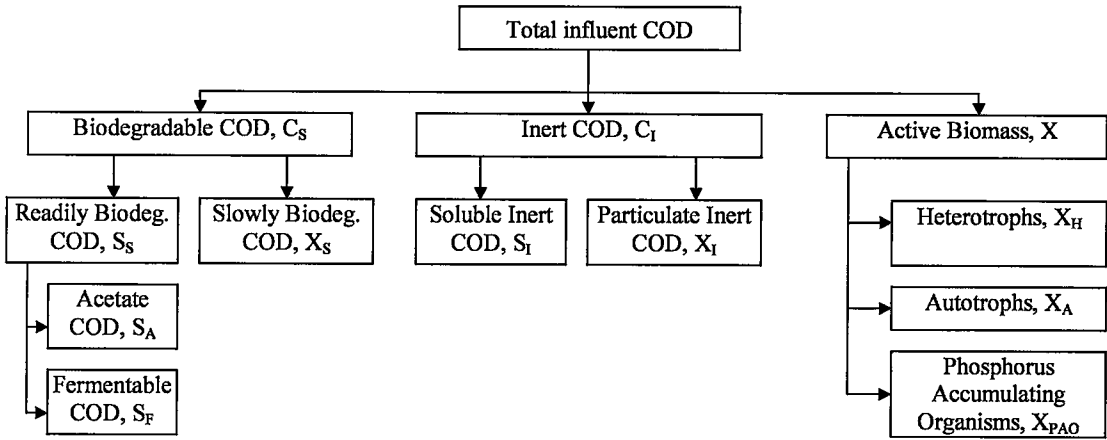


Figure 1.26 ASM2d based influent wastewater COD fractionation

With physical methods, the selection of filter pore size for the separation of soluble and particulate COD components is still in question since the colloidal organics are partially trapped or pass through the filter (Levine *et al.*, 1991). Currently, a pore size of 0.45 μm membrane filters is mostly used for the separation of soluble and particulate COD. On the other hand, short-term or long-term respirometric methods are utilized for the accurate estimation of readily and slowly biodegradable COD together with kinetic and stoichiometric model parameters (Figure 1.27). The details of those respirometric tests can be found in Chapter 2,3 and 4.

For model simplification, assumptions can also be made considering the operational mode of the activated sludge plant and plant effluent analyses. For instance, the rapidly hydrolyzable COD fraction (S_H) (Orhon *et al.*, 1999a) can be incorporated as part of the slowly biodegradable form (X_S) if the system is operated in extended aeration mode.

The active biomass fractions in influent wastewater are assumed to be negligible and they can be added to influent X_S according to Henze (1992). Alternatively, the heterotrophic biomass fraction in wastewater can be measured via long-term respirometric experiments applied to raw wastewater without any biomass inoculation (Sperandio and Paul, 2000).

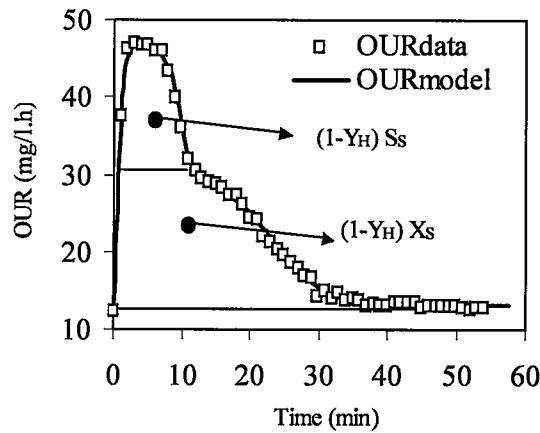


Figure 1.27 Estimation of biodegradable COD fractions from respirograms

The effluent soluble inert COD (S_I) is assumed to be equal to the influent inert soluble COD of the treatment plant if it is operated at an SRT at least higher than 3 days (Ekama *et al.*, 1986; Mamais *et al.*, 1993) disregarding the inert soluble microbial products (S_P) due to endogenous biomass activity (Orhon *et al.*, 1989). In a practical way, 90% of the effluent COD can be regarded as the inert influent soluble COD (Siegrist and Tschui, 1992) for domestic wastewater. The inert COD fractions can also be experimentally calculated via long-term COD measurements as described in Germirli *et al.* (1991). Another important issue is that the diurnal, weekly or seasonal changes in wastewater characteristics (load, water temperature, flow, rain and storm events etc.) should be considered if the actual performance of the system is to be evaluated (Metcalf and Eddy, 2003). Moreover, aside from modelling, the planning of sampling time and measurement frequency are of great importance in mimicking the actual behavior of the activated sludge plant (De Pauw *et al.*, 2004).

1.5.3 Main processes in activated sludge models

1.5.3.1 Nitrification

The nitrification takes place in two consecutive reactions. These are (1) the ammonia ($\text{NH}_4\text{-N}$) oxidation to nitrite ($\text{NO}_2\text{-N}$) by a group of bacteria known as *Nitrosomonas* and (2) nitrite ($\text{NO}_2\text{-N}$) oxidation to nitrate ($\text{NO}_3\text{-N}$) by another group of bacteria, *Nitrobacter*. Based on process stoichiometry, the oxidation of $\text{NH}_4\text{-N}$ to $\text{NO}_2\text{-N}$ requires

3.43 gO₂/gN₂ and the oxidation of NO₂-N to NO₃-N necessitates 1.14 gO₂/gN₂. To sum up, 4.57 gO₂/gN₂ is consumed for the complete oxidation of NH₄-N to NO₃-N (Metcalf and Eddy, 2003; Orhon and Artan, 1994). The oxygen utilization due to the two reaction can be expressed as:

$$OUR_{ex} = (3.43 - Y_{A1}) \cdot \frac{\mu_{maxA1} \cdot X_1}{Y_{A1}} \cdot \frac{S_{NH}(t)}{K_{N1} + S_{NH}(t)} + (1.14 - Y_{A2}) \cdot \frac{\mu_{maxA2} \cdot X_2}{Y_{A2}} \cdot \frac{S_{NO2}(t)}{K_{N2} + S_{NO2}(t)}$$

where Y_A is the autotrophic yield; μ_{maxA} is the maximum autotrophic growth rate; X indicates the active biomass concentration, K_N is the nitrogen half saturation constant for NH₄-N and NO₂-N. The indices '1' and '2' indicate the reactions pertaining to the activity of *Nitrosomonas* and *Nitrobacter*, respectively. An experimental respirogram obtained from a batch test initially fed with NH₄ is given in Figure 1.28. Basically, the first plateau represents the NH₄ oxidation to NO₂. The tailing of the second plateau indicates the end-point of NO₂ oxidation to NO₃ as a final step. However, it is sometimes difficult to observe the second plateau from the respirogram and the kinetics can often be simplified to a one step nitrification when NH₄ is directly oxidized to NO₃ (Petersen, 2000; Brouwer *et al.*, 1998). In the literature, high nitrite concentrations in the effluent have been reported to be due to possible inhibition of the second step because of environmental conditions (i.e. temperature, dissolved oxygen, pH).

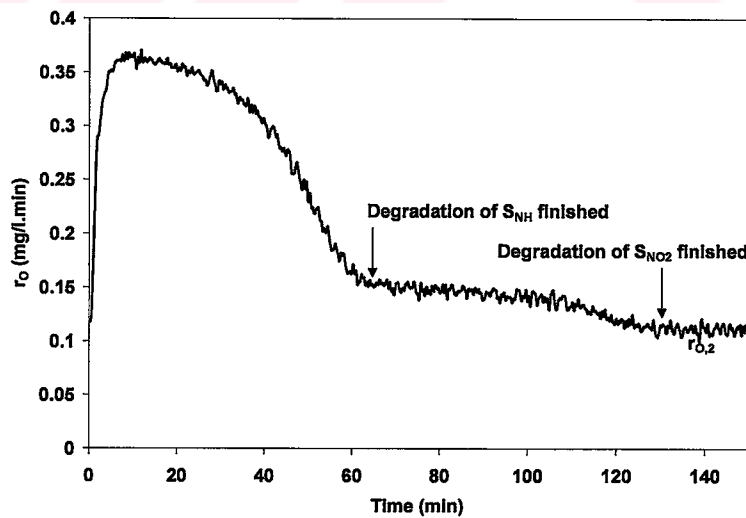


Figure 1.28 Respirometric batch test for nitrifiers (Petersen, 2000)

The nitrification kinetics are influenced by a number of environmental factors: dissolved oxygen concentration, temperature, pH, inhibitory substances (Orhon and Artan, 1994). Considering those environmental factors of substrate concentration (S_{NH}), dissolved oxygen concentration (S_O), temperature (T), the actual growth rate for the single step nitrification can be expressed with the equation given below at pH around 7-8.5.

$$\mu_A = \mu_{\max A_{20}} \cdot \theta_{20}^{(T-20)} \cdot \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_O}{K_{OA} + S_O} \quad (1.4)$$

The temperature is incorporated in the equation with an Arrhenius type equation and controls the maximum specific autotrophic growth rate (Orhon *et al.*, 2000). The oxygen dependency can be described by a dissolved oxygen (S_O) Monod expression where K_{OA} is the saturation constant for autotrophs, depending upon the diffusional limitations of S_O into floc matrix. It is important to note that nitrification is more susceptible to low S_O levels than the activity of heterotrophs. This is expressed with higher K_{OA} values. In addition, the nitrifying bacteria can be inhibited by many different substances especially from industrial discharges (i.e. Leather tanning, metal finishing, textile effluents) (Orhon *et al.*, 2000). The reaction rate constants for nitrifying bacteria are listed in Table 1.3 below (Henze *et al.*, 1995b).

Table 1.3 Reaction rate constants for nitrifying bacteria at 20 °C (Henze *et al.*, 1995b)

	Parameter	Unit	Quantity		
			<i>Nitrosomonas</i>	<i>Nitrobacter</i>	Overall Process
Maximum specific growth rate	$\mu_{\max A}$	d ⁻¹	0.6-0.8	0.6-1.0	0.6-0.8
Saturation contant for NH ₄	K_{NA}	gN/m ³	0.3-0.7	0.8-1.2	0.3-0.7
Oxygen half saturation contant	K_{OA}	gO ₂ /m ³	0.5-1.0	0.5-1.5	0.5-1.0
Maximum yield constant	$Y_{\max A}$	gVSS/gN*	0.10-0.12	0.05-0.07	0.15-0.20
Decay constant	b_A	d ⁻¹	0.03-0.06	0.03-0.06	0.03-0.06

*per gram NO₃ formed

1.5.3.2 Heterotrophic activity

Ordinary Heterotrophic Organisms (OHOs) and Phosphorus Accumulating Organisms (PAOs) are heterotrophic biomass. The OHOs are responsible for several biological reactions in the activated sludge process. These are mainly the anaerobic, anoxic and

aerobic hydrolysis, aerobic/anoxic growth, fermentation and decay processes which are of great importance in carbon and nutrient removal from wastewaters.

The hydrolysis mechanism describes the slow degradation of slowly biodegradable matter in such a way that larger molecules are converted to small, biodegradable forms prior to heterotrophic utilization (Sollfrank and Gujer, 1991; Orhon and Artan, 1994). The total COD of raw wastewater is constituted by more than 50% hydrolyzable COD (Henze, 1992); this can be regarded as an important organic carbon source for the design and upgrade of BNR type activated sludge systems with appropriate process applications (Hatziconstantinou *et al.*, 1996; Bannister and Pretorius, 1998). Literature studies reveal that the hydrolyzable COD fraction shows wide variation in the range of 15-70% for industrial wastewaters, as well (Orhon *et al.*, 2001; Rozzi *et al.*, 1999, Görgün *et al.*, 1995). Lishman and Murphy (1994) stated that the hydrolysis rate is the rate limiting step that would be appreciably slower than either death or synthesis on the basis of the ASM1 model. In this respect, the determination of the amount of slowly biodegradable COD fraction together with its degradation kinetics is important for process selection.

In most activated sludge models, the reaction kinetics for hydrolysis process are mostly expressed with a surface saturation type reaction (Contois type). The reaction rate is also proportional to the concentration of active heterotrophic biomass (X_H):

$$-\frac{dX_S}{dt} = \frac{dS_S}{dt} = k_h \frac{X_S / X_H}{K_X + X_S / X_H} X_H = k_h \frac{X_S}{K_X X_H + X_S} X_H \quad (1.5)$$

where

X_S : slowly biodegradable COD [mgCOD/l]

S_S : readily biodegradable COD [mgCOD/l]

k_h : maximum hydrolysis rate [d⁻¹]

K_X : half saturation hydrolysis constant [gCOD/gcellCOD].

The variation of the hydrolysis constants depending upon electron acceptor conditions are given in Table 1.4.

Table 1.4 Variations of the hydrolysis constants (Henze *et al.*, 1995b; Orhon *et al.*, 2002)

Electron Acceptor	Unit	Oxygen	Nitrate	Without oxygen/nitrate
Hydrolysis rate constants (dissolved), k_{hs}	day ⁻¹	3-20	1-15	2-20
Hydrolysis rate constants (suspended), k_{hx}	day ⁻¹	0.6-1.4	0.15-0.4	0.3-0.7
Hydrolysis half saturation constants (suspended), K_{xx}	gCOD/gcellCOD	0.01-0.05	0.01-0.05	0.01-0.05

Although the incorporation of reduction factors for anoxic and anaerobic conditions is considered to adjust the hydrolysis kinetics when modelling (Henze *et al.*, 1987; Henze and Mladenovski 1991; Goel *et al.*, 1997), some studies indicated that the hydrolysis process is an enzymatic reaction and thus, the electron acceptor conditions do not influence the reaction rates (Goel *et al.*, 1998; Mino *et al.*, 1995b; Gujer *et al.*, 1999).

Under anaerobic conditions, the slowly biodegradable COD is hydrolyzed to fermentable COD (S_F). Then, the S_F is fermented to volatile fatty acid (S_A) via heterotrophic activity by the first order reaction (Henze *et al.*, 1995a; Barker and Dold, 1997; Gujer *et al.*, 1999). In BNR plants, the anaerobic reactor prior to the anoxic/aerobic compartments is designed to promote EBPR. From a modelling point of view, the anaerobic hydrolysis reduction factor (η_{fe}) is one of the most sensitive and unknown parameters since it not only enables the use of biodegradable COD source (as fermentable and VFA-COD) for EBPR but also liberates the nitrogen and phosphate into the bulk liquid (Ekama and Wentzel, 1999). The reduction factors for anaerobic (η_{fe}) and anoxic (η_{HNO}) conditions are reported in the ranges of 0.1-1.0 and 0.3-1.0, respectively (Henze and Mladenovski 1991; Mino *et al.*, 1995b; Henze *et al.*, 2000; Sözen *et al.*, 1998). In the same way, an increase in the anoxic reduction factor can promote the denitrification under anoxic conditions, yielding higher denitrification removal if the slowly biodegradable COD source is available in the anoxic reactor. Hence, depending upon the operating conditions, the hydrolysis process may be crucial under all electron acceptor conditions in terms of biological nutrient and carbon removal.

Biological denitrification involves the oxidation of organic carbon using nitrate or nitrite as the final electron acceptor when oxygen is unavailable (Grady *et al.*, 1999; Orhon and

Artan, 1994). The organic carbon source can be (1) the readily biodegradable COD in raw wastewater (2) the readily biodegradable COD hydrolyzed from slowly biodegradable COD and/or (3) the endogenous biomass. Depending on the dissolved oxygen concentration (S_O) nitrate concentration (S_{NO}), the denitrification rate can be expressed as:

$$-\frac{dS_{NO3}}{dt} = \eta_g \cdot \mu_{\max H} \frac{S_S}{K_S + S_S} \frac{S_{NO}}{K_{NO} + S_{NO}} \frac{K_{OH}}{K_{OH} + S_O} X_H \quad (1.6)$$

where

$\mu_{\max H}$: maximum heterotrophic growth rate COD [d^{-1}]

K_S : half saturation constant [mg/l]

η_g : anoxic reduction factor for growth [-]

S_S : readily biodegradable COD (S_A and S_F) [mgCOD/l]

K_{NO} : nitrate half saturation constant [gNO₃-N/l]

K_{OH} : oxygen half saturation constant [gO₂/l]

According to this equation, the inhibition term of oxygen limits denitrification. On the other hand, the denitrification is controlled by a nitrate Monod function. If the nitrification process is maintained with reduced oxygen transfer, the Simultaneous Nitrification and Denitrification (SND) process (Rittmann and Langeland, 1985; Pochana and Keller, 1999; Munch *et al.*, 1996; Bertanza, 1997) can be activated depending upon the reference K_O value. The K_O value is reported to be a plant specific parameter and falls in the range of 0.1-0.2 mgO₂/l (Barker and Dold, 1997). The SND process was reported for full-scale oxidation ditches (Cinar *et al.*, 1998; Grady *et al.*, 1999; Rittmann and Langeland, 1985) and SBR systems (Munch *et al.*, 1996; Insel *et al.*, 2004) based on modelling and observation of high total nitrogen removal up to 95%.

The SBR studies of Oh and Silverstein (1999) revealed that 0.09 mgO₂/l was found to significantly inhibit the denitrification. The denitrification efficiency was reduced by 85% when the mixed liquor S_O was around 2.0 mgO₂/l.

The denitrifying heterotrophs and phosphorus accumulating organisms (PAOs) compete for VFA (S_A) utilization in the availability of nitrate. The substrate (VFA) utilization for denitrification can be accelerated by increasing the heterotrophic growth rate under anoxic conditions, $\eta_g \cdot \mu_{Hmax}$. On the other hand, EBPR can be promoted by elevating the maximum acetate storage rate of X_{PAOs} , q_{PHA} to give the advantage of VFA uptake to X_{PAOs} . As a result, the VFA will be taken up by the X_{PAOs} for further phosphate uptake under anoxic or aerobic conditions (Henze *et al.*, 2000; Barker and Dold, 1997; Kuba *et al.*, 1993). In addition to that, reduced dissolved oxygen levels may activate nitrification, denitrification and biological phosphorus removal reactions and finally result in simultaneous nutrient removal (Daigger and Littleton, 2000) in a single bioreactor. In this respect, the simultaneous VFA uptake, nitrification and denitrification together with EBPR requires model-based evaluation in order to understand the complex process kinetics and the interaction of those processes under dynamic operating conditions (i.e. aeration, temperature).

2 IDENTIFICATION AND MODELLING OF AEROBIC HYDROLYSIS- APPLICATION OF OPTIMAL EXPERIMENTAL DESIGN

2.1 Introduction

Hydrolysis is an important process which initiates the degradation of slowly biodegradable substrate in wastewaters. This process is an integral part of activated sludge models for the kinetic description of the utilization of the slowly biodegradable substrate. It is, by nature, defined as a process slower than heterotrophic growth and this way, it usually becomes the rate-limiting step for the biodegradation of organic carbon. The slowly biodegradable fraction, X_S , represents the bulk of the biodegradable substrate in the majority of wastewaters (Henze, 1992). As a relatively slow process, hydrolysis is generally the decisive step for the quality of the biological effluent. This statement is especially true for industrial wastewaters with more complex substrate compositions (Orhon *et al.*, 2002; Rozzi *et al.*, 1999). Hydrolysis also plays a dominant role in the delicate balance of electron donor/electron acceptor ratio in BNR and EBPR systems (Bannister *et al.*, 1998; Moser-Engeler *et al.*, 1998; Hatziconstantinou *et al.*, 1996). Appropriate design, control and upgrade of wastewater treatment plants therefore necessitates an accurate and rapid information gathering on the degradation kinetics and quantity of substrate available.

The quantity and kinetic information for substrate present in the wastewater can rapidly be collected by lab-scale batch tests with an appropriate mixture of wastewater and biomass (Sözen *et al.*, 1998; Spanjers and Vanrolleghem, 1995; Chudoba *et al.*, 1992; Ekama *et al.*, 1986b). In the literature, many batch and semi-continuous respirometric methods have been proposed together with alternative hydrolysis rate equations (Spanjers and Vanrolleghem, 1995; Chudoba *et al.*, 1992; Sperandio and Paul, 2000;

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Kappeler and Gujer, 1992; Dold *et al.*, 1980; Ekama and Marais, 1979) but still difficulties remain with respect to the appropriate modelling concept. The difficulties for the accurate and representative characterization of wastewater and biomass are not only based upon the modelling pitfalls but also upon the microbiological aspects. From the modelling point of view, the accurate identifiability of hydrolysis kinetics depends on the complexity and structure of the model and on the experimental conditions. A large number of parameters led the activated sludge models difficult to identify and may result in parameter correlation leading to significant uncertainties in the model. One solution is to assume that some of the parameters -difficult to determine from the experiment- have to be fixed to default values. The assessed bio-kinetic parameters can be used as default values, which favor the estimation of the remaining unknown model parameters (Brouwer *et al.*, 1998). The second solution is to break up the complete model into sub-models. However, the batch experiments designed for sub-model identification must be sufficiently informative for the parameter subsets under study. The information content of the experiment and improvement in the accuracy of the estimation of model parameters can be evaluated with the application of Optimal Experimental Design methodology (Dochain and Vanrolleghem, 2001; Vanrolleghem *et al.*, 1995).

In batch tests, the initial substrate to biomass, S_0/X_0 ratio plays a crucial role for the accurate assessment of the parameters related to microbiological and modelling aspects. If the ratio of S_0/X_0 is very large, significant changes can occur in the culture during the assay, resulting in parameters that are not reflective of the culture as it existed in the environment from which it was removed (Chudoba *et al.*, 1992). From a microbiological point of view, the adaptation period and response of mixed culture population can be observed during the sequential addition of substrate in kinetic batch tests (Vanrolleghem *et al.*, 1998). The nature of the kinetic experiments is important because some of them may alter the history of the activated sludge culture and cause biased characterization of biomass (Grady *et al.*, 1996; Novak *et al.*, 1994; Chudoba *et al.*, 1992). The reason is that activated sludge is composed of a population of microorganisms that each interact differently to biodegradable components. Through competition, the sludge composition may alter and therefore the history of the experiment is important. In the literature, different substrates are classified according to their different degradation rates and

accordingly, the biodegradation kinetics of slowly biodegradable substrate in activated sludge systems is represented by the hydrolysis mechanism. In activated sludge models, the hydrolysis mechanism is commonly described by means of a surface-saturation-type of reaction. This equation can be expressed as:

$$k_h \frac{X_S / X_H}{K_X + X_S / X_H} X_H \quad \text{or} \quad k_h \frac{X_S}{K_X X_H + X_S} X_H \quad (2.1)$$

where, k_h : maximum hydrolysis rate [d^{-1}]

K_X : half saturation constant for hydrolysis [$mgCOD \cdot mgCOD^{-1}$]

X_S : slowly biodegradable COD [$mgCOD \cdot dm^{-3}$]

X_H : heterotrophic active biomass [$mgCOD \cdot dm^{-3}$]

In this approach, the rate of hydrolysis depends upon the magnitude of two kinetic coefficients, namely, the maximum hydrolysis rate, k_h , and the half saturation constant for hydrolysis, K_X . Numerical values of these coefficients are wastewater specific and exhibit a significant variation, especially for industrial wastewaters (Orhon *et al.*, 2001; Germirli Babuna *et al.*, 1998). The generally adopted procedure for the experimental assessment of k_h and K_X under aerobic conditions involves model evaluation and curve fitting of respirograms. There is extensive data presented in the literature based on this procedure, for different wastewaters. A careful evaluation of the procedure reveals that it is more likely to generate, not a single set, but a relatively large number of different coefficient pairs equally applicable to the experimental data. The calibration of the model can be ended up successfully even using a domain of parameter values to be estimated.

In this context, the scope of the study was first to define a systematic approach for the determination of the most appropriate coefficients that can be extracted from respirograms within the framework of surface saturation-type of hydrolysis kinetics. In the second step, the proposed approach was experimentally tested on textile effluent, a typical wastewater with a significant slowly biodegradable substrate fraction. It also covered the accurate estimation of the hydrolysis coefficients for two different initial experimental conditions. This step also included the comparative evaluation of the information content of the experiments through the Fisher Information Matrix (FIM) for the two runs.

2.2 Materials and Methods

2.2.1 Model and wastewater selection

Multi-component activated sludge models (Gujer *et al.*, 1999; Henze *et al.*, 1995a; Novak *et al.*, 1995; Orhon and Artan, 1994; Henze *et al.*, 1987) are becoming more popular, since the degradation kinetics and fate of different substrates can be easily interpreted by means of experimental observations and modelling studies. In this study, commonly used surface-saturation-type hydrolysis mechanism was investigated for an industrial wastewater. Textile wastewater was selected as a case study since it contains high amounts of slowly biodegradable substrate (Rozzi *et al.*, 1999; Germirli Babuna *et al.*, 1998; Ubay Çokgör *et al.*, 1998). This feature is advantageous for the characterization of the kinetics of slowly biodegradable substrate in the framework of selected simple model presented in Table 2.1.

Table 2.1. Matrix representation of activated sludge model

Parameters Process	S _S	X _S	X _H	S _O	Rate
Growth	-1/Y _H		1	-(1-Y _H)/Y _H	$\hat{\mu}_H \frac{S_S}{K_S + S_S} X_H$
Hydrolysis	+1	-1			$k_h \frac{X_S / X_H}{K_X + X_S / X_H} X_H$
Decay			-1	(1-f _E)	b _H X _H
Parameter, ML ⁻³	COD	COD	Cell COD	O ₂	

defaults: Y_H=0.67 [cellCOD.COD⁻¹]; b_H=0.19 day⁻¹

The state and parameter vectors of the selected model shown in Table 1 where $\tilde{S}=[S_O, S_S, X_S, X_H]$ and $\tilde{p}=[k_h, K_X, \hat{\mu}_H, K_S, Y_H, f_E]$ respectively. The heterotrophic yield coefficient, Y_H was assumed to be known and the inert fraction of endogenous biomass, f_E was accepted as 0.2 in all similar activated sludge models. The endogenous decay rate, b_H was determined with the method proposed by Ekama *et al.* (1986).

2.2.2 Theoretical identifiability

The investigation of identifiable parameters of a selected model has an important role in view of reliable unique parameter estimations. There are few available methods are applicable to non-linear models to derive identifiable parameter subsets (Walter and

Pronzato, 1995; Godfrey and DiStefano, 1985; Walter, 1992; Pohjanpalo, 1978). Since the application to non-linear model is relatively simpler than the other methods, the Taylor Series Expansion method was used here to study the theoretical identifiability (Pohjanpalo, 1978). This method was applied to activated sludge models by other researchers, too (Gernaey *et al.*, 2002; Petersen *et al.*, 2001a; Dochain *et al.*, 1995). The Maple V (Waterloo) software package was used for the Taylor series expansion of the hydrolysis model.

The model was investigated through two different modelling approaches together with the Taylor series expansion. In the first approach, no growth of X_H was assumed during the experimentation time. The expansion of the hydrolysis model showed that the parameter subsets for the growth and the hydrolysis processes can be estimated simultaneously under the assumption that no X_H change took place. For this case, 6 parameter subsets can be derived from the respirogram (Table 2.2, column [1] and [3]). In the second approach, the growth of X_H equation was additionally included in the series expansion (see Equation 2.2). Thus, the maximum hydrolysis constant, k_h could be separated from the parameter subsets (Table 2.2, column 4). However, a *pseudo steady state approximation* (Dochain and Vanrolleghem, 2001) for the growth process was made since it became too complex for Maple V to solve the growth and hydrolysis processes together. The change in the S_S concentration was assumed to be zero as shown in equation 2.3. According to the model, the growth process is limited by the hydrolysis rate. It should be noted here that the parameters for the growth and the hydrolysis could not be found simultaneously, because the solution of the series expansion became too complex to solve as mentioned above.

$$\frac{dX_H}{dt} = \hat{\mu}_H \frac{S_S}{K_S + S_S} X_H \quad (2.2)$$

$$\frac{dS_S}{dt} = 0 \text{ where } 0 < t < t_{\text{end}} \quad (2.3)$$

According to the Taylor series expansion method, two different parameter subsets can be found for the hydrolysis kinetics depending on whether the biomass growth during the

experiment is considered or not. The identifiable parameter subsets that can be found by parameter estimation are listed in Table 2.2. This means that the parameter combinations give unique values, but the individual parameters of that combination can vary as long as the value of the combination is maintained. As a result, the hydrolyzable COD fraction, X_{S0} , the maximum hydrolysis rate, k_h , the half saturation constant for hydrolysis, K_X , the initial active heterotrophic biomass, X_{H0} are found to be structurally identifiable if the heterotrophic yield coefficient, Y_H is known.

Table 2.2 Identifiable parameter combinations for hydrolysis model

Growth Kinetics (Dochain <i>et al.</i> , 1995)		Hydrolysis Kinetics (This Study)	
No biomass growth	Biomass growth	No biomass growth	Biomass growth*
[1]	[2]	[3]	[4]
$(1-Y_H) \frac{\hat{\mu}_H X_{H0}}{Y_H}$	$(1-Y_H) \frac{X_{H0}}{Y_H}$	$(1-Y_H) k_h X_{H0}$	$(1-Y_H) X_{H0}$
$(1-Y_H) S_{S0}$	$(1-Y_H) S_{S0}$	$(1-Y_H) K_X X_{H0}$	$(1-Y_H) K_X X_{H0}$
$(1-Y_H) K_S$	$(1-Y_H) K_S$	$(1-Y_H) X_{S0}$	$(1-Y_H) X_{S0}$
-	$\hat{\mu}_H$	-	k_h

* based on the pseudo steady state approximation

2.2.3 Practical identifiability

In a theoretical identifiability study the data, in this case OUR data are assumed to be noise-free. In reality, however, this situation is not practically achievable due to the lack of precision of equipment and environmental conditions (Vanrolleghem *et al.*, 1995). Moreover, problems such as finding highly correlated parameters may arise if insufficient and/or highly noise corrupted data are collected from real lab-experiments. For instance, the Monod type growth model is a good example when the maximum heterotrophic growth rate, $\hat{\mu}_H$ and the half saturation constant for growth, K_S are found to be highly correlated if the experiments are poorly designed (Petersen, 2000). The information content of the experiments can be augmented either by setting better initial conditions or applying different experimental techniques (e.g. fed batch operation, multiple additions of substrate) which makes the experiment much more informative for reliable and accurate parameter estimation (Vanrolleghem *et al.*, 1995; Gernaey *et al.*, 2002; Holmberg, 1982; Petersen, 2000; Versyck and van Impe, 2000; Munack, 1989;

Vialas *et al.*, 1986). In addition, the mathematical techniques used for the estimation of the model parameters may have numerical problems such as slow convergence to the solution or getting stuck in a local minimum (Dochain *et al.*, 1995). Fisher Information Matrix (FIM) is regarded as a corner stone of optimum experiment design (OED) methodology (Vanrolleghem *et al.*, 1995). In general, the FIM summarizes the sensitivity functions for output variables and measurement errors with respect to quantification especially the shape of the joint confidence regions of parameters (Munack, 1989; Vialas *et al.*, 1986). The FIM can be expressed as the formula given below:

$$\text{FIM} = \sum_{i=1}^N Y(t_i, p)^T Q_i Y(t_i, p) \quad (2.4)$$

where $Y(t_i, p)$ is the output sensitivity function with respect to the parameters. The weighting matrix, Q_i is typically the inverse of the measurement error covariance matrix. There are several scalar functions that can be derived from the FIM in order to compare the information content of the experiments which have, for instance, different initial conditions. Within the scope of this study, two of these scalar functions will be examined. The first one is the D-Criterion which is calculated as the determinant of the FIM known to be inversely proportional to the volume of confidence region: the higher the value of determinant, the smaller the confidence region. The second one is the Mod-E criterion that deals with the shape of the confidence region. It corresponds to the condition number of the FIM. The condition number is the ratio of the largest eigenvalue over the smallest eigenvalue. If the minimum eigenvalue of FIM is found to be zero, the information content of the experiment becomes zero. This is for instance, when there is a strong dependency or high correlation between the estimated parameters. This brings the condition number to approach infinity. WEST software package was used for the simulation and calculation of the sensitivity trajectories for the estimated parameters.

2.2.4 Experimental setup

In this study, textile wastewater was sampled from a textile mill with a COD value of 1200 mg/l. Biomass was acclimated to the textile wastewater before conducting the respirometric batch experiments. Two different batch experiments were carried out

under different initial conditions with different dilutions and S_0/X_0 ratios as proposed by Ekama *et al.* (1986b). A nitrification inhibitor (Formula 2533TM, Hach Company) was added to suppress the oxygen utilization due to nitrification. The S_0/X_0 ratio was adjusted to 0.16 and 0.09 gCOD·gVSS⁻¹ for the first and second experiments, respectively.

Table 2.3 Initial conditions for Experiments 1 and 2

Initials	Unit	Experiment 1	Experiment 2
S_0/X_0 ratio	gCOD·mg dm ⁻³ VSS ⁻¹	0.16	0.09
Total Biomass, X_{MLVSS}	mgVSS·dm ⁻³	1530	1400
Total Volume, V_T	dm ³	2.700	2.230
Wastewater Volume, V_{ww}	dm ³	0.500	0.230

The oxygen uptake data was measured with a Manotherm RA-1000 continuous type respirometer with a sampling rate of sample per minute (Spanjers, 1993). COD and Mixed Liquor Volatile Suspended Solid (MLVSS) measurements were carried out according to the Standard Methods (APHA, 1998). The initial conditions of the experiments are summarized in Table 2.3.

2.3 Results and Discussion

2.3.1 Parameter estimation and sensitivity analysis

Parameter estimation study using the OUR profiles was carried out for the initial values of the following state variables: the initial readily biodegradable COD, S_{S0} , slowly hydrolysable COD, X_{S0} and the initial active heterotrophic biomass, X_{H0} and kinetic parameters: the maximum hydrolysis rate, k_h , the half saturation for hydrolysis, K_X , the maximum heterotrophic growth rate, $\hat{\mu}_H$ and the half saturation constant for heterotrophic growth, K_S . In order to test model validity, the parameter estimation study was conducted in two stages. In the first stage, the parameter estimation was carried out for the experiments individually. However, in the second step, multi-experimental fit (Dochain and Vanrolleghem, 2001) was applied using two sets of OUR data.

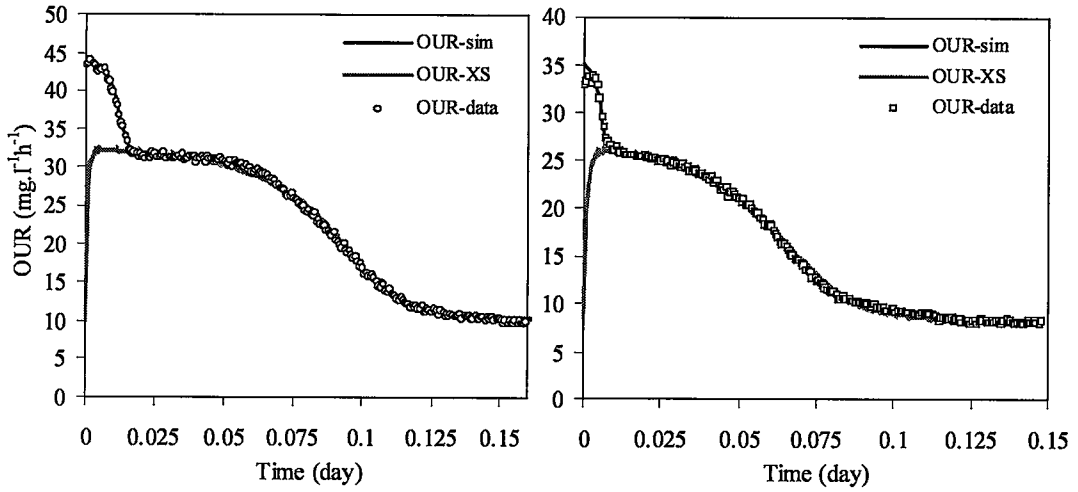


Figure 2.1 Simulated and measured OUR values for Experiment 1 (left), Experiment 2 (right)

As illustrated in Figure 2.1 by the simulated OUR profile that correspond to the slowly biodegradable COD, the period in which the hydrolysis process is rate limiting is clearly observed. As can be seen in Figure 2.1, the degradation of the readily biodegradable COD, S_S was terminated after 0.02 and 0.01 days for Experiment 1 and 2, respectively. Evidently, the first OUR experiment started with a much higher initial S_0/X_0 ratio (0.16) reached the endogenous level later than Experiment 2.

According to the results, the individual and the multi-experimental estimations give nearly identical results exerting nice simulated fits on the experimental respirograms. It can be concluded from Table 2.4 and Table 2.5 that the relative error for K_S has comparably higher values than that of the other parameters (Vanrolleghem *et al.*, 1995; Holmberg, 1982). The error contribution of each estimated parameters were also checked by the eigenvalue decomposition of the covariance matrix. The most uncertainties pertaining to the parameters of K_S , K_X and $\hat{\mu}_H$ are found to be important (results not shown). For the first experiment, the sensitivity analysis was carried out using the absolute-relative sensitivity function. This function measures the absolute change in OUR for a 100 % change in the parameter.

Table 2.4 Estimated initial state variables and parameters and deduced sludge and wastewater characteristics

Parameter	Experiment 1		Experiment 2	
	Value	STD*	Value	STD*
$\hat{\mu}_H$ (day ⁻¹)	1.088	0.015	1.081	0.027
K_S (mgCOD·dm ⁻³)	0.46	0.08	0.65	0.11
k_h (day ⁻¹)	1.140	0.005	1.146	0.009
K_x (COD·cellCOD ⁻¹)	0.0102	0.0003	0.0107	0.0004
S_{sini} (mgCOD·dm ⁻³)	9.84	0.13	5.00	0.09
X_{sini} (mgCOD·dm ⁻³)	137.01	0.31	77.20	0.26
X_{Ha} (mgcellCOD·dm ⁻³)	1585	3.7	1367	4.6
S_{Sww} (mgCOD·dm ⁻³)**	53		49	
X_{Sww} (mgCOD·dm ⁻³)**	740		748	
C_{Sww} (mgCOD·dm ⁻³)**	793		797	
X_T (VSS)-Experimental	1530		1400	
X_{Ha}/X_T (cell-COD)	0.72		0.69	

*Standard Deviation, **Concentration in wastewater

The sensitivity trajectories for the estimated parameters are illustrated in Figure 2.1. The sensitivity trajectories for the growth process (Figure 2.1-left) show that the effects of $\hat{\mu}_H$, K_S and S_{S0} are negligible after the first plateau (Compare Figure 2.1-right). The excitation of the sensitivities are confined in the first OUR plateau. Figure 2.2 reveals that the shapes of the sensitivity trajectories obtained for $\hat{\mu}_H$ and K_S are quite similar but follow opposite directions with time. Since the magnitude of the sensitivity for K_S is lower than that of $\hat{\mu}_H$, the uncertainty pertaining to K_S is higher.

This conclusion can also be derived from the parameter estimation results. As discussed above, the relative standard deviation is calculated to be around 16 % for K_S , which is approximately 10 times larger than for the other parameters. However, the situation is different for the hydrolysis process. The parameters of k_h , K_X and X_{S0} have influences on the OUR profile during the complete experimentation time. The sensitivity of k_h shows that the effect of this parameter reaches its maximum during the transition between OUR plateaus (the first and second drops in OUR).

The sensitivity trajectory for S_{S0} is only visible during the first plateau. As expected, after the first plateau the sensitivity of S_{S0} is zero since hydrolysis process is then the rate limiting step according to the simulation. However, the sensitivity profile of the initial slowly biodegradable COD component, X_{S0} , is active until the endogenous level is

reached. Maximum sensitivities for X_{S0} were obtained when the OUR was between the hydrolysis and the endogenous levels, indicating that this provides important information on this parameter.

Table 2.5 Estimated initial states and parameters (multi-experimental fit)

Parameter	Multi Experimental Fit	
	Value	STD*
$\hat{\mu}_H$ (day ⁻¹)	1.104	0.011
K_S (mgCOD·dm ⁻³)	0.509	0.049
k_h (day ⁻¹)	1.168	0.011
K_x (COD·cellCOD ⁻¹)	0.0106	0.0002
S_{sini1} (mgCOD·dm ⁻³)	9.97	0.117
S_{sini2} (mgCOD·dm ⁻³)	4.55	0.15
X_{sini1} (mgCOD·dm ⁻³)	139.73	0.59
X_{sini2} (mgCOD·dm ⁻³)	76.39	0.38
X_{Ha1} (mgCOD·dm ⁻³)	1571	8
X_{Ha2} (mgCOD·dm ⁻³)	1317	8

* Standard Deviation, indice 1 and 2 is attributed to experiment number

The sensitivity trajectories presumably look similar for K_X and k_h possibly leading to a correlation between these parameters. Indeed, an increase in one parameter can be compensated by the increase in the other parameter. The contour plots of the sum of squared errors (SSE) with respect to the different parameters exert a valley-like shape of the confidence region illustrating the extent of this correlation (Figure 2.3). The larger sensitivity for the slowly biodegradable COD fraction, X_{S0} is located between the second and the third OUR plateau (compare Figure 2.1-left). This period contains much more information for the estimation of the X_{S0} fraction.

However, it should be noted here that some difficulties may arise for the accurate estimation of this fraction if the hydrolysis plateau cannot easily be distinguished from the endogenous level. This situation is quite common, especially for respirometric measurements carried out for domestic wastewater under low initial S_0/X_0 (substrate/biomass) ratios (Ekama *et al.*, 1986b; Brouwer *et al.*, 1998; Orhon *et al.*, 2002).

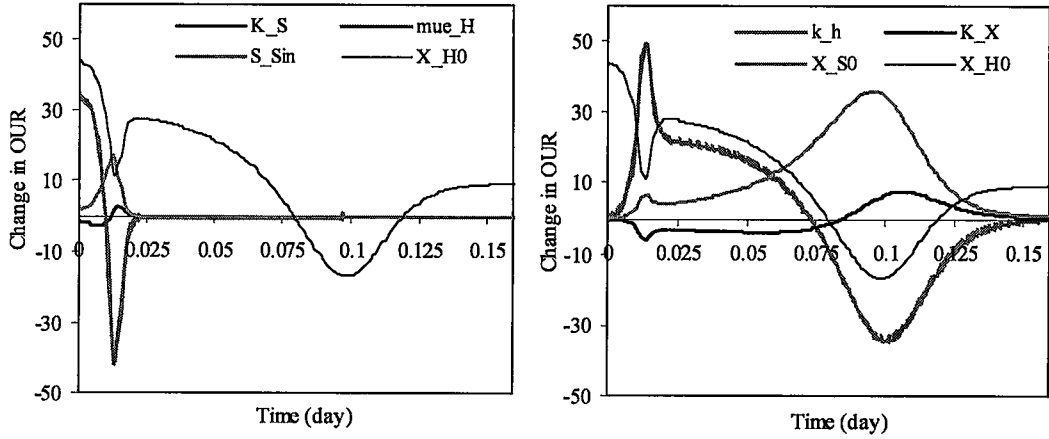


Figure 2.2 Absolute-Relative (AR) sensitivity trajectories of the parameters for Growth (left) Hydrolysis (right) (Experiment 1)

Therefore, the initial experimental condition should be optimized in order to gain more information both on the X_{S0} fraction and the kinetic constants *via* optimal experimental design (OED) techniques (Vanrolleghem *et al.*, 1995). As expected, the parameters for the hydrolysis kinetics are not effective during the endogenous level and at the beginning ($t = 0$) of the OUR experiment because the sensitivities are almost zero.

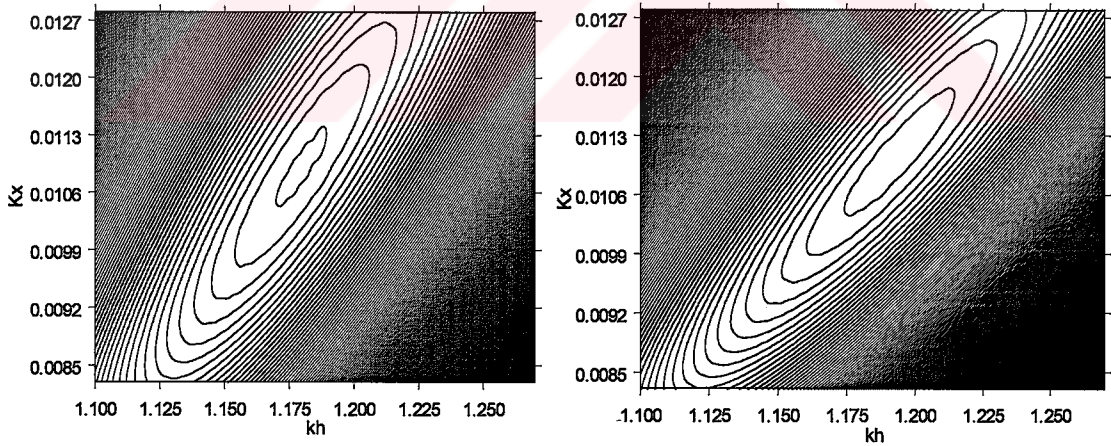


Figure 2.3 SSE contour plots for k_h and K_X experiment 1 (left) experiment 2 (right)

The contours of the sum of squared errors (SSE) concerning the hydrolysis constants, k_h , K_X and the initial heterotrophic active biomass, X_{H0} are plotted two by two against each other as illustrated in Figure 2.3 in two coordinate system. These figures give

information about the uncertainties of the parameters relative to each other. For instance, it can be concluded from Figure 3 that the estimation of X_{H0} is much more accurate than that of K_X . The optimum values of the parameters (i.e. their estimates) are located in the middle of the inner circle. From a modelling point of view, the parameter ranges are also quite small both for X_{H0} and K_X . However, the shape of the confidence region is valley-like. On the contrary, the k_h and K_X parameters are inversely proportional to each other according to Figure 2.4. The shapes of the contour plots are circle-like which is a desirable situation for accurate parameter estimation. Still note that, one should consider the overall effect of the estimated parameters in a multi-dimensional vector space (with dimension = number of parameter).

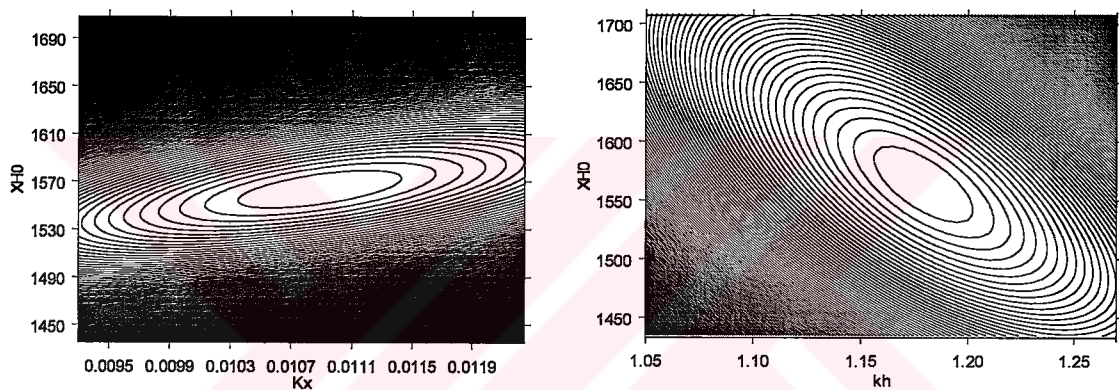


Figure 2.4 SSE contour plots for K_X and X_{H0} (left) k_h and X_{H0} (right) for Experiment 1

2.3.2 Optimal Experimental Design (OED) concept

In this section, two experimental runs are evaluated on the basis of the OED concept using the scalar functions of the Fisher Information Matrix (FIM). For these batch experiments, only the initial biomass concentration in the reactor is considered as a degree of freedom. However, absolute value of this component cannot be determined without calibration. Still, the added mixed liquor and the calibrated active biomass are proportional. In this respect, the effect of different initial active heterotrophic biomass concentrations on the information contents can be evaluated by means of the D-criterion and the Modified-E criterion (Figure 2.5). According to the D-criterion, the volume of the multi-dimensional confidence ellipsoid is getting smaller by increasing the initial active biomass, X_{H0} as illustrated in Figure 2.5. However, the shape of the confidence ellipsoids becomes more elongated with the X_{H0}

increase. In other words, by lowering the S_0/X_0 ratio, the parameters can be estimated more accurately, but they become more correlated.

It should be stressed here that the first OUR plateau which is important for the growth kinetics ($\hat{\mu}_H$, K_S , X_{H0}) can be non-informative due to the sudden (too short) peak in the first plateau under very low S_0/X_0 ratios (Brouwer *et al.*, 1998; Vanrolleghem and Verstraete, 1993). The multi-experimental fits can be suggested for the experiments performed under high and low S_0/X_0 ratios for accurate and unbiased estimation of the parameters for growth and hydrolysis kinetics. Because, a shift in the value of one parameter may inevitably influences the values of the other parameters. On the other hand, the confidence regions only for k_h and K_X were found to be comparably smaller and elongated for lower S_0/X_0 ratios (Insel *et al.*, 2002). If these two experiments are compared with respect to their information contents, as it can be seen from Figure 5 that the first experiment contains comparably more information than the second one.

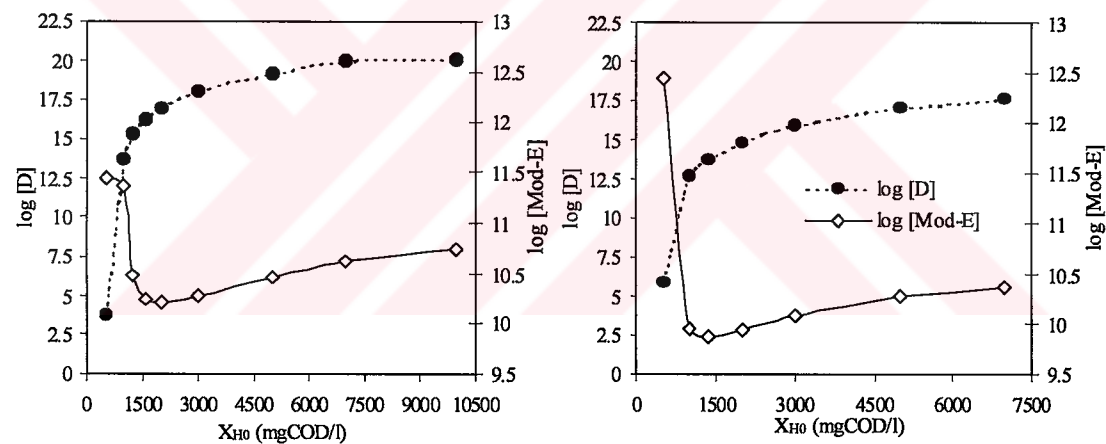


Figure 2.5 Information content of experiments, experiment 1 (left) experiment 2 (right)

The new method proposed in this thesis is shown to allow accurate estimation of kinetic constants for surface saturation type hydrolysis kinetics. According to the proposed method, besides readily and slowly biodegradable COD fractions, the kinetic constants for hydrolysis can be estimated from a batch respirogram. Accurate estimation of parameters can be provided by the application of Optimal Experimental Design (OED) techniques. Since the optimal initial conditions of the experiment are dependent on the parameter values and wastewater type, experimental design should be applied for each case. Generalized conclusions on parameter values may lead to erroneous and biased

parameter estimation of hydrolysis parameters. Therefore, for each case hydrolysis parameters should be estimated.

Evaluation of two sets of parallel experiments carried out at markedly different initial ratios of wastewater and sludge provides a refinement to the procedure, without providing however a definitive solution to the problem. It is therefore essential to define an experimental evaluation system that would enable identification of the most appropriate set of coefficients associated with the hydrolysis kinetics.

2.4 Conclusions

The proposed method allows to estimate the kinetic constants and initial states of the surface saturation type hydrolysis model. The information content of the experiment can be improved by starting the respirometric experiment under low S_0/X_0 ratio. Although the confidence region gets smaller by adjusting the initial conditions to low S_0/X_0 ratio, the parameter correlations become greater with the increase of initial heterotrophic biomass concentration.

Accurate estimation and model validation can be performed using the multi-experimental fit approach. It also provides a solution for the correlated parameters and high standard deviations known as common problems for the parameter estimation from batch experiments. As a result, the initial conditions of the experiments should be well defined depending upon the selected model.

The parameters of the growth and the hydrolysis processes can be estimated quite easily from the batch respirogram if two plateaus are observable. However, the hydrolysis parameters and the concentration of the initial slowly biodegradable COD fraction can only be estimated with the aid of the second plateau and the endogenous OUR levels. In this study, as an example a textile wastewater was tested and for this wastewater, the growth, hydrolysis and endogenous phases can easily be distinguished from each other.

3 IMPORTANT LIMITATIONS IN THE MODELING OF ACTIVATED SLUDGE BIASED CALIBRATION OF THE HYDROLYSIS PROCESS

3.1 Introduction

Recent developments on the modeling of activated sludge may be regarded as one of the most significant achievements in environmental science and technology today. They provided a giant improvement in the mechanistic understanding of activated sludge. With the support of a few pioneering scientific studies (Dold *et al.*, 1980; Ekama and Marais, 1979; van Haandel *et al.*, 1981), the introduction of ASM1 brought about a complete revision in the concept of traditional modeling (Henze *et al.*, 1987). It was soon modified for endogenous decay and generation of residual metabolic products, a concept quite significant for the biological treatment of industrial wastewaters (Orhon and Artan, 1994). ASM1 was expanded into ASM2 and ASM2d to cover enhanced biological phosphorus removal (Henze *et al.*, 1995a; 1999). Recently ASM3 was proposed, advocating biochemical storage as the primary mechanism of substrate utilization for organic carbon and nitrogen removal (Gujer *et al.*, 2000).

This rapid improvement however, increased the structural complexity of the models, because it is achieved by introducing new concepts that translated as additional *model components* and new *biochemical processes*, each involving a new set of *kinetic and stoichiometric parameters*. It should be noted that the merit of the new models mainly depends on the accuracy and reliability of the information they reflect on the wastewater to be treated and the biochemical mechanisms involved. This information must be experimentally determined. It forms the experimental basis of activated sludge modeling. It has to cover (i) wastewater fractions included as model components; (ii) biomass fractions in activated sludge and wastewater, and (iii) various kinetic and stoichiometric parameters defining biochemical processes in the models.

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The progress in the modeling of activated sludge covering all aspects of carbon, nitrogen and phosphorus removal has been so fast that experimental backup lagged behind. It is time now to make the necessary scientific effort to close the gap between modeling and the experimental support it requires. It should be noted that wastewater characterization and experimental evaluation of process kinetics, although an integral part of the comprehensive kinetic evaluation of activated sludge systems, requires a different experience and expertise as compared to modeling. Generally, activated sludge models are regarded as *over-parameterized* and the order of the model should be reduced or simplified with appropriate applications of mathematical techniques. This way, splitting of a complete experimental data set in terms of time segments (Keesman *et al.*, 1998) and/or estimating only the best parameter combinations (Dochain *et al.*, 1995; Weijers and Vanrolleghem, 1997) may be necessary in order to provide correct information on the kinetics. As a result, much more accurate predictions can be derived on the overall performance of an activated sludge process.

The objective of the study is to highlight selected experimental aspects of activated sludge modeling, mainly for organic carbon removal as it is the major concern for most agro-industries, emphasizing weak points and drawbacks, and this way underlining expected future developments in this area.

3.2 Relevance for Agro Industry

Biological processes constitute the major treatment step for industrial wastewaters and especially, the effluents from agro-industries. Experimental support for the understanding of biological treatment is more important for industrial wastewaters compared to domestic sewage, mainly because the latter is well studied and defined in terms of commonly accepted parameters, whereas industrial effluents are much more diversified.

Agro-industries generate strong wastewaters with high COD and generally low total N and P. Therefore, the common concern is mainly organic carbon removal and rarely N removal as in the case of leather tanning and meat processing effluents. External phosphorus supply is usually needed as a remedy for nutrient deficiency in biological treatment. Characteristics of a number of selected industrial effluents, together with

domestic sewage, are given in Table 3.1. COD fractionation as shown in the table reveals high residual COD fractions as a common feature of most industrial effluents. Slowly biodegradable COD represents the bulk of their COD content, with magnitudes highly exceeding that in domestic sewage.

ASM 1 modified for endogenous decay and soluble residual COD generation (Henze *et al.*, 1987; Orhon and Artan, 1994; Orhon *et al.*, 1992) is usually suitable for the modeling of activated sludge for agro-industries. Limited to organic carbon removal for simplicity, it involves, as defined in Table 3.2, a minimum of 8 model components, 3 processes and a total of 8 kinetic and stoichiometric parameters. The appropriate values of these parameters for industrial wastewaters should be expected to be different as compared to domestic sewage, depending on the processes/chemicals used in each different industrial category. With high slowly biodegradable COD fractions, hydrolysis should be underlined as the important mechanism with the main concern that hydrolysis rates may be significantly lower as compared to domestic sewage, due to organic compounds that are not totally compatible with biological treatment.

Table 3.1 Typical characteristics of selected industrial effluents (Orhon *et al.*, 1999a)

Parameters (mg l ⁻¹)	Agro Industries				Domestic
	Tannery	Poultry Processing	Textile	Dairy	
<i>Conventional characterization</i>					
Total COD	2285	2490	2400	1410	430
Soluble COD	1298	1770	1700	1075	170
TSS	770	418	500	190	350
TKN	160	343	35	63	47
Total P	6	30	34	7	8
<i>COD fractions</i>					
S _{SI} /C _{T1}	0.19	0.11	0.14	0.28	0.10
X _{SI} /C _{T1}	0.60	0.78	0.82	0.64	0.80
S _{II} /C _{T1}	0.10	0.10	0.14	N*	0.03
X _{II} /C _{T1}	0.11	0.01	N*	0.08	0.07

*N: negligible

3.3 Respirometry as a Tool for Experimental Evaluation

Respirometry has been used as a very convenient and useful instrument for providing the experimental information required for the modeling of activated sludge systems (Spanjers and Vanrolleghem, 1995; Spanjers *et al.*, 1998, Vanrolleghem *et al.*, 1999;

Petersen *et al.*, 2001b). The assessment of inert COD components and related model parameters obviously require other techniques (Germirli Babuna *et al.*, 1991; Orhon *et al.*, 1999b; Petersen *et al.*, 2001b) and mass balancing is sufficient for the assessment of the biodegradable COD components, aside from the readily biodegradable COD. A detailed account of wastewater characterization is presented elsewhere (Henze, 1992; Petersen *et al.*, 2001b) and it is beyond the scope of this work. Respirometric approaches generally involve observing the electron acceptor utilization profiles in batch reactors initially started with a wastewater/biomass mixture. The oxygen utilization rate (OUR) in an aerated reactor is used for the characterization of aerobic processes and the nitrate utilization rate (NUR) for the computation of correction factors applicable to anoxic conditions.

Table 3.2 Matrix representation of an activated sludge model involving residual COD generation

Components → Processes ↓	S _I	S _P	S _S	X _S	X _H	X _P	X _I	S _O	Process Rate
Growth			$-\frac{1}{Y_H}$		1			$-\frac{(1-Y_H)}{Y_H}$	$\hat{\mu}_H \frac{S_S}{K_S + S_S} X_H$
Hydrolysis			1	-1					$k_h \frac{X_S/X_H}{K_X + X_S/X_H} X_H$
Decay		f _{ES}			-1	f _{EX}		(1-f _{ES} -f _{EX})	b _H X _H
Unit [ML ⁻³]	COD	COD	COD	COD	CellCOD	COD	COD	O ₂	

A suitable substrate to biomass ratio (F/M ratio) needs to be selected for each particular application (Dochain and Vanrolleghem, 2001). Figure 3.1 shows typical OUR curves that would be obtained for domestic sewage and textile wastewater. Both curves were generated for characteristics generally accepted to describe these wastewaters and an initial heterotrophic active biomass of 200 mg cell COD l⁻¹ corresponding to an F/M ratio of 1.35 g COD(g cell COD)⁻¹ for domestic sewage and 1.70 g COD(g cell COD)⁻¹ for textile wastewater (Table 3.3). The difference in the shape of the OUR profile is mainly due to a much slower rate of hydrolysis for the textile effluent, requiring a longer period to reach the final endogenous phase, a common pattern for most industrial wastewaters. Accordingly, it would be a mistake to end the experimental observation after a shorter period, as it is necessary to reach the endogenous phase for an accurate evaluation of the OUR test.

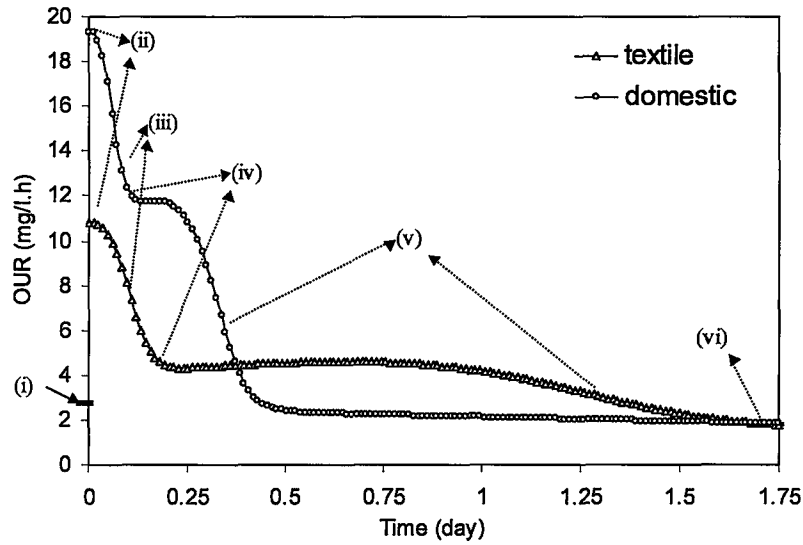


Figure 3.1 Typical OUR profiles for domestic sewage and textile wastewater

Parts of the OUR curve reflect different levels of sensitivity to the sequence of biological processes in the batch reactor, a valuable asset for kinetic evaluation. Basically, (i) the initial OUR level before substrate addition is determined by the endogenous decay activity, $b_H X_H$; (ii) the starting level of the first plateau is set by the growth activity, $\mu_H X_H$; (iii) the ascending slope of the first plateau, if any, is due biomass growth; (iv) the half saturation constant, K_S is most effective on the slope of the drop after the first plateau; (v) the shape of the OUR curve after the first plateau is mainly governed by the hydrolysis rate, namely, k_h and K_X , and (vi) the last phase reflects again endogenous respiration.

The area under the OUR curve as a whole depends upon the specific biodegradable COD fractions (S_S , S_H , X_S) defining the particular wastewater tested in the respirometric experiment. The relative impact of different kinetic parameters on the OUR curve is best assessed by a sensitivity analysis. Figure 3.2 illustrates separately the sensitivity analysis for growth and hydrolysis processes carried out for the OUR curve associated with domestic sewage for the half of the experiment shown in Figure 3.1.

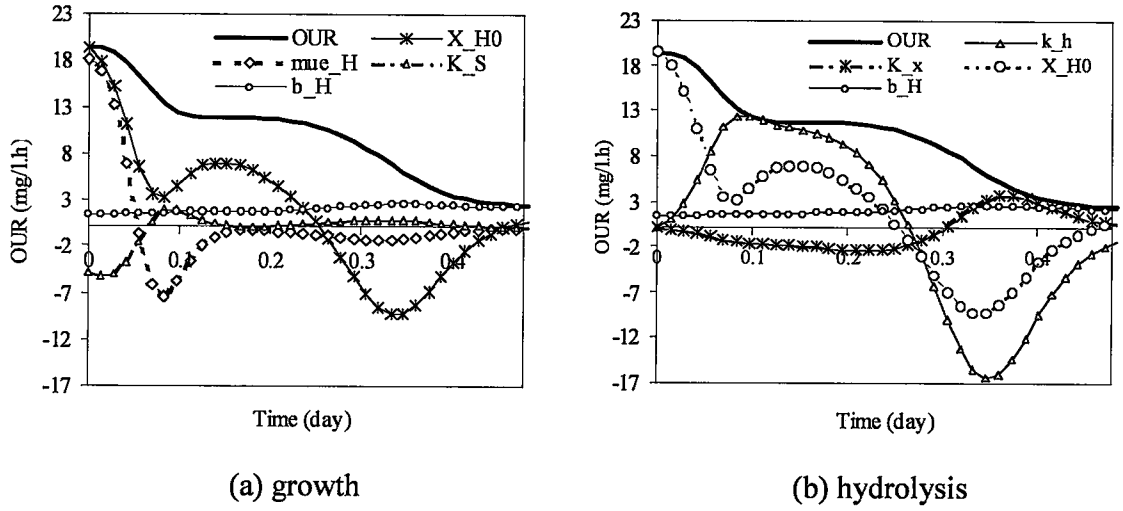


Figure 3.2 Sensitivity analysis for (a) growth and (b) hydrolysis processes on the OUR curve obtained for domestic sewage [$F/M = 1.35 \text{ gCOD(g cell COD)}^{-1}$]

It should be noted here that if the sensitivity trajectories of the parameters are proportional and have the same sign, there is *inverse correlation* between those parameters. On the contrary, if the shapes of the sensitivity trajectories are proportional but with different sign, inevitably, there is a *direct correlation* between these parameters. In this context, the figure reflects, as expected, a strong inverse correlation between $\hat{\mu}_H$ and X_{H_0} , with the indication that the increase in one parameter can be compensated with a corresponding decrease in the other. The correlation between $\hat{\mu}_H$ and K_S is somewhat different in the sense that the shape of the sensitivity functions is the same but the trajectories follow opposite directions. The figure indicates a similar and strong correlation between the hydrolysis rate parameters k_h and K_X . As will be elaborated on later, this correlation cannot be removed completely for batch tests but may be minimized using Optimal Experimental Design (OED) techniques (Vanrolleghem *et al.*, 1995; Insel *et al.*, 2003a; Dochain and Vanrolleghem, 2001).

3.4 Experimental Evaluation of Model Parameters

Currently, techniques using respirometry are widely used for the experimental assessment of individual kinetic parameters such as $\hat{\mu}_H$ and b_H . Similar techniques are also defined to assess the active heterotrophic biomass, X_H , a significant model

component. Assessment of the hydrolysis parameters k_h and K_X still requires model calibration of the experimental OUR data, provided that necessary information on wastewater characteristics and other kinetic and stoichiometric parameters are previously obtained and included in the evaluation (Vanrolleghem *et al.*, 1999; Petersen *et al.*, 2001b).

3.4.1 Experimental assessment of $\hat{\mu}_H$

There are inherent difficulties associated with the traditional methods that use the linearized Monod expression and overall COD and VSS measurements, yielding consistently low $\hat{\mu}_H$ values. New respirometric techniques were developed in accordance with the structure of the new models, based upon the interpretation of the maximum OUR observed during a period with no substrate limitation. Ekama *et al.* (1986b) suggested running an aerated batch reactor at a suitably low initial F/M ratio that would generate an observable initial OUR plateau. They defined a basic relationship showing that $\hat{\mu}_H X_H$ was proportional to the OUR level in this plateau. Another and somewhat tedious procedure was also given to calculate X_H this way leading to the experimental assessment of $\hat{\mu}_H$. It is important to note that the shape of the OUR profile in this experiment is very sensitive to the initial amount of active biomass in the reactor. At the low F/M ratios recommended for the test, it may not be justifiable to neglect the effect of endogenous respiration on the OUR. With this viewpoint, Kappeler and Gujer (1992) developed a similar test initiated with a high F/M ratio, yielding a totally different and exponentially ascending OUR profile. With the assumption that maximum growth can be sustained in the reactor during the period where the readily biodegradable substrate concentration remains sufficiently high, $\hat{\mu}_H$ can be calculated without knowledge of the initial level of X_H in the reactor. The approach used was criticized by Novak *et al.* (1994) with the argument that it may create a microbial growth medium different from conditions associated with continuous-flow activated sludge systems and that during the test fast-growing organisms may be selected giving rise to an overestimation of the maximum growth rate. Grady *et al.* (1996) further stated that conditions before the kinetic set may have an impact on the measured parameters and

suggest that such impacts are best prevented when disturbances during the test remain small and the duration of the test is relatively short.

Based on existing experimental information, a $\hat{\mu}_H$ value of around 5-6 d⁻¹ is generally adopted for domestic sewage. Results in the same range were also reported for different industrial effluents provided that compounds with inhibitory action were removed prior to the test (Sözen *et al.*, 1998). This observation was explained with the argument that new models related microbial growth only to readily biodegradable substrate, S_S and the nature of S_S , by definition, should not change from one wastewater to the other.

3.4.2 Experimental assessment of b_H

In the traditional modeling approach, the endogenous decay parameter is determined as a lump term, k_d , from the linear relationship between the sludge age and the specific substrate removal rate (Pearson, 1968). The procedure can only define an apparent decay parameter of around $k_d = 0.05$ d⁻¹ which is lower than the true b_H value and the underestimation becomes more pronounced as the sludge age increases (Orhon and Artan, 1994). This explains the wide range of k_d values reported in the literature.

The currently developed models, which differentiate between active biomass and inert organic particulate matter, often rely on respirometry for the experimental assessment of b_H . The procedure proposed by Ekama *et al.* (1986b) is now widely recognized and routinely used for this purpose. It involves observing the OUR profile obtained from the aerobic digestion of activated sludge with no external substrate over a period of several days. The slope of the plot of $\ln(\text{OUR})$ versus time yields the value of b_H . A b_H value of 0.24 d⁻¹ at 20 °C was reported for domestic sewage and was adopted as a default value in recent models. Similar evaluations for industrial effluents resulted in variable and generally lower b_H values. Spanjers and Vanrolleghem (1995) proposed a method for the determination of endogenous decay parameter coupled with the growth rate from a single respirogram. Avcioglu *et al.* (1998) also argued that the OUR levels induced by $b_H X_H$ were too low and likely to bring sensitivity and accuracy problems. Their experiments yielded scattered data, sometimes with cyclic variations that were attributed to sequential release and utilization of endogenous residues, making numerical evaluation almost impossible. They have defined another respirometric method that

consisted of measuring changes in the $\mu_H X_H$ response. The method reflected the variation of X_H with time by always sustaining a constant $\hat{\mu}_H$ level during the course of the experiment. They obtained a significantly lower b_H value of around 0.1 d^{-1} at 20°C for domestic sewage. Van Loosdrecht and Henze (1999), in a comprehensive review on this subject, stated that what was simply defined as endogenous decay, could be in reality a spectrum of different mechanisms such as maintenance energy requirements, decay of cells, endogenous respiration, grazing by higher organisms, effect of toxic substances or adverse conditions that result in cell lysis. In this respect, aerobic digestion tests, like the one proposed by Ekama *et al.* (1986), may be subject to severe interference by either external particulate slowly biodegradable substrate, X_S enmeshed with biomass or by internal storage products, X_{STO} , included as a model component in some new models (Gujer *et al.*, 2000).

3.4.3 Experimental assessment of X_H

Identification of the viable fraction in activated sludge, X_H , requires an OUR measurement that reflects the balance between the utilization of the electron acceptor and the process rates for growth and endogenous decay. Henze (1986) used this relationship to determine the viable biomass in wastewater with the assumption that the maximum specific substrate utilization rate at 20°C is $1 \text{ e}^{\cdot}\text{eq. (g VSS d)}^{-1}$, corresponding to $133 \text{ mgCOD (g VSS h)}^{-1}$. A value of $150 \text{ mgCOD (g VSS h)}^{-1}$ was adopted for the evaluation of experimental results. A range of $0.5\text{--}2.0 \text{ e}^{\cdot}\text{eq (g VSS d)}^{-1}$ is reported in the literature as a function of substrate and temperature for different types of heterotrophic bacteria (McCarty, 1972). Ekama *et al.* (1986b) suggested that active biomass could be expressed in terms of the initial OUR value in the experiment for endogenous decay rate, provided that the values of b_H and f_{EX} are known. Similarly, as part of the high F/M ratio batch test for the assessment of $\hat{\mu}_H$, Kappeler and Gujer (1992) directly calculated X_H as a function of the initial OUR provided that $\hat{\mu}_H$, b_H , Y_H and f_{EX} are previously estimated. Ubisi *et al.* (1997) proved that the active heterotrophic biomass estimated with batch tests is in good agreement with the one calculated theoretically using steady state equations (Scheer *et al.*, 1996). Recently, Sözen *et al.* (1998) used two batch OUR tests conducted at different F/M ratios and evaluated the

viable fraction of the biomass by calibrating the initial OUR plateau of the test suggested by Ekama *et al.* (1986b) with the $\hat{\mu}_H$ value computed from a similar test conducted at a much higher F/M ratio as defined by Kappeler and Gujer (1992).

3.4.4 Experimental assessment of k_h and K_X

Hydrolysis of the slowly biodegradable substrate, X_S , is a very important step of activated sludge modeling, because X_S accounts, as previously mentioned, for the bulk of the biodegradable COD content of both domestic sewage and industrial wastewaters. Depending upon their nature and size, different organic compounds lumped into this fraction undergo a sequence of complex reactions. As identification and description of these reactions in wastewater is impossible, they are conveniently collected into an overall single hydrolysis mechanism defined by means of a surface-limited reactions kinetics, with k_h and K_X as the rate parameters. Experimental assessment of the parameters concerning the surface saturation type hydrolysis was first proposed by Ekama *et al.*, (1986) using the “square feed” method that depends upon OUR measurement. In addition, batch respirometric tests are proposed by adjusting the appropriate wastewater/biomass mixtures (Orhon *et al.*, 1999c). For this purpose, the model equations are made operational with known values of COD fractions and kinetic parameters, either defined by direct experiments or adopted by experience prior to curve fitting with the selected OUR profile. Many researchers argued that it might be difficult and sometimes misleading to characterize the entire slowly biodegradable COD fraction by a single hydrolysis rate and suggested a dual hydrolysis mechanism for rapidly hydrolysable COD, S_H , and slowly hydrolysable COD, X_S , as different model components (Orhon *et al.*, 1999c; Sollfrank and Gujer, 1991; Spanjers and Vanrolleghem, 1995). It should be noted here that if the sensitivity trajectories of the parameters are proportional and have the same sign, there is *inverse correlation* between those parameters. On the contrary, if the shapes of the sensitivity trajectories are proportional but with different sign, inevitably, there is a *direct correlation* between these parameters. In this context, the figure reflects, as expected, a strong inverse correlation between $\hat{\mu}_H$ and X_H , with the indication that the increase in one parameter can be compensated with a corresponding decrease in the other. The correlation between

$\hat{\mu}_H$ and K_S is somewhat different in the sense that the shape of the sensitivity functions is the same but the trajectories follow opposite directions. The figure indicates a similar and strong correlation between the hydrolysis rate parameters k_h and K_X . As will be elaborated on later, this correlation cannot be removed completely for batch tests but may be minimized using Optimal Experimental Design (OED) techniques (Vanrolleghem *et al.*, 1995; Insel *et al.*, 2003a; Dochain and Vanrolleghem, 2001).

3.5 Interpretation of the OUR Profiles

For the interpretation of the OUR data, acetate, a simple well-studied readily biodegradable organic compound, and domestic sewage were selected as typical substrates. A model simulation approach, using default values listed in Table 3.3, was adopted for acetate and domestic sewage. Random noise of $0.5 \text{ mgO}_2 \text{ L}^{-1} \text{ h}^{-1}$ was added to approximate an experimental OUR profiles with selected characteristics. Model evaluation of the OUR data was performed using AQUASIM computer program. (Reichert *et al.*, 1998).

Table 3.3 Wastewater characteristics adopted for the model simulations

Parameter	Unit	Acetate	Domestic Sewage	Textile Effluent
Maximum heterotrophic growth rate, $\hat{\mu}_H$	day^{-1}	7.0	6.0	3.2
Half saturation parameter for growth, K_S	mg COD l^{-1}	4	20	20
Heterotrophic yield parameter, Y_H	$\frac{\text{mg cell COD}}{(\text{mg COD})^{-1}}$	0.78	0.67	0.67
Endogenous decay parameter, b_H	day^{-1}	0.2	0.2	0.14
Inert fraction of endogenous biomass, f_E	-	0.2	0.2	0.2
Maximum hydrolysis rate parameters, k_h	day^{-1}	-	3.0	1.0
Half saturation parameters for hydrolysis, K_X	$\frac{\text{mgCOD}}{(\text{mg cell COD})^{-1}}$	-	0.1	0.16
Initial readily biodegradable COD, S_{S0}	mg COD l^{-1}	344	54	60
Initial slowly biodegradable COD, X_{S0}	mg COD l^{-1}	-	216	280
Initial active heterotrophic biomass, X_{H0}	$\text{mg cell COD l}^{-1}$	430	200	200
F/M Ratio	$\frac{\text{mg COD}}{(\text{mg cell COD})^{-1}}$	0.80	1.35	1.70

3.5.1 Relationship between endogenous decay and microbial growth

The measured OUR profile reflects the true electron acceptor utilization response of the microbial community under the operating conditions of the experimental reactor. This response is interpreted in terms of a model that assumedly describes the kinetic behavior

of the community. For this purpose, kinetic parameters related to growth and endogenous decay, namely $\hat{\mu}_H$ and b_H , are generally determined beforehand, by means of differently structured OUR experiments, and incorporated into the model to fit the experimental OUR data. $\hat{\mu}_H$ and b_H are correlated by the active biomass concentration in the reactor, X_H which is difficult to determine at the start of the experiment. As the initial OUR value before substrate addition reflects $b_H X_H$, and after the substrate addition, $\mu_H X_H$, the OUR curve is fitted by searching for the most appropriate X_H value that correlates the two kinetic parameters, b_H and $\hat{\mu}_H$.

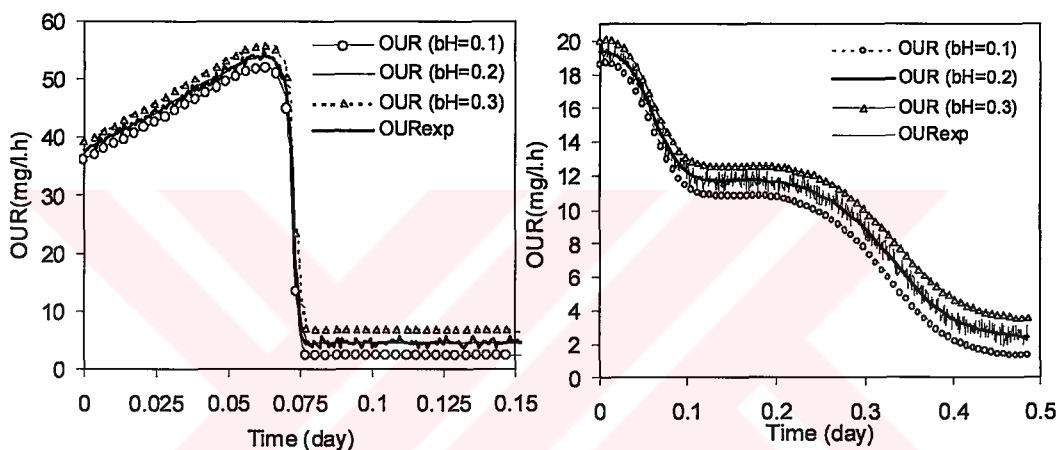


Figure 3.3 Effect of b_H on the OUR profile of acetate (left) and domestic sewage (right)

As previously mentioned, it is also difficult to come up with an accurate assessment of b_H and $\hat{\mu}_H$ and the values experimentally computed may not correctly reflect the response of the microbial community to the selected wastewater. Often, values of these parameters are adopted from another source that is not compatible with the wastewater under investigation. The degree of uncertainty involved may seriously affect the interpretation of the OUR data, both for the relationship between endogenous decay and microbial growth and for the following hydrolysis phase.

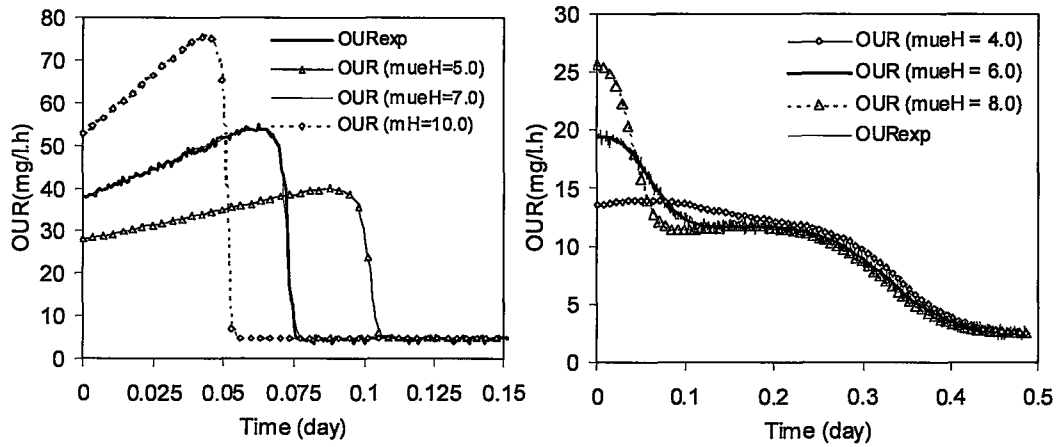


Figure 3.4 Effect of $\hat{\mu}_H$ on the OUR profile of acetate (left) and domestic sewage (right)

An important observation in this respect is the fact that the OUR profile is sensitive to the chosen values of b_H and $\hat{\mu}_H$ and consequently, any change from the intrinsic values of the kinetic and stoichiometric parameters is likely to affect the profile. With all other parameters kept constant, a b_H value different than the one selected to characterize the wastewater shifts the total OUR curve as shown in Figure 3.3. Similarly, a different $\hat{\mu}_H$ value significantly changes the shape of the plateau, while the area under the curve is conserved as illustrated in Figure 3.4. These discrepancies from the experimental data may easily be detected if both b_H and $\hat{\mu}_H$ are previously known. The main problem remains in the fact that with one of the parameters determined or adopted with a certain degree of error, there is the possibility of fitting the OUR profile by adjusting other parameters to values that do not totally relate to the wastewater tested. Basically, the $b_H X_H - \hat{\mu}_H X_H$ correlation automatically selects an X_H level different from the true value, and this will directly reflect on the values of other kinetic parameters. The effect of b_H and $\hat{\mu}_H$ on the estimation of other parameters is illustrated with model simulations outlined in Tables 3.4 and 3.5.

Table 3.4 The effect of b_H on the estimation of other kinetic parameters

	Parameter	Initial Active Biomass, X _{H0} (mgCOD.l ⁻¹)	Growth Kinetics		Hydrolysis Kinetics		χ^2
	<u>b_H value (d⁻¹)</u>		$\hat{\mu}_H$	K _s	k _h	K _x	
			(d ⁻¹)	(mg.l ⁻¹)	(d ⁻¹)	-	
Acetic	0.30	311	9.12	5.87	-	-	501.13
	0.25	359	8.11	4.89	-	-	174.42
	0.20*	427	7.02	4.12	-	-	47.40
	0.15	537	5.79	3.12	-	-	187.82
	0.10	779	4.18	2.23	-	-	715.36
Domestic	0.30	111	10.47	20.51	4.71	0.19	129.84
	0.25	146	8.07	19.92	3.83	0.14	83.36°
	0.22	176	6.80	20.43	3.32	0.12	70.72
	0.20*	202	5.93	19.80	2.99	0.10	68.54
	0.17	254	4.78	20.03	2.46	0.08	74.24
	0.15	300	4.11	21.00	2.14	0.06	83.42
	0.13	363	3.44	21.31	1.82	0.05	96.28
	0.10	506	2.56	23.42	1.36	0.04	121.21°

*default used in the generation of the “true” data;^ofit shown in Figure 3.5.

In the case of acetate, this effect reflects a straightforward relationship between b_H and $\hat{\mu}_H$. For more complex wastewaters such as domestic sewage, it also involves hydrolysis parameters. Inspection of Table 3.4 shows that adoption of a b_H value between 0.1-0.3 d⁻¹ leads to a significant $\hat{\mu}_H$ variation in the range of 2.56 – 10.47 d⁻¹ for domestic sewage. The corresponding K_S variation remains negligible for domestic wastewater.

Table 3.5 The effect of $\hat{\mu}_H$ on the estimation of kinetic parameters for $b_H = 0.2$ d⁻¹ (domestic wastewater)

	Parameter	Initial Active Biomass, X_{H0}	Growth Kinetics	Hydrolysis Kinetics		χ^2
			K_S	k_h	K_X	
μ_H value	3.00	252	10.80	2.40	0.07	206.33
	5.00	221	15.30	2.73	0.08	90.09
	5.93	202	19.80	2.99	0.10	68.54
	7.00	189	26.05	3.19	0.11	84.15
	8.00	181	32.43	3.34	0.12	113.54

It should be remembered that the parameter estimation procedure minimizes the objective function of χ^2 . As shown in Table 3.4 for domestic wastewater, estimation of the default values of the kinetic parameters corresponds to χ^2 of 47.40 and 68.54,

respectively. OUR profiles generated by model simulation for the b_H range of 0.1-0.25 d^{-1} yield reasonably close χ^2 values and consequently fit well with the default OUR curve (Figure 3.5), despite the fact that they provide totally misleading information about the magnitude of the growth kinetics.

3.5.2 Assessment of the hydrolysis rates

Two major concerns exist in the experimental assessment of the hydrolysis parameters. The first concern is the effect of inaccurately pre-selected parameters on the evaluation of the OUR data. They lead to a distorted image of the hydrolysis process as far as the kinetic parameters are concerned: As given in Table 3.4, selection of a b_H value in the 0.13 – 0.25 d^{-1} interval induces a significant, yet statistically acceptable ($\chi^2 = 83.36 - 96.28$) shift in the corresponding k_h levels in the range of 1.82 – 3.83 d^{-1} . A similar variation of 0.05 – 0.14 is also inflicted upon K_X .

At this point, it may be interesting to note the contrast between the minor impact of b_H on the OUR curve (Figure 3.3) and its significant implications on resulting information related to the hydrolysis kinetics. This can be explained on the basis of sensitivity analysis, indicating a uniform sensitivity for b_H throughout the entire OUR curve. Therefore, b_H can only be compensated by changing X_H , $\hat{\mu}_H$ and k_h parameters, where appropriate. From a modeling point of view, the effect of one parameter on a state variable (OUR) can be compensated by other parameter(s) when the parameter(s) has similar sensitivities in shape. In this situation, the shape of the sensitivity function for b_H is completely different from those of the others. However, since the parameter b_H is active during the entire OUR experiment, the change in b_H can only be balanced with relevant combinations of other parameters. Simulation studies also show that $\hat{\mu}_H$ exerts a similar but relatively limited impact on the hydrolysis parameters due to the rate limiting effect of the hydrolysis process after the first plateau (Table 3.5). This is also obvious from the sensitivity profiles where the effect of $\hat{\mu}_H$ and K_S on the OUR profile is negligible after the initial growth phase.

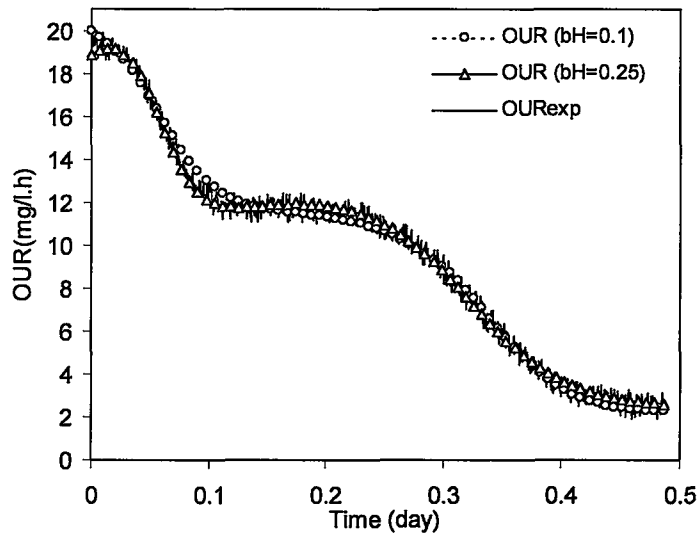


Figure 3.5 Fitting the OUR profile for domestic sewage for b_H 0.1 and 0.25 d^{-1}

The second concern is the inherent property of the OUR test to generate not one, but a series of parameter couples for hydrolysis with equal statistical validity, even if all other kinetic and stoichiometric parameters are assessed or selected properly. In statistical terms, a confidence domain for the parameter couple with a given χ^2 value may be defined for each experimental OUR data set. Figure 3.6 gives the confidence ellipses delineated for different χ^2 contours for an OUR test run with an F/M ratio of 1.35 $gCOD(g\ cell\ COD)^{-1}$ for domestic sewage. If $\chi^2 = 128$ is visually estimated to be the limit for conformity with the experimental OUR profile, then all k_h - K_X couples within the $\chi^2 = 128$ contour may secure model calibration (Figure 3.7). In a more explicit way, $k_h = 3.2\ d^{-1}$; $K_X = 0.13$ and $k_h = 2.8\ d^{-1}$; $K_X = 0.075$ define the limits of the $\chi^2 = 128$ contour.

It is usually helpful to run a second experiment at a different preferably lower F/M ratio. Figure 3.8 gives a model evaluation for $F/M = 0.33\ gCOD(gcellCOD)^{-1}$ obtained by increasing X_H to 800 $mg\ l^{-1}$. The figure also includes the results obtained with $F/M = 1.35\ gCOD(gcellCOD)^{-1}$ for comparison. It is important to note that a lower F/M ratio is much more informative in the sense that it gives smaller areas within the same χ^2 contours; also the confidence regions are more inclined towards the k_h axis and therefore

indicate observed more sensitive for K_X . The χ^2 contours rotate, as may be depicted in Figure 3.8 around the *optimum point* for the model simulation in this study.

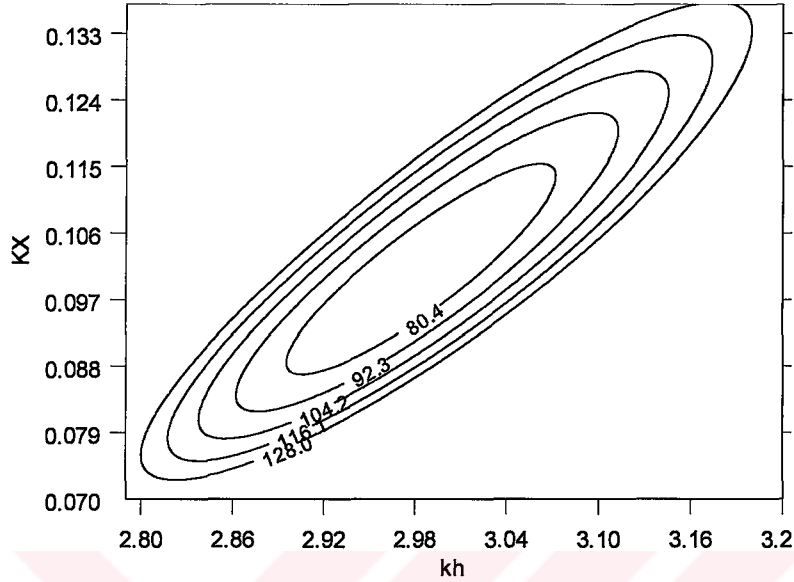


Figure 3.6 χ^2 contour plots for the estimation of k_h and K_X for $F/M = 1.35 \text{ g COD(gcellCOD)}^{-1}$

This rotation property may be used to identify the optimum k_h - K_X couple that is associated with the wastewater tested, by means of two sets of OUR data generated at different F/M ratios (Sperandio and Paul, 2000; Orhon *et al.*, 2001; Insel *et al.*, 2003a). However, this approach does not always yield the same optimum parameter estimates for two experiments with different initial conditions. A multi-experimental fitting procedure (Dochain and Vanrolleghem, 2001) has to be performed in order to acquire joint solution.

3.6 Evaluation and Conclusion

The above evaluations of the model in relation to the available experimental data fit into the major question “Why do we use models?” for activated sludge systems. If the answer is performance calibration and prediction, then the next equally important issue is to ascertain which parameter, whether it be a model component or a kinetic parameter, has

priority for that purpose and to give emphasis on its accurate assessment for the specific wastewater of concern.

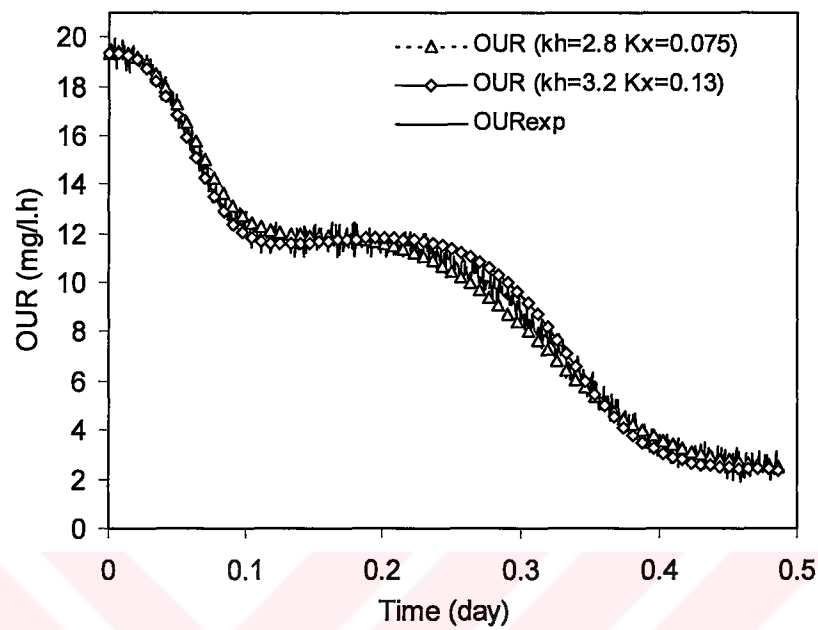


Figure 3.7 Simulation results for limiting k_h - K_X values for $\chi^2 = 128$ ($b_H=0.2\text{ d}^{-1}$)

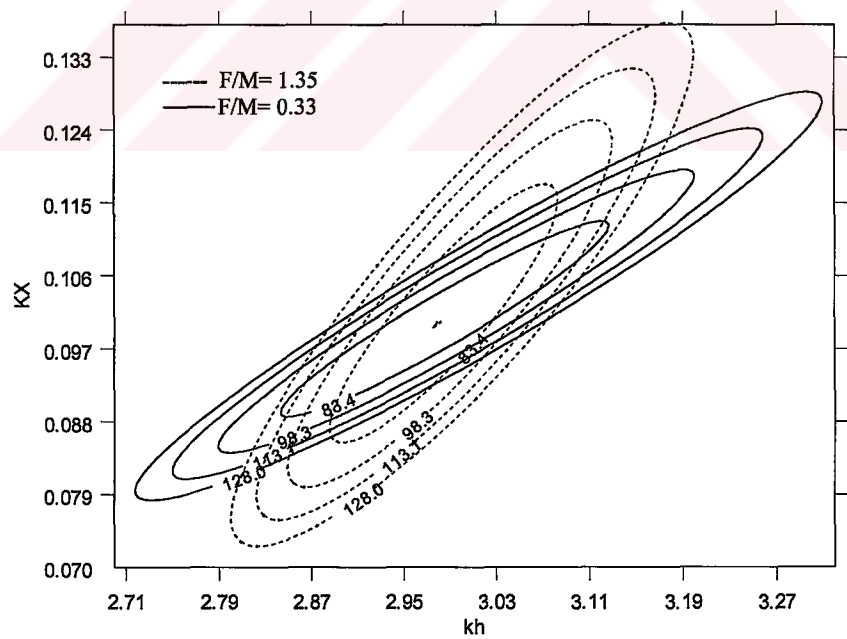


Figure 3.8 χ^2 contour plots for k_h - K_X values obtained with F/M ratios of 0.33 and 1.35 $\text{gCOD}(\text{gcellCOD})^{-1}$

A modeling exercise, without the experimental assessment complement as exemplified in this study, may show that a given parameter may be assigned a secondary significance and adopted without too much concern as to whether it reflects the intrinsic process property. The paper addressed this problem as one of the major pitfalls in modeling, in the sense that an unjustifiable flexibility or a bias in one parameter may cause a significant propagation towards all parameters to be estimated from the experiment. Depending upon the modeling purpose, this problem should be given prime consideration as it exerts a direct influence on the prediction of overall performance of an activated sludge system.

For most effluents from agro-industries, hydrolysis of slowly biodegradable substrate appears to be the major issue. Respirometry, while very useful and promising, still involves a number of pitfalls for an accurate assessment of the rate parameters for this process. Moreover, all other parameters play a major role in the evaluation process and a joint estimation should be preferred over a sequential estimation.

Despite the important body of knowledge and experience now available, experimental evaluation still requires substantial additional effort for improvement. Sensitivity analysis and optimal experimental design techniques should be given major emphasis in this endeavor.

4 IDENTIFIABILITY ANALYSIS FOR AEROBIC HYDROLYSIS KINETICS BASED ON SHORT TERM RESPIROMETRIC DATA

4.1 Introduction

The use of activated sludge models necessitates accurately estimated model parameters and wastewater characteristics to provide useful information for design and optimization of activated sludge plants. Knowledge of biodegradable COD components in wastewaters is of great importance to maintain effective biological nutrient removal performance (Wentzel *et al.*, 1990). Short-term respirometric batch tests provide rapid and accurate information on the biomass activity and the amount of biodegradable substrate available in wastewaters (Brouwer *et al.*, 1998; Spanjers and Vanrolleghem, 1995; Ekama *et al.*, 1986; Dold *et al.*, 1980). Moreover, they allow process engineers to evaluate the degradation kinetics and amount of substrate, the potential inhibition effect of substances *etc.* with the aid of appropriate mathematical models in a short period of time.

The respirogram -the oxygen uptake rate (OUR) data profile- to be used in parameter and state estimation is crucial in terms of data quality/quantity, initial conditions and the limitations of batch experiments. The data quality/quantity is important for the selection of the best model and the accurate estimation of the model parameters (Dochain and Vanrolleghem, 2001). Furthermore, the initial experimental conditions such as the S_0/X_0 ratio (food/microorganism) may alter the biomass characteristics (Novak *et al.*, 1994) or may result in non-informative and insufficient data for parameter estimation (Brouwer *et al.*, 1998; Insel *et al.*, 2003a). In addition, fast dynamic transient responses in respirometric batch experiments may cause a delay time before reaching the maximum OUR level (Vanrolleghem *et al.*, 2004). The model parameters and states can be estimated if the oxygen uptake rate data are properly collected and the initial experimental condition

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are relevant. In other words, the experiments must be optimized to collect necessary information for modeling. Few studies have been devoted to maximize (or optimize) the number of parameters extracted from a single respirometric measurement under certain initial conditions (Insel *et al.*, 2003a; Sperandio and Paul, 2000; Dochain *et al.*, 1995).

The theoretical and practical identifiability serve as useful step to find identifiable parameters. As a preliminary step, the theoretical identifiability analysis is the investigation of reliable, uniquely identifiable model parameters from the data without noise, even if the non-linear model structure and complexity allows mathematical techniques to be applied (Dochain *et al.*, 1995; Petersen, 2000). However, without model simplification, it is mostly difficult to derive the uniqueness parameter estimates with existing mathematical methods. Contrary, practical identifiability concerns the quality of the extraction of model parameters using real data by considering probable parameter correlations and success of model fits (Vanrolleghem *et al.*, 1995; Baltes *et al.*, 1994). In the literature, different practical identifiability methods are applied to detect identifiability problems. So far, the most commonly used method is the parametric sensitivity analysis through visual inspection of sensitivity trajectories (Holmberg, 1982). However, it is difficult to compare the parametric sensitivities visually if the model has many parameters (Dochain and Vanrolleghem, 2001; Brun *et al.*, 2001; Weijers and Vanrolleghem, 1997). Thus, other widely accepted methods such as the use of the Fisher Information Matrix, FIM (Hidalgo and Ayesa, 2001; Vanrolleghem *et al.*, 1995; Walter and Pronzato, 1990; Munack, 1989) and eigen-value decomposition of the covariance matrix (Brouwer *et al.*, 1998) methods are used. Another, systematic approach of Brun *et al.* (2001) is applied for large environmental simulation models. The above-mentioned methods have different measures and interpretation point of views for the detection of identifiability problems.

In this study, a practically identified endogenous decay hydrolysis model (see Chapter 2) was tested using two respirograms obtained for raw domestic and slaughter-house wastewaters, with the aid of the three practical identifiability methods discussed above. The identifiable parameters for the aerobic hydrolysis model and identification problems were interpreted through the utilization of these methods.

4.2 Materials and Methods

4.2.1 Model and wastewater selection

4.2.1.1 Hydrolysis model and estimation of parameters

An activated sludge model including heterotrophic growth and surface saturation type hydrolysis under aerobic conditions (Orhon and Artan, 1994) was selected to characterize the experimentally obtained respirograms (see matrix in Table 4.1). The model is constituted of state variables of readily biodegradable COD fraction, S_s [mgCOD/l], a slowly biodegradable COD fraction, X_s [mgCOD/l] and the active heterotrophic biomass, X_H [mgcellCOD/l] as model states. The kinetic parameters are: maximum heterotrophic growth rate, $\hat{\mu}_H$ [day^{-1}], half saturation constant for growth, K_s [mgCOD/l], the maximum hydrolysis rate, k_h [day^{-1}] and the half saturation constant for hydrolysis, K_X [mgCOD.mgcellCOD $^{-1}$.l $^{-1}$]. In the model, the endogenous decay rate for heterotrophs, b_H [day^{-1}] and inert fraction of endogenous biomass, f_E [-] were kept constant because of practical identifiability problems which will be explained in the following sections.

Table 4.1 Matrix representation of aerobic hydrolysis model

Parameters Process	S_s	X_s	X_H	S_o	Rate
Growth	$-1/Y_H$		1	$-(1-Y_H)/Y_H$	$trans \cdot \hat{\mu}_H \frac{S_s}{K_s + S_s} X_H$
Hydrolysis	+1	-1			$k_h \frac{X_s / X_H}{K_X + X_s / X_H} X_H$
Decay			-1	$(1-f_E)$	$b_H X_H$
Unit, ML $^{-3}$	COD	COD	cell COD	O $_2$	

Defaults: $Y_H=0.66$ gcellCOD/gCOD, $b_H=0.20$ day $^{-1}$, $f_E = 0.2$

The transition term, *trans* was included in the model to reflect the fast transient phase at the beginning of the initial oxygen uptake rate measurement just after the addition of substrate (Vanrolleghem *et al.*, 2004). Hence, the oxygen uptake rate (r) is expressed as follows:

$$r = trans \cdot \left(\frac{1 - Y_H}{Y_H} \right) \cdot \hat{\mu}_H \cdot \frac{S_s}{K_s + S_s} X_H + (1 - f_E) \cdot b_H \cdot X_H \quad (4.1)$$

where *trans*: $(1 - e^{-t/\tau})$ and t: time [T] and τ : first order time constant [T]

The theoretically identifiable parameter subsets were adopted from Chapter 2. Possible combinations of model parameters to be estimated from a batch respirogram for growth and hydrolysis are listed in Table 4.2.

Table 4.2 Parameter combinations for growth and hydrolysis

Growth (Dochain <i>et al.</i> , 1995)	Hydrolysis (Chapter 2)
$(1 - Y_H) \frac{\hat{\mu}_H X_{H0}}{Y_H}$	$(1 - Y_H) k_h X_{H0}$
$(1 - Y_H) S_{S0}$	$(1 - Y_H) X_{S0}$
$(1 - Y_H) K_S$	$(1 - Y_H) K_x X_{H0}$

It should be noted that the solution for hydrolysis kinetics is possible if the respirogram exerts a second tailing after the first plateau. The reason is that the pseudo steady state approximation (Dochain and Vanrolleghem, 2001) then becomes valid. In this approximation, after the first OUR plateau for growth, the reaction rate is limited by the hydrolysis kinetics during the second plateau, which consolidates information on the hydrolysis kinetics and the amount of slowly biodegradable COD (Insel *et al.*, 2003a). Although the parameter combinations were found to be identifiable as given Table 4.2, the estimation of model parameters is activated in the estimation procedure. The secant algorithm was used for parameter estimation of AQUASIM software. A linearized uncertainty analysis was done by simulating the upper and lower bounds of the OUR profiles using the equation below (Reichert *et al.*, 1998). In equation 4.2 below, σ_{θ_i} indicates the absolute-standard deviation of the parameter. However, it is important to note that equation 4.2 does not consider correlation of parameter estimates.

$$\Delta \text{OUR} = \sqrt{\sum_{i=1}^8 \left(\frac{\partial \text{OUR}}{\partial \theta_i} \right)^2 \sigma_{\theta_i}^2} \quad (4.2)$$

4.2.1.2 Practical identifiability methods

The comparison of sensitivity trajectories visualizes both the magnitude sensitivity and also the possible correlation between the model parameters. Absolute-Relative sensitivity

trajectories of OUR with respect to the parameters are obtained according to Reichert *et al.* (1995). However, it is difficult to compare the parametric sensitivities of various parameter combinations if the model is complex (Dochain and Vanrolleghem, 2001; Brun *et al.*, 2001). In order to deal with this problem, the method of Brun *et al.* (2001) that combines the sensitivity measures and determines the linear dependency of the parameters described with the collinearity index (γ_K) can be applied. Briefly, this method provides a systematic approach and compares the collinearity indices of parameter subsets and checks the degree of identifiability of a parameter subsets. According to Brun *et al.* (2001), subset K out of k model parameters is first decided using the dimension-free sensitivity function, $s_{i,j}$ and their sensitivity measures of δ_j^{msqr} and δ_j^{mabs} as expressed in equations 4.3 and 4.4 by ranking in ascending order. Hence, the constitution of a parameter subset is carried out via grouping the parameters from the top of the ranking.

$$s_{i,j} = \frac{\Delta\theta_j}{sc_i} \frac{\partial y_i}{\partial \theta_j} \quad (4.3)$$

$$\delta_j^{msqr} = \sqrt{\frac{1}{n} \sum_{i=1}^n s_{i,j}^2} = \frac{1}{\sqrt{n}} \|s_{i,j}\| \text{ and } \delta_j^{mabs} = \frac{1}{n} \sum_{i=1}^n |s_{i,j}| \quad (4.4)$$

where

$s_{i,j}$ = scaled sensitivity matrix

sc_i = scaling factor for measurements

$\partial y_i / \partial \theta_j$ = sensitivity function of parameter, θ_j to model output, y

n = number of observations (i)

m = number of model parameters (j)

The collinearity index, γ_K (see equation 4.5) is the measure of approximate linear dependency of selected parameter subsets and it also has a close relationship to the condition number (see Mod-E Criterion in Chapter 2). In equation 4.5, $\tilde{S}_K$ is a submatrix of $\tilde{S}$ that

corresponds to the parameters in K ; β is the vector of coefficients and λ_K is the smallest eigenvalue of $\tilde{S}_K^T \tilde{S}_K$.

$$\gamma_K = \frac{1}{\min_{\|\beta\|=1} \|\tilde{S}_K \beta\|} = \frac{1}{\sqrt{\lambda_K}} \quad (4.5)$$

For instance, a collinearity index of 20 means that the effect of an estimated parameter on the measurement can be compensated to 5% by appropriate changes in other parameters (Brun *et al.*, 2002; 2001). Practically, it is suggested that critical values for γ_K fall in the range between 5 and 20. On the contrary, condition number above 100 results in severe parameter identifiability problems. In this study, nearly all parameters (8 out of 11) can be estimated according to the theoretical identifiability of the hydrolysis model. So, the selection of parameter subsets is not considered in this study. AQUASIM software with the UNCSIM module (Reichert *et al.*, 1998; 2003) is used for the calculation of collinearity indices, γ_K .

Another method uses the Fisher Information Matrix (FIM) and its scalar functions (Munack, 1989; Walter and Pronzato, 1990). As seen in equation 6, the FIM summarizes the sensitivities of the model parameters and the measurement errors expressed in a quadratic form:

$$FIM = \sum_{i=1}^N Y(t_i, \theta)^T Q_i Y(t_i, \theta) \quad (4.6)$$

where $Y(t_i, \theta)$ is the output sensitivity function with respect to the parameters. The weighting matrix, Q_i is the inverse of the measurement error covariance matrix (Vanrolleghem *et al.*, 1995). The determinant of FIM (D-Criterion) is inversely proportional to the volume of the confidence region of the parameter estimates (Hidalgo and Ayesa, 2001; Dochain and Vanrolleghem, 2001). In this study, only the D-Criterion was calculated for each parameter combination derived in the method of Brun *et al.* (2001).

The third method used in this study is the eigenvalue decomposition of the parameter estimation covariance matrix, $Cov \hat{\theta}_N$, which is the inverse of the FIM (Brouwer *et al.*, 1998; Vanrolleghem *et al.*, 1995). The eigenvalue decomposition of $Cov \hat{\theta}_N$ can be expressed as:

$$V^T \cdot Cov \hat{\theta}_N \cdot V = \Lambda \quad (4.7)$$

where V is the orthogonal matrix of eigenvectors and Λ is the diagonal matrix composed of eigenvalues. Here, a small eigenvalue (λ_i) corresponds to a large uncertainty in the direction of the V_i vector. Thus, the higher elements of V_i with smaller eigenvalue (λ_i) show that the corresponding model parameter is difficult to estimate using the available data and the uncertainty on this parameter is relatively high (Brouwer *et al.*, 1998). After obtaining Absolute-Absolute (Reichert *et al.*, 1995) sensitivity trajectories, the MATLAB software package was used for the eigen-value decomposition of the parameter estimation error covariance matrix.

4.2.2 Experimental setup

Two characteristic OUR profiles (respirograms) obtained for domestic and slaughter-house effluents were selected for this study. The batch respirograms were obtained after the addition of wastewater to aerated biomass acclimated to the wastewater in the presence of a nitrification inhibitor (ATU). The wastewater was added after obtaining a relatively constant endogenous OUR which also indicates the end of the experiment. The respirogram for domestic wastewater was obtained after adding 70 ml of wastewater having 817 mg/l total-COD to an aerated reactor with an initial volume of 1500 ml. The S_0/X_0 (initial food/microorganism ratio) was adjusted to approximately 0.01 mgCOD/mgcellCOD. The second batch experiment for slaughter-house wastewater was done for a S_0/X_0 ratio of approximately 0.07. A wastewater volume of 395 ml having a total COD of 572 mgCOD/l was added to 2000 ml mixed liquor. The measurement time was about 60 min for both experiments. A Manotherm-RA 1000 type continuous respirometer was used with a sampling interval of one minute.

4.3 Identifiability Results and Discussion

The model parameters including the time constant of the transition term (*trans*) were estimated using two batch respirometric data sets selected for domestic and slaughter house wastewaters (see Figure 4.1). Table 4.3 depicts the estimated parameter values, standard deviations and the correlation matrix of the parameter estimates. It should be noted that the uncertainty of the parameters YH, bH and fE was ignored since they were set to their default values. Otherwise, the overall uncertainty is likely to increase. For the domestic wastewater, higher relative

standard deviations (STD%) for K_S , $\hat{\mu}_H$, τ and K_X were calculated as 48%, 28%, 24% and 22%, respectively. As a result, the linear uncertainty bounds are wider for the parameters of domestic wastewater than of the slaughter-house wastewater. The reason is that the transition phase in the OUR measurements caused uncertainty on the estimates of the growth-related parameters. This can also be concluded from the correlation matrix where a high correlation (approx. 90%) between the parameter couples K_S - $\hat{\mu}_H$, τ - $\hat{\mu}_H$ and K_S - τ is observed. The sensitivity analysis also shows the degree of correlations since the shapes of the trajectories are similar (Figure 4.2b and 2d). In addition, one can see from the sensitivity plots in Figure 4.2 that there is a high degree of correlation between k_h - X_{H0} and k_h - X_{H0} . A lower correlation is expected at the maximum OUR but for domestic wastewater, insufficient data is available compared to the slaughter-house respirogram (Figure 4.1.b). For the slaughter-house experiment, there is sufficient data to estimate growth parameters and time constant simultaneously. Sufficient data characterizing the maximum activity during growth phase lead to lower correlations among the growth parameters. Thus, lower standard deviations on parameters are obtained with narrow uncertainty bounds (Figure 4.1.b).

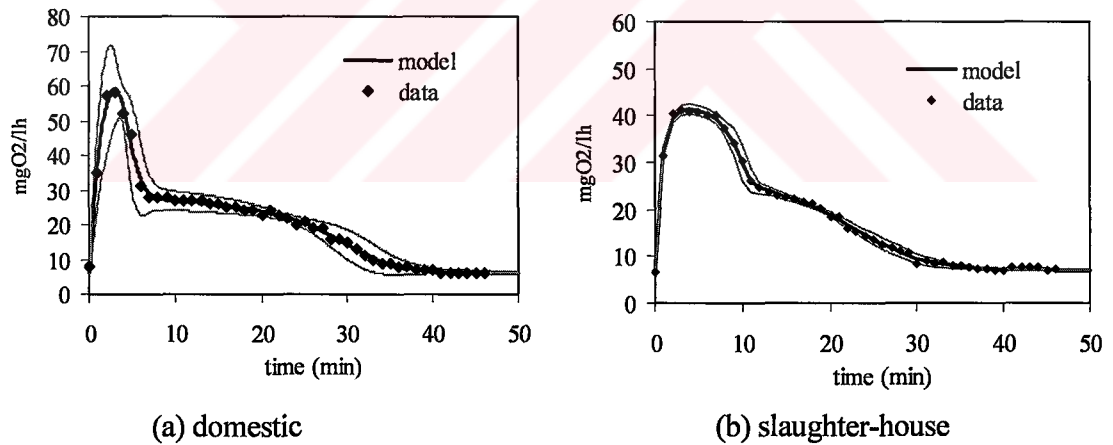


Figure 4.1 Data and model for batch respirometers for (a) domestic and (b)slaughter-house wastewaters

The readily biodegradable (S_{S0}) and slowly biodegradable (X_{S0}) initial COD concentrations in raw wastewater can be estimated accurately as indicated by the sensitivity plots (see Figure 4.2.a). The hydrolysis process characterized by the second OUR tailing especially where the sensitivities for the hydrolysis parameters are effective and the growth parameter sensitivities

stay around zero. It should be noted that the accuracy of the estimates, and, consequently, the model uncertainty depends not only upon the collected data at the maximum OUR but also on the hydrolysis rate. Hence, the complete respirometric degradation curve should be observed. Another important point is that the estimated parameters can be used as combinations as listed in Table 4.2 or individually. The practical identifiability of the hydrolysis model based on respirometric measurements was verified with the method of Brun *et al.* (2001). In Table 4.4, the maximum and minimum values of collinearity indices are given together with the normalized D-Criteria for the parameter subsets of 2 up to 8 parameters pertaining to the experiments of domestic and slaughter-house wastewaters (Reichert and Vanrolleghem, 2001). The collinearity indices were calculated to be 22.13 and 13.90 for domestic and slaughter-house wastewater, respectively. According to the method, without giving any identifiability problems, an acceptable value of 20 (Brun *et al.*, 2001; 2002) is advised and therefore, the collinearity is still acceptable for this study.

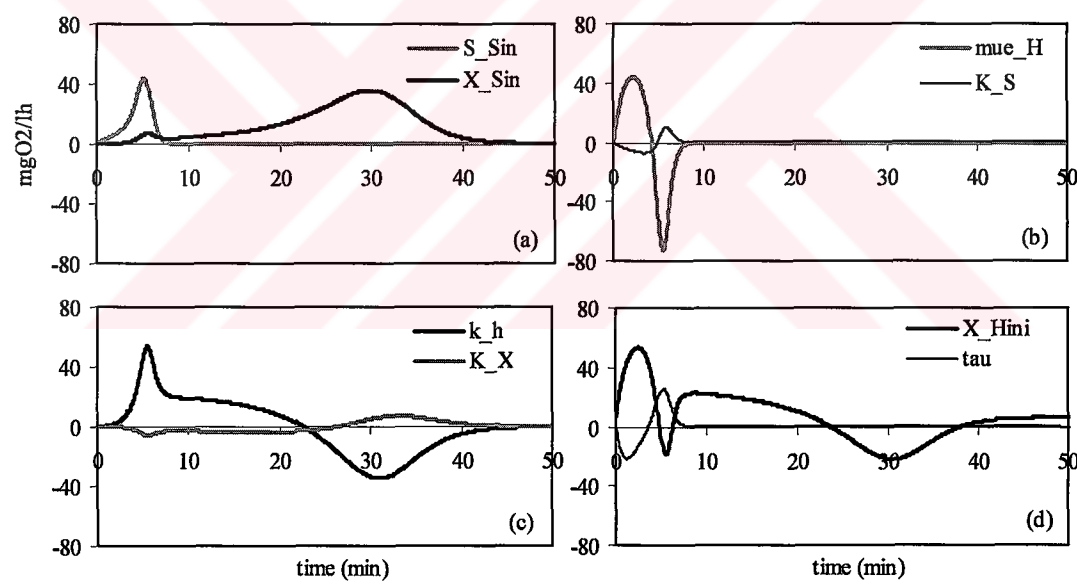


Figure 4.2 Absolute-Relative sensitivity simulations for model parameters and state variables for domestic wastewater

In this study, the collinearity index, γ_K reaches a 200 when the endogenous respiration rate, b_{H_0} is included in the parameter group to be estimated. The search algorithm also failed to find to estimate 9 parameters from the respirograms. It is also obvious that the respirogram length is too short to gather sufficient information on b_{H_0} .

Table 4.3 Estimated parameters and correlation matrix for hydrolysis model (defaults: $Y_H=0.66$ geellCOD/gCOD, $b_H=0.20$ day⁻¹ $f_E = 0.2$)

Estimated			Domestic wastewater					Estimated			Slaughter House wastewater				
STD			STD					STD			STD				
Value	Abs	%	Value	Abs	%	Value	Abs	Value	Abs	%	Value	Abs	%	Value	Abs
k_h	1.8573	0.2034	0.11	1.00		1.6453	0.0853	0.05			1.00				
K_S	2.7214	1.2954	0.48	-0.30	1.00	0.3026	0.0486	0.16			-0.45	1.00			
K_x	0.0034	0.0008	0.22	0.92	-0.35	1.00	0.0039	0.0005	0.12		0.97	-0.40	1.00		
μ_H	6.1480	1.7500	0.28	-0.04	0.94	-0.12	1.00	1.6318	0.0367	0.02	0.39	0.48	0.34	1.00	
S_{SO}	6.0234	0.3119	0.05	-0.41	0.70	-0.50	0.54	5.6784	0.2706	0.05	-0.81	0.71	-0.76	0.13	1.00
τ	0.0015	0.0004	0.24	-0.28	0.88	-0.31	0.92	0.0006	0.0001	0.04	-0.16	0.50	-0.13	0.35	0.20
X_{HO}	920.67	64.05	0.07	-0.94	0.17	-0.78	-0.08	1057.15	16.08	0.02	-0.68	0.13	-0.58	-0.76	0.25
X_{SO}	27.443	1.018	0.04	0.95	-0.40	0.86	-0.15	20.4464	0.4135	0.02	0.94	-0.56	0.88	0.30	-0.83

Table 4.4 Calculated collinearity indices and D-Criterion

Subset#			Domestic wastewater					Subset#		Slaughter wastewater				

The collinearity index with respect to the parameter subsets, which include K_S - $\hat{\mu}_H$ - τ group has a maximum collinearity index around 20 (Figure 4.3.a). This finding is in agreement with the correlations between these parameters as discussed in the sensitivity analysis above. Contrary, the parameter subsets corresponding to the low γ_K -indicating good identifiability- always consist of S_{S0} and X_{S0} components for domestic wastewater (Table 4.4). However, the situation is different for slaughterhouse wastewater. The collinearity index (γ_K) increased up to 13.90 gradually with the increase in the size of parameter subset without causing instant jumps in γ_K as observed in Figure 4.3.a.

Thus, highly correlated parameter groups may change the overall history of γ_K . The worst parameter subset for slaughter wastewater is k_h , K_X , X_{S0} and S_{S0} probably due to a smooth transition of OUR from the first plateau to the second one. But, the γ_K values always stay below 20 indicating that the system is still identifiable.

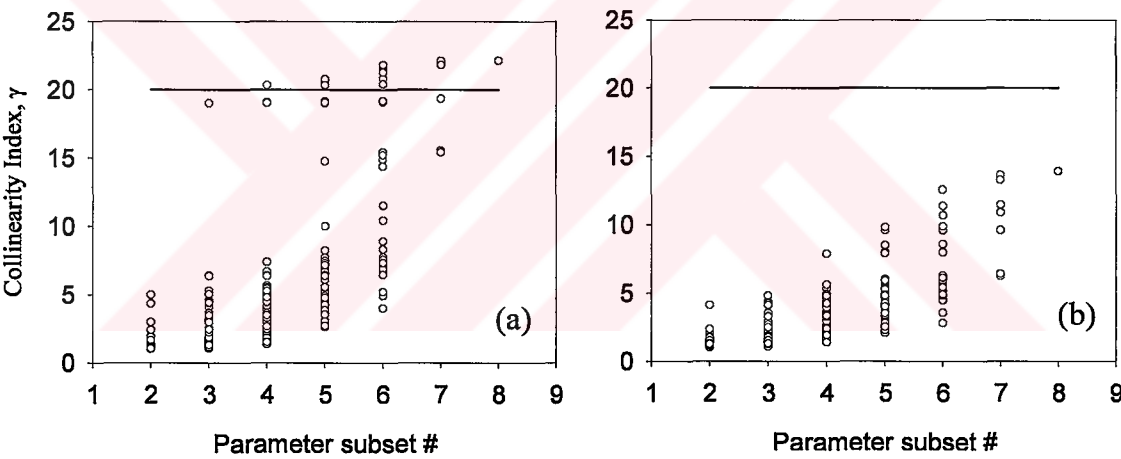


Figure 4.3 Identifiability measures according to Brun *et al.* (2001) (a) domestic and (b) slaughter house wastewater

Regarding the parameter subsets corresponding to small γ_K values, subset #4 has the maximum information content expressed with normalized D-Criterion (Reichert and Vanrolleghem, 2001) since the diagonal elements of the Fisher Information Matrix, FIM are maximized where parameter correlations are at minimum levels (Table 4.4). For the case of large γ values, the normalized D-Criterion decreased in parallel to the gradual decline in collinearity index to 16.50 and 17.20, respectively. This indicates that the

information content is lowered and the parameter correlations improve when extending the number of subsets for the two experiments.

The third measure of practical identifiability results from the eigenvalue decomposition of the parameter estimation covariance matrix. The eigenvalue decompositions are carried out for the 8*8 model matrix for two experimental layouts in order to detect the parameters causing identifiability problems. In this respect, the parameters and initial states having higher elements of the matrix corresponding to smaller eigenvalues (λ_i) are: τ , S_{S0} , K_X , k_h , K_S and $\hat{\mu}_H$ as indicated in Table 4.5 for domestic wastewater. These parameters have larger standard deviations as shown in the parameter estimation step (see Table 4.3). It should be noted that the initial state S_{S0} was also identified with this method indicating similar results as Brun *et al.* (2001). A combined utilization of these methods allows the determination of identifiable parameter subsets, parameter correlations and uncertainty. In that way, the initial conditions of the experiments can be improved to make the experiment more informative in order to decrease the uncertainty on certain parameter groups.

Table 4.5 Eigenvalue decomposition of the parameter estimation covariance matrix (domestic wastewater)

k_h	0.9957	0.0000	0.0000	-0.0004	0.0020	0.0912	-0.0122	0.0030
K_S	0.0237	-0.0018	0.0002	-0.0002	-0.7949	-0.1633	0.5839	-0.0034
K_X	-0.0005	0.0111	-0.0535	-0.9985	0.0000	0.0005	-0.0001	0.0000
μ_H	-0.0146	0.0013	0.0001	0.0001	0.5374	0.2554	0.8036	0.0022
S_{S0}	0.0001	0.9656	-0.2587	0.0245	-0.0021	-0.0006	0.0001	0.0000
τ	0.0000	-0.2596	-0.9645	0.0488	0.0004	0.0001	0.0002	0.0000
X_{H0}	0.0016	0.0000	0.0000	0.0000	0.0000	0.0147	-0.0019	-0.9999
X_{S0}	-0.0878	0.0000	0.0000	0.0006	-0.2818	0.9484	-0.1147	0.0140
<i>Eigen Values</i>	-0.03066	-2.06E-07	1.88E-08	1.52E-07	0.05108	0.18755	4.6704	4103.6

4.4 Conclusions

Respirograms provide information-rich data for accurate estimation of kinetic parameters and initial states within the context of a selected model. But, different characteristics in respirograms may bring along different identifiability problems on certain parameters depending on wastewater, biomass characteristics and initial conditions. Appropriate utilization of identifiability analysis methods allows to

maximize the number of model parameters which can be extracted from dedicated respirometric tests. However, the respirometric experimental conditions (i.e. initial S_0/X_0 ratio, fast transient response of biomass) also play an important role on model identifiability.

Simultaneous utilization of practical identifiability methods yields similar or complementary results for the identification of identifiable parameter subsets to be extracted from respirometric measurements. As a further step, the initial experimental conditions can be adjusted in order to deal with identifiability analysis problems on certain parameter groups.



5 EFFECT OF TEMPERATURE ON THE NITROGEN REMOVAL PERFORMANCE OF A SEQUENCING BATCH REACTOR TREATING TANNERY WASTEWATER

5.1 Introduction

Stringent effluent limitations apply to domestic and industrial wastewaters, often without any concern for the restricting effect of temperature on treatment performance. Systems treating domestic and especially high-strength industrial wastewaters face severe limitations, imposed by the nature of biological processes related to nitrogen removal, in meeting effluent restrictions during the cold season. This limitation is sometimes overlooked in the process of compliance monitoring. When the temperature effect is considered, the rate of nitrification becomes the rate limiting parameter for the overall nitrogen removal, as it directly controls the level of nitrogen oxidized to nitrate. It is well known that the temperature effect reflects most on the maximum specific autotrophic growth rate, μ_{Amax} . Previous experiments (Orhon *et al.*, 2000) conducted on the same tannery wastewater suggest that the effect of temperature on μ_{Amax} may be evaluated by an Arrhenius type of equation with a temperature coefficient, θ of 1.127, slightly higher than what is normally associated with domestic sewage (Henze *et al.*, 1995b; Sözen *et al.*, 1996).

The sequencing batch reactor (SBR) offers full flexibility and potential for simultaneous carbon and nutrient removal (Taşlı *et al.*, 1999, 2001; Wilderer *et al.*, 2001). Its operation can now be interpreted, defined and modeled using fundamentals of related stoichiometry and process kinetics (Artan *et al.*, 2001, 2002a). This process applies also well to tannery wastewater both for organic carbon and nutrient removal (Carucci *et al.*, 1999b; Murat *et al.*, 2002).

This chapter was published as:

Murat, S., Insel, G., Artan, N. and Orhon, D., 2004. Effect of temperature on the nitrogen removal performance of a sequencing batch reactor treating tannery wastewater, *Wat. Sci. Tech.*, **48(11-12)**, 319-326.

This study was undertaken with the main objective of highlighting the effect of temperature on the nitrogen removal performance of an SBR treating tannery wastewater. The results were interpreted and evaluated using both basic stoichiometry and mass balances related to nitrification and denitrification and also, model calibration of the system performance in terms of major parameters such as COD, oxidized nitrogen ($\text{NO}_x\text{-N}$) and ammonia nitrogen ($\text{NH}_4\text{-N}$) concentrations observed during the cyclic operation of the SBR at steady state.

5.2 Materials and Methods

A pilot-scale SBR unit installed on site, was operated at the treatment facilities of the *Istanbul Organized Leather Tanning Industrial District*, located in Tuzla/Istanbul. The industrial district, originally planned for a capacity equivalent to a wastewater flow rate of $36,000 \text{ m}^3 \text{ d}^{-1}$, presently operates with 110 tanneries processing both cattle hide and sheep skin and generates a daily wastewater flow of around $10,000\text{--}12,000 \text{ m}^3$. The SBR unit used in the study was a cylindrical PVC tank of 1 m diameter, with an effective volume of around 844 L. The SBR installation was equipped with a PLC control sustaining the desired sequence of anoxic/aerobic phases. Two 30 cm diameter membrane diffusers connected to a compressor through a solenoid valve, provided air and mixing for the aerobic phase. Mixing in the anoxic phase was secured by a combination of a mechanical mixer and internal recirculation using a submerged pump. Other details of the SBR units are described elsewhere (Murat *et al.*, 2002).

All analyses for conventional characterization were performed as defined in *Standard Methods* (APHA, 1995). The soluble and filtered COD was defined as the filtrate through Whatman GF/C glass fiber filters with an effective pore size of $1.2 \text{ }\mu\text{m}$, also used in the analysis of volatile suspended solids (VSS) and suspended solids (SS). The kinetic and stoichiometric constants for selected models under different temperatures were adopted from previous similar works (Orhon *et al.*, 1999d; Murat *et al.*, 2002). Model simulation was performed using the AQUASIM software package developed by Reichert (1994). ASM1 (Henze *et al.*, 1987) modified for endogenous decay (Orhon and Artan, 1994) and ASM2 (Henze *et al.*, 1995) were used for model evaluations and comparisons.

5.3 Results and Discussion

5.3.1 SBR Performance for nitrogen removal

The plain-settled wastewater, which served as the influent for the SBR operation, reflects all the characteristics of a typically strong tannery wastewater with a high COD level around $2,000 \text{ mg l}^{-1}$ and similarly high total kjeldahl nitrogen (TKN) concentration in the range of $110\text{--}160 \text{ mg l}^{-1}$. The SBR was operated at steady state in terms of the mixed liquor volatile suspended solids concentration (MLVSS) for more than 6 months, at three different wastewater temperature ranges between 9°C and 30°C . The corresponding influent wastewater characteristics are outlined in Table 5.1.

In this study, the SBR operation for carbon and nitrogen was designed for two cycles a day (A *total cycle time*, $T_C = 12 \text{ h}$), where 10 h was devoted to *the process phase*, TP and the remaining 2 h for *settle, draw and idle* phases ($T_S + T_D + T_I = 2 \text{ h}$). The *anoxic phase*, T_{DN} was selected as 1.5 h , with continuous wastewater feeding ($T_F = T_{DN}$) and the reactor was aerated for 8.5 h ($T_A = 8.5 \text{ h}$), during the remaining portion of the process phase. The system was ultimately adjusted to a total sludge age, θ_x , of 15 days to ensure complete nitrification. A *fill volume*, V_F of 141 L was selected, leaving 703 L for the *stationary volume*, V_0 and corresponding to $V_0/V_F = 5$. Under these operating conditions, the nominal hydraulic retention time, θ_h , of the system was set to 3 days.

In terms of nitrogen components, SBR operation with the selected pre-denitrification mode was observed to be quite efficient, producing an effluent with an average $\text{NO}_x\text{-N}$ concentration of 14 mg l^{-1} at $28\text{--}30^{\circ}\text{C}$ and 11 mg l^{-1} at $20\text{--}28^{\circ}\text{C}$. Under these conditions, the corresponding average $\text{NH}_4\text{-N}$ concentrations were observed to remain at 1.0 mg l^{-1} and 4.0 mg l^{-1} respectively. As expected, nitrification was quite sensitive to temperature effects but full nitrification could be secured at temperatures higher than 20°C . The operation was continued at increasingly lower wastewater temperatures and the performance of the system was observed to drop, mainly due to the kinetic effect of temperature on nitrification. The effluent $\text{NH}_4\text{-N}$ concentration increased to around $20\text{--}30 \text{ mg l}^{-1}$ depending on temperature.

Table 5.1 Influent wastewater characterization

	Operating Parameters										
	Total COD	Soluble COD	TKN	NH ₄ -N	Total P**	SS	VSS	S ⁻²	Total Cr	Cl ⁻¹	pH
	mg l ⁻¹										-
<i>This Study</i>											
Steady-state Operation											
28-30°C	1935	1080	163	91	>20	644	441	80	66	5842	7.7
20-28°C	1982	1164	148	98	>20	614	428	63	38	6844	8.0
9 -14°C	1691	1017	111	73	>20	494	387	59	45	5005	8.0
Cyclic Operation											
20°C	2475	1570	150	110	22	610	575	49	18	5910	7.9
14°C	1440	1195	109	66	22	375	310	89	NA	3375	7.8
Murat <i>et al</i> (2002)*	2514	1564	224	126	>20	621	463	45	52	5760	8.1
Orhon <i>et al.</i> (1999)	2255	1300	214	164	5.9	768	467	36	40	5400	7.9

* Steady state operation, ** External addition

Nitrification was heavily affected but never ceased at wastewater temperatures above 8 °C. The performance of the SBR was appreciably better than that of the full-scale plant during the same period. These results can be justified on the basis of a basic mass balance concerning the fate of different nitrogen compounds. Details of the related stoichiometry are presented elsewhere (Artan *et al.*, 2001). It should be noted that aside from nitrification, which determines the magnitude of oxidized nitrogen, the V_0/V_F ratio plays a dominant role in setting the available nitrate for denitrification and therefore the effluent NO_x-N concentration.

Table 5.2 Significant parameters of SBR performance

	Mixed Liquor		Effluent Quality					
	MLSS	MLVSS	Tot. COD	Sol. COD	VSS	SS	NO _x -N	NH ₄ -N
<i>This Study</i>								
Steady-state Operation								
28-30°C	3406	2727	172	142	13	20	14	1.0
20-28°C	2927	2252	215	141	NA	31	11	4.0
9 -14 °C	2365	1941	180	142	34	51	3	31
Cyclic Operation								
20°C	2670	2150	280	140	NA	34	11	1.1
14°C	2190	1770	125	80	19	54	2.8	28
Murat <i>et al.</i> , 2002 (20 °C)	4030	3150	250	164	23	28	25	1.0
Full Scale Plant								
28-31 °C	4932	3749	236	161	NA	65	NA	4.6
17-25 °C	5630	4385	257	161	NA	74	NA	35

In this study, an effluent NO_x-N level in the range of 11–14 mg l⁻¹ could be achieved with a V_0/V_F ratio of 5, whereas in a similar previous study, a single cycle operation corresponding to $V_0/V_F = 2$ could only secure a much higher NO_x-N concentration of 25 mg l⁻¹ (Murat *et al.*, 2002).

5.3.2 Modeling nitrogen removal at steady state

SBR performance for nitrogen removal was evaluated by model simulation of the cyclic operation at steady state. Kinetic and stoichiometric coefficients adopted for this purpose are listed in Table 5.3. A part of these coefficients were experimentally determined in this study, others were taken from previous experiments on the same wastewater and the rest reflect default values suggested in literature.

Table 5.3 Model coefficients characterizing treatment of plain-settled tannery wastewater

Parameter	Symbol	Value		Unit	Reference
		RUN 1 20 °C	RUN 2 14 °C		
Heterotrophic maximum growth rate	μ_{Hmax}	2.1	2.0	day ⁻¹	Murat <i>et al.</i> (2002)
Half saturation coefficient for heterotrophic growth	K_S	30	30	mgCOD.l ⁻¹	Orhon <i>et al.</i> (1999)
Autotrophic maximum growth rate	μ_{Amax}	0.21	0.12	day ⁻¹	Murat <i>et al.</i> (2002)
Half saturation coefficient for autotrophic growth	K_{NH}	1.0	1.0	mgNI ⁻¹	ASM1
Heterotrophic endogenous decay	b_H	0.12	0.1	day ⁻¹	Murat <i>et al.</i> , 2002
Autotrophic endogenous Decay	b_A	0.05	0.045	day ⁻¹	ASM1
Maximum specific hydrolysis rate for S_H	K_{hS}	1.0	1.0	day ⁻¹	Murat <i>et al.</i> (2002)
Half saturation coefficient for hydrolysis of X_S	K_{XS}	0.18	0.05	mgCOD(mgcell COD) ⁻¹	Murat <i>et al.</i> (2002)
Maximum specific hydrolysis rate for S_H	K_h	0.23	0.3	day ⁻¹	Murat <i>et al.</i> (2002)
Half saturation coefficient for hydrolysis of X_S	K_X	0.08	0.013	mgCOD(mgcell COD) ⁻¹	Murat <i>et al.</i> (2002)
Heterotrophic yield coefficient	Y_H	0.63	0.64	mgCOD(mgcell COD) ⁻¹	Orhon <i>et al.</i> , 1999d
Autotrophic yield coefficient	Y_A	0.24	0.24	mgCOD(mgN) ⁻¹	ASM1
COD equivalent of biomass	f_x	1.42	1.42	mgcellCOD(mgVSS) ⁻¹	Orhon and Artan (1994)
Particulate inert fraction of biomass	f_e	0.2	0.2	mgCOD(mgcell COD) ⁻¹	ASM1
Soluble inert fraction of biomass	f_{es}	0.1	0.1	mgCOD(mgcell COD) ⁻¹	Orhon <i>et al.</i> , (1999b)
N content of biomass	i_{NBM}	0.085	0.085	mgN(mgcell COD) ⁻¹	Orhon <i>et al.</i> , (1999d)
N content of X_I	i_{NXI}	0.01	0.014	mgN(mgCOD) ⁻¹	Gujer <i>et al.</i> , (1999d)
N content of S_I	i_{NSI}	0.027	0.07	mgN(mgCOD) ⁻¹	Gujer <i>et al.</i> , (1999d)
Anoxic correction factor for growth	η_g	0.8	0.8		ASM1
Anoxic correction factor for hydrolysis	η_h	0.8	0.8		This study

Model calibration was carried out using the NH₄-N and NO_x-N concentration profiles experimentally determined during two selected complete cycles within the steady state operation of the SBR at two different temperatures of 20°C and 14°C. The model structure for calibration was completed with the COD fractions experimentally

determined for the tannery effluent at the beginning of the selected cycles, as given in Table 5.4.

In this step, SBR performance for nitrogen removal was simulated over a 60-day period in order to reflect system behavior with a heterotrophic/autotrophic biomass composition at steady state for a wastewater temperature of 20⁰C. Figure 5.1 shows the one-day simulation trajectories and experimental data illustrating a good fit under steady state operation. During the anoxic fill phase ammonia accumulates and the available nitrate, sustained in the anoxic phase by the selected V_0/V_F ratio, is used through denitrification. In the following aerobic period, ammonia is oxidized and nitrate is generated. As can be seen from Figure 5.1, the change in the ammonia level under aerobic conditions is higher than that of nitrate, due to the fact that the ammonia is also used for biomass growth.

Table 5.4 COD fractionation of plain settled tannery wastewater

	C _T	C _S	S _S	S _H	S _I	X _S	X _I
	mg l ⁻¹						
This Study							
RUN 1 (20 ⁰ C)	2475	2100	530	815	225	755	150
RUN 2 (14 ⁰ C)	1440	1240	288	756	150	196	50
Murat <i>et al.</i> (2002)*	2330	2000	460	700	65	840	265
Orhon <i>et al.</i> (1999d)	2284	1807	434	649	214	724	263

*Analysis during cyclic operation

5.3.3 Modelling nitrogen dynamics at low temperatures

A superficial interpretation of the experimental data with no emphasis on system kinetics and related model evaluation may easily lead us to conclude that nitrification persists at temperatures as low as 14⁰C. In reality, what happens is that the SBR maintains an apparent steady state in terms of its heterotrophic biomass, but a dynamic disturbance and a gradual washout starts for the autotrophs. This statement may be confirmed using the basics of nitrification kinetics. Using the data in Table 5.3, applicable to tannery wastewater, the minimum operational temperature for the autotrophic growth may be calculated to be around 16.5–17.1⁰C with an Arrhenius type equation.

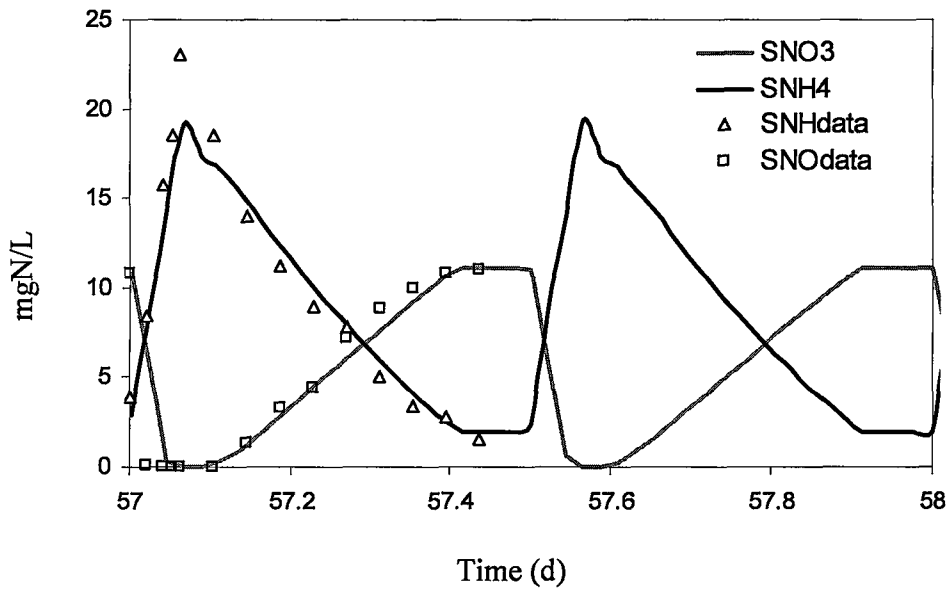


Figure 5.1 Steady state simulation for temperature at 20°C

Consequently, autotrophic biomass will be washed out if the temperature goes below 16.5°C during the current operating strategy of the SBR. In order to maintain autotrophic biomass, the aerobic sludge age should be increased. The minimum aerobic sludge age at 20°C and 14°C can be calculated as follows:

$$1/\text{SRT}_A = \mu_{A_{\max}} - b_A = 0.21 - 0.05 \rightarrow \text{SRT}_A = 6.5 \text{ days (at } 20^\circ\text{C)}$$

$$1/\text{SRT}_A = \mu_{A_{\max}} - b_A = 0.12 - 0.045 \rightarrow \text{SRT}_A = 14.0 \text{ days (at } 14^\circ\text{C)}$$

where, SRT_A = aerobic sludge age (day).

The above calculations show that the current aerobic sludge age of 10.5 days is not sufficient for operation at 14°C and the autotrophic biomass is bound to be washed out from the system. This mechanism is visualized in the second simulation study where the system performance was simulated over 11 days for an average temperature of 14°C. The simulation results for nitrogen compounds are shown in Figure 5.2 and Figure 5.3.

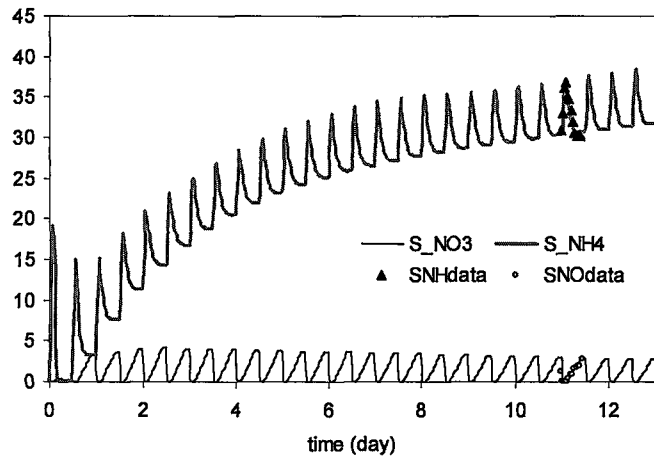


Figure 5.2 Simulation for Temperature: 10°C (initials states of 20°C used)

It should be noted here that the temperature is decreased from 20°C to 14°C at time zero and the initial values of the state variables were taken from the steady state simulation under 20°C in order to maintain the consistency of the evaluation. As discussed above, the simulation confirms the gradual increase of the ammonia concentration with time as a result of the decreasing autotrophic biomass in the reactor. Figure 5.3 indicates that complete washout of the autotrophs will occur in 60 days, if the wastewater temperature continually remains under the critical level for nitrification. The observation of the fate of the nitrogen compounds during the cyclic operation at 14°C is shown in Figure 5.4 and Figure 5.5.

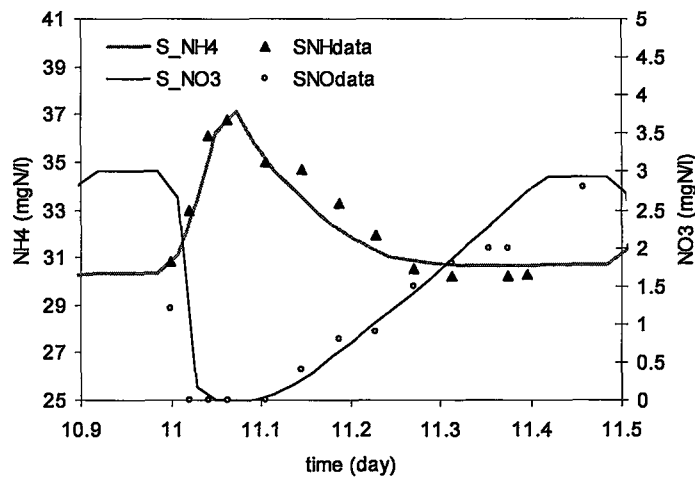


Figure 5.3 Simulation for Temp: 10°C (initials of 20°C used)

It is interesting to note that the observation remains within the period where the autotrophic biomass is dynamically disturbed and the simulation provides a good prediction of the system performance in the selected time frame within this period. The simulation also gives a clear picture of the fact that the SBR performance in terms of the nitrogen compounds for the observed cyclic operation as shown in Figure 5.5, is not stable at 14°C.

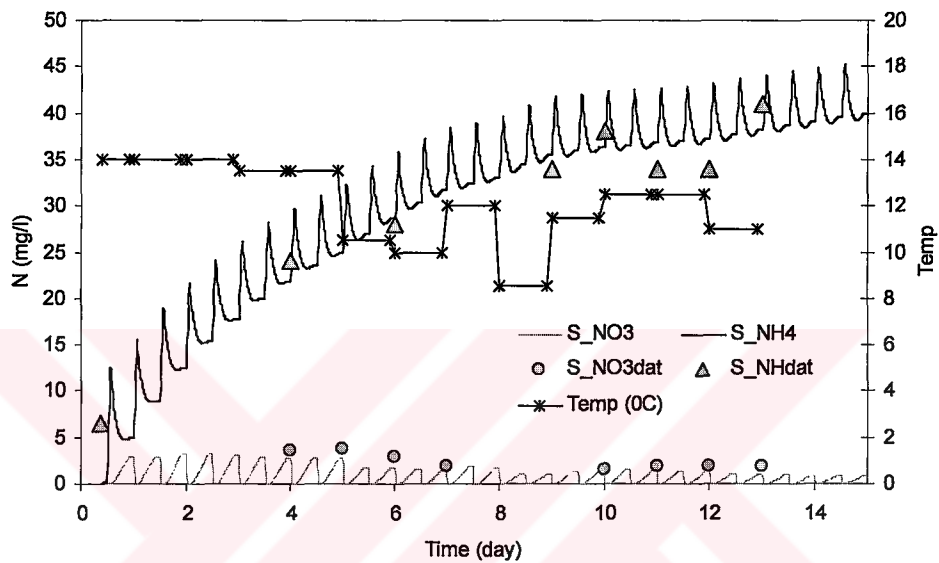


Figure 5.4 Dynamic temperature effect on nitrogen fractions

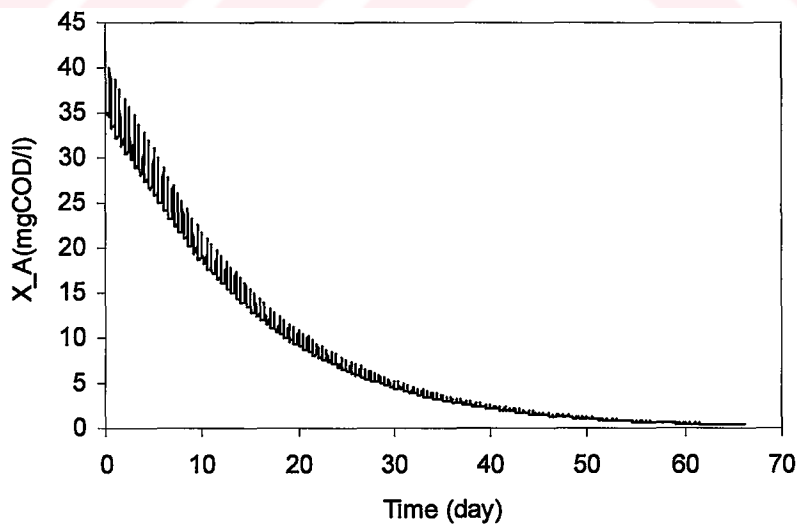


Figure 5.5 Simulated autotrophic biomass concentration under low temperature

5.4 Conclusions

This study provides experimental proof of the potential of SBR technology in achieving effective nitrogen removal from tannery effluent, a typically strong wastewater in terms of its high nitrogen content. SBR operation at steady state with two cycles a day, secures an effluent $\text{NO}_x\text{-N}$ concentration of 11–14 mg l^{-1} and a $\text{NH}_4\text{-N}$ concentration below 4 mg l^{-1} , at wastewater temperatures above 20°C. The V_0/V_F ratio is confirmed to be the essential parameter in manipulating operation for the desired denitrification efficiency. At temperatures critically lower than required to sustain nitrification, experimental observations verified by the dynamic model evaluation indicate that SBR operation, while practically remaining at steady state for heterotrophic biomass, becomes dynamically unbalanced in terms of its nitrifiers. As a result, an increase in the effluent $\text{NH}_4\text{-N}$ concentration occurs due to gradual washout of the autotrophic biomass. In the study, nitrification is observed to continue, although at increasingly reduced rates, mainly because the low temperature period lasted shorter than what was required for a complete washout. This evaluation underlines the danger in interpreting the results in a way to conclude that nitrification may be sustained at temperatures lower than the critical level necessary to sustain nitrifiers growth for tannery wastewaters.

6 EFFECT OF AERATION ON THE PERFORMANCE OF SMALL SEQUENCING BATCH REACTORS FOR ORGANIC CARBON AND NITROGEN REMOVAL

6.1. Introduction

Accumulated experiences indicate that Sequencing Batch Reactor (SBR) is a promising technology and it serves as a viable alternative for efficient removal of organic carbon and nutrients from industrial and domestic wastewaters. A greater flexibility in the design/retrofit of existing SBR, greater amenability to automation and advanced process control provide competitive potential use compared to continuous flow activated sludge plants (Wilderer *et al.*, 2001; Tilche *et al.*, 2001; Demuyne *et al.*, 1994).

An appropriate design of SBR should meet the desired effluent quality with respect to carbon and nutrients. In the literature, few methodologies have been proposed for the design of SBR by providing delicate stoichiometric relationships between biomass, biodegradable substrate and nitrogen (Artan *et al.*, 2002a; Teichgraber *et al.*, 2001). However, in reality, some important factors may alter the response of the system, which were not considered during the design step of SBR system. Although, the applicable design procedures are well formulated for the nitrogen removal, in general, the importance of the selection of aeration capacity is underestimated. Hence, the oxygen profiles -starting from zero to saturation level at the end of the phase- may occur depending upon the trade off between the oxygen uptake rate, OUR and the oxygen transfer rate, OTR whilst the aeration is relatively limited. In this case, real nutrient removing performance of SBR deviates from the predicted because of the fact that oxygen limitation influences the nitrification and denitrification processes (Insel *et al.*, 2003; Artan *et al.*, 2002b).

This chapter was presented in 6th Specialist Conference on Small Water and Wastewater Systems: Insel, G., Artan, N. and Orhon, D., 2004. Effect of aeration on the performance of small sequencing batch reactors for organic carbon and nitrogen removal, 6th Specialist Conference on Small Water and Wastewater Systems, 11-14 February, Perth, Australia.

In this part of this thesis, the objective is to investigate the effect of volumetric oxygen transfer coefficient, K_{La} on dissolved oxygen profile through the aerated phase in relation to the nitrification and denitrification processes with the aid of calibrated model simulations. In this study, the nitrogen removal efficiency of a pilot-scale SBR treating the tannery wastewaters is investigated with the aid of model calibration.

6.2 Conceptual Basis for Oxygen Transfer Modeling

The amount of oxygen transfer rate, OTR_f per volume of the tank, V can be expressed with the equation (6.1) where K_{La_f} [day^{-1}] is the volumetric oxygen transfer coefficient and $S_{O_{\infty f}}$ [gO/l] is the dissolved oxygen concentration (indicated with indice-f) at infinite aeration time under process conditions (WEF, 1996). The S_O parameter stands for the average dissolved oxygen concentration desired in the aeration tank (mostly taken as 1-2 mgO_2/l).

$$\frac{OTR_f}{V} = K_{La_f} (S_{O_{\infty f}} - S_O) \quad (6.1)$$

Based on the mass balance over dissolved oxygen in an aerated activated sludge tank, the changes in the dissolved oxygen concentration, S_O with time can be expressed with the formula given by equation 6.2. (Mueller and Stensel, 1990). According to the formula, the dissolved oxygen concentration at a time t is the function of net effect of the oxygen transfer rate and oxygen uptake rate, OUR. In this respect, the selection of K_{La_f} is of great importance since sufficient oxygen levels should be provided in order to sustain heterotrophic and autotrophic activity. The OUR term governs the sum of oxygen uptake rates of heterotrophic, autotrophic activities and endogenous biomass.

$$\frac{dS_O}{dt} = K_{La_f} (S_{O_{\infty f}} - S_O) - OUR \quad (6.2)$$

In SBRs, variations in reactor volume and the cyclic operational characteristic (i.e. aerated, unaerated periods) should be considered in the calculation of daily oxygen to be supplied to the system. First, the actual volume during aerated period (T_A) within a cycle (T_C) is important since the K_{La} is dependent upon the volumetric air supply as given in (see equation 6.3). For instance, the effect of actual volume is

more pronounced if aerated-fill period is available in the SBR operation. Second important factor is that the air can only be supplied during the aerated periods (TA). Therefore, a correction should be placed upon K_{La_f} calculation where unaerated durations of mixed (TM), settling (TS), draw (TD) and idle (TI) phases are subtracted from the total cycle time (TC) as given in equation 6.4. Then, the volumetric oxygen transfer rate (K_{La_f}) for SBR systems can be calculated according to equation 6.5:

$$K_{La_f} = \frac{OR}{V_T(S_{O_{\infty f}} - S_O)} \frac{24}{m \cdot T_A} \quad (6.3)$$

where

$$T_A = T_C - (T_M + T_S + T_D + T_I) \quad (6.4)$$

m = number of SBR cycle in a day

OR = Daily oxygen requirement (kg/day)

6.3. Materials and Methods

The operational data of sequencing batch reactor and the average characteristics of leather tanning wastewater to be used in the aeration capacity calculations and modelling/simulations studies are adopted from the previous work of Murat *et al.* (2002). The SBR was operated in predenitrification mode with mixed filled phase followed by aeration phase. A total cycle time, T_C of 12 hrs (two cycles a day) was set for the SBR operation for carbon and nitrogen, where 10 hrs was devoted to the *process phase*, T_P and the remaining 2 h for *settle*, *draw* and *idle* phases ($T_S + T_D + T_I = 2$ hrs). The *mixed*, T_M was selected as 1.5 hrs, with continuous wastewater feeding ($T_{Fill} = T_M$) and the reactor was aerated for 8.5 hrs ($T_A = 8.5$ h), during the remaining portion of the process phase. A *fill volume*, V_F of 141-l was selected, leaving 703-l for the *initial volume*, V_0 and corresponding to $V_0/V_F = 5$. The nominal hydraulic retention time, θ_h of the system was set to 3 days. The total sludge age, θ_x was adjusted to 10 days. The mixed liquor temperature and pH were recorded steadily around 23°C and 7.5, respectively. For additional information, one should consult to Murat *et al.* (2002).

The wastewater characteristics on the basis of COD fractions and nitrogen can be summarized as follows: The total biodegradable COD is 1050 mgCOD/l (out of COD_{total}: 1340 mg/l) and the biodegradable total kjeldahl nitrogen, TKN is taken as 125.3 mgN/l (TKN_{total}: 139 mg/l). The readily biodegradable COD (S_S: 530 mgCOD/l), soluble hydrolysable COD (S_H: 280 mgCOD/l), soluble inert COD (S_I: 200 mgCOD/l), particulate hydrolysable COD (X_S: 240 mgCOD/l) and finally the particulate inert COD (X_I: 90 mgCOD/l).

In the first step of the study, the daily biological oxygen requirement, OR_{BIO} is calculated using the stoichiometric balance between biomass, COD and the nitrogen components (ammonia and nitrate) according to the method proposed by Artan *et al.*, (2002). Then, the biological oxygen requirement is compared to the oxygen requirements due to mixing, accordingly.

In the second step, the activated sludge model is calibrated manually using in-cycle ammonia-nitrogen (S_{NH}), nitrate-nitrogen (S_{NO}) and dissolved oxygen (S_{O2}) measurements. In order to visualize the influence of important parameters on system performance and identifiability, in-cycle absolute-relative sensitivity trajectories are simulated for the volumetric oxygen transfer coefficient (K_{La}), oxygen half saturation coefficient for heterotrophs (K_O) and ammonia half saturation constant for autotrophs (K_{NH}). The K_{La} parameter found in the calibration work is compared with calculated theoretically using the equation 6.1.

The last stage of the study deals with simulation study investigating the effect of process K_{La} on nitrogen removal efficiency of system as a result of different dissolved oxygen, S_O profiles obtained. The values of kinetic and stoichiometric coefficients were adopted from the previous study of Murat *et al.* (2002). The endogenous decay concept and dual hydrolysis kinetics were introduced in the model by considering only the carbon and nitrogen removal (Orhon and Artan, 1994). The AQUASIM (Reichert, 1998) simulation software is used for model simulations.

6.4 Results and Discussion

6.4.1 Calculation of volumetric oxygen transfer coefficient, K_{La_f}

The biological oxygen requirement, OR_{Bio} can be calculated using the stoichiometric equation 6.5. (Orhon and Artan, 1994). According to equation 6.5 As seen from the equation, the oxygen requirement which corresponds to the denitrified nitrate in mixing phase should be subtracted from the total oxygen requirement where E_{DEN} represents the denitrification efficiency of the system. By incorporating the components of ammonia nitrogen utilized for heterotrophic growth, N_x (equation 6.7) and oxidized nitrogen, N_{OX} (equation 6.8) in equation 6.5, the overall biological oxygen requirement, OR_{Bio} can be calculated as follows:

$$OR_{Bio} = Q [(1-Y_{NH})C_{S1} + 4.57 N_{OX} - 2.86 E_{DEN} N_{OX}] \quad (6.5)$$

$$OR_{Bio} = 0.282 [(1-0.38) \cdot 1050 + 4.57 \cdot 91 - 2.86 \cdot (5/6) \cdot 91]$$

$$OR_{Bio} = 0.282 [651 + 416 - 217] = 0.240 \text{ kg/day}$$

where,

$$Y_{NH} = Y_H \frac{1 + f_E b_H \theta_{XE}}{1 + b_H \theta_{XE}} = \frac{1 + 0.2 \cdot 0.15 \cdot 8.33}{1 + 0.15 \cdot 8.33} = 0.38 \quad (6.6)$$

$$N_X = i_{XB} Y_{NH} C_{S1} = 0.086 \cdot 0.38 \cdot 1050 = 34.3 \text{ mgN/l} \quad (6.7)$$

$$N_{OX} = C_{TKNbd} - S_{NHeffluent} - N_X = 125 - 34 = 91 \text{ mgN/l} \quad (6.8)$$

The K_{La_f} value of 66 day^{-1} can be calculated using equation 6.3 by incorporating the biological oxygen requirement obtained from equation 6.5. The aeration should also fulfill the mixing requirements during aeration phase if no other mixing devices are available. A generalized formula can be derived for the calculation of the oxygen transfer during mixing with air (see equation 6.9). Regarding the information on diffused aeration systems: (a) air flow rate necessary for sufficient mixing in the tank is $0.3 \text{ l-air /m}^3 \cdot \text{sec}$ (b) the weight of the air $0.239 \text{ kgO}_2/\text{m}^3 \text{ air}$ (c) the height of the water is 1.0 m . (d) the oxygen transfer efficiency, OTE is 20% for fine bubble aeration system (at $H_{water} = 4.5 \text{ m}$), the oxygen requirement for mixing, OR_{MIX} can roughly be calculated as:

$$OR_{MIX} = Q_{air} \cdot V \cdot W_{O2} \cdot (OTE/H_{water}) \cdot (T_A/T_C) \cdot 86400 \text{ sec/day}$$

$$\begin{aligned}
&= 0.003 \text{ m}^3/\text{m}^3 \cdot \text{sec} \cdot 0.844 \text{ m}^3 \cdot 0.239 \text{ kgO}_2/\text{m}^3 \cdot 20\% \div 4.5 \text{ m} \cdot (T_A/T_C) \cdot 86400 \text{ sec/day} \\
&= 1.62 \text{ kgO}_2/\text{d}
\end{aligned} \tag{6.9}$$

By assuming 2.0 mgO₂/l average dissolved oxygen concentration, S_O in the reactor. According to the results, the biological oxygen requirement (OR_{Bio}) is much lower than that of mixing by the factor of around 1/7. It should be noted that this calculation should be regarded as a comparison basis for the oxygen transfer due to biological requirement and mixing. However, in this study, the mixing was always provided by rotating mixers through the overall cycle time (TC). Hence, the aeration was not regarded as a bottle-neck during aeration phase of the SBR.

6.4.2 Model calibration and sensitivity analysis

In this section, a model calibration is needed due to the mismatch between the data and simulation results. The model calibration is performed by keeping the number of calibrated parameters at minimum level using the data of ammonia nitrogen, S_{NH4}, nitrate nitrogen, S_{NO3} and dissolved oxygen profiles, S_{O2} (see Figure 6.1). It should be noted that the NO₂-N concentration was always below 0.5 mg/l during the complete cycle. The half saturation constant for autotrophs, K_{NH} and oxygen half saturation for heterotrophs, K_O are manually calibrated and adjusted to 3 mgN/l and 0.4 mgO₂/day, respectively. Additionally, the K_{La}f value of 66 day⁻¹ has to be fine tuned and it is adjusted to 86 day⁻¹ to obtain a best model fit on all data set. In addition, the MLVSS concentrations (≈1600 mg/l) together with nitrogen content of the mixed liquor suspended solids (142 mgN/l) are also checked during the calibration and it was found to be in good agreement with the measurements taken from the end of aeration phase.

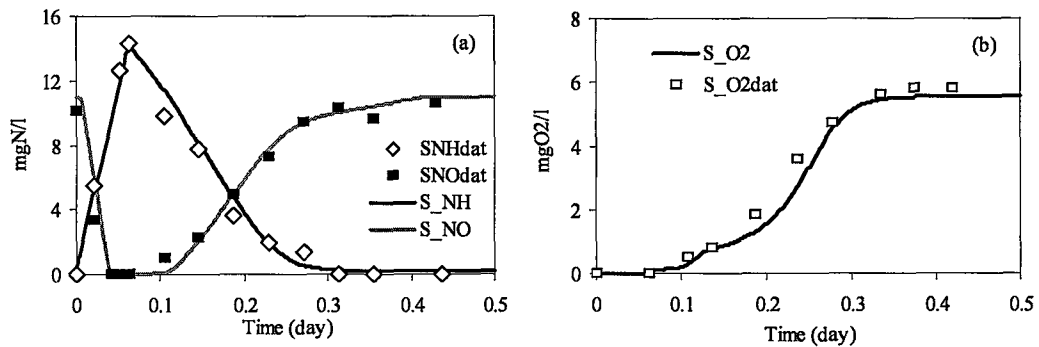


Figure 6.1 Simulation profiles for (a) nitrogen and (b) oxygen profiles

The simulated absolute relative parameter sensitivity trajectories for the ammonia, S_{NH} , nitrate, S_{NO} and dissolved oxygen, S_O (Figures 6.2 and 6.3) reveal that it is difficult to estimate K_{NH} and K_{OA} simultaneously since the trajectory profiles (for S_{NH} and S_{NO}) are nearly symmetrical. The K_{NH} parameter is used in the calibration because it is more sensitive to the simulation outputs rather than K_{OA} . In this respect, K_{OA} is set to its default value, 0.5 mgO_2/l as proposed in ASM2d (Henze *et al.*, 1999). In addition, the volumetric oxygen transfer coefficient, K_{La}^* yields maximum sensitivity level during the oxygen transition phase with respect to the oxygen, ammonia and nitrate (Figure 6.2 and Figure 6.3).

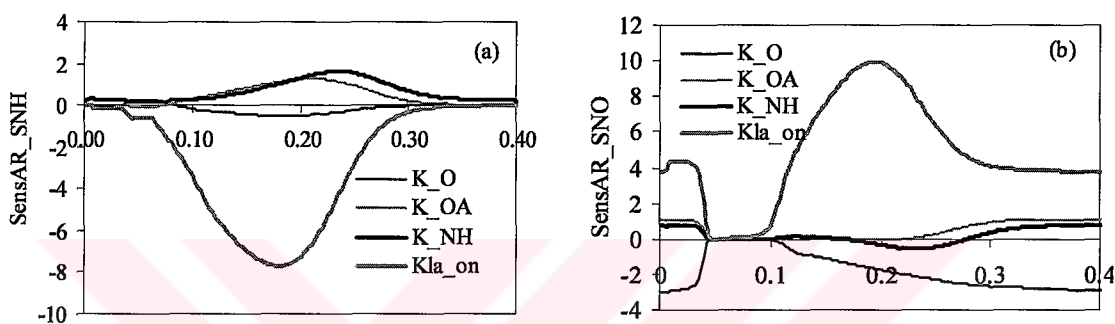


Figure 6.2 Absolute-relative sensitivity trajectories for (a) ammonia and (b) nitrate

6.4.3 Effect of aeration intensity on system performance

The selection of volumetric oxygen transfer coefficient, K_{La} for nutrient removing SBR is of great importance not only for maintaining sufficient aerobic sludge age, θ_{XA} for autotrophs but also for optimizing the effluent total nitrogen concentration. The Figure 6.4a illustrates the oxygen uptake rate, OUR segments for autotrophic and heterotrophic activities. According to the figure, the total oxygen uptake rate, OUR_{tot} increases up to 27 $mgO_2/l.h$ depending on oxygen switch functions incorporated in growth equations when the aeration is commenced. It should be noted that the maximum OUR values are limited by low oxygen levels at the start of the aeration. And the aeration only provides an OTR around 28 mgO_2/l with the calibrated K_{La_f} value of 86 day^{-1} . At the start of the aeration phase, the oxygen requirement is higher due to high oxygen requirement for heterotrophic growth running on remaining biodegradable COD.

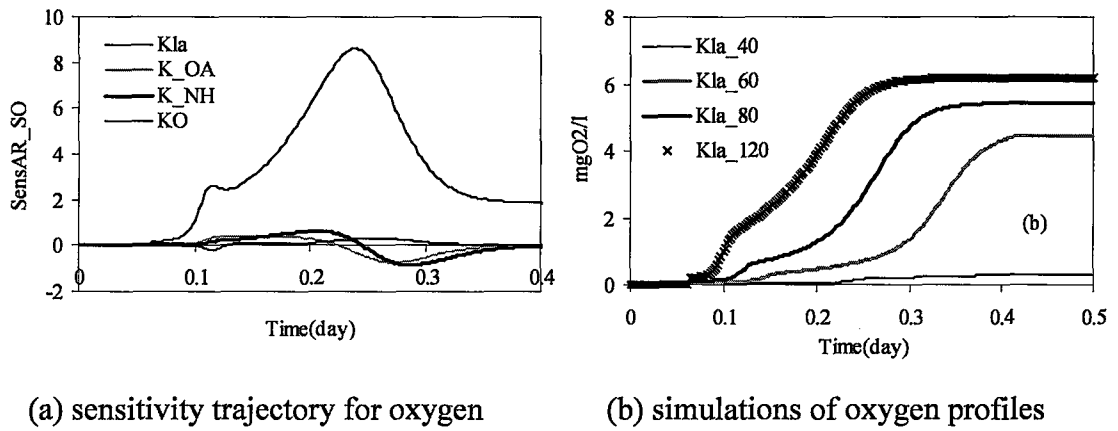


Figure 6.3 Simulations of (a) sensitivity trajectory for oxygen and (b) simulations of oxygen profiles for different K_{La} values

The distribution of oxygen utilization is not uniformly distributed and 5 times greater at the start of aeration phase (Figure 6.4a) compared to values at the end of the cycle. It is also expected that oxygen limitation resulted in a reduced autotrophic activity delineated with OUR_{aut} in Figure 6.4a. The OUR_{aut} increases from 5 $\text{mgO}_2/\text{l.h}$ up to 16 $\text{mgO}_2/\text{l.h}$ when the readily biodegradable COD is completely consumed around 0.12 days. Concomitantly, this gives rise to the oxygen concentration in the tank nearly in the mid of the aeration phase (Figure 6.1b).

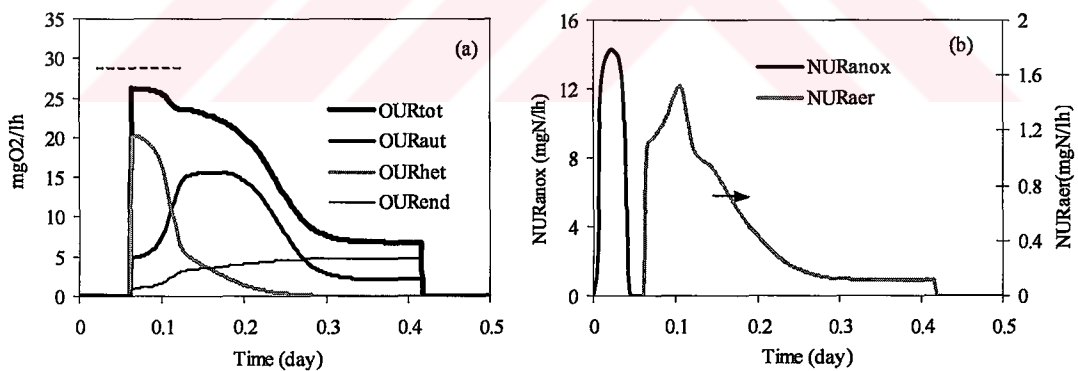


Figure 6.4 The simulations for (a) oxygen uptake rate, OUR and (b) nitrate utilization rate, NUR.

Another issue is the simultaneous nitrification and denitrification, SND (Rittman and Langland, 1985) during the transient phase of oxygen profile of SBR system (Figure 6.3b). Figure 6.4b shows the nitrate utilization rate, NUR in one SBR cycle. In the anoxic phase, NUR_{anox} increases to a maximum level of 14 $\text{mgN}/\text{l.h}$. Later, nitrate utilization rate in the following aeration phase (NUR_{aer}) is simulated to be 10 times

lower than the maximum level reached in anoxic (filling) phase (see Figure 6.4b-right axis). Based on the simulated profiles, NUR_{aer} increases until 1.6 mgN/L.h in parallel to the increase in the autotrophic activity at the start of aeration phase. Total area under the NUR_{aer} profile gives additional nitrate removed during SND at the beginning of the aeration phase.

A sudden drop in NUR_{aer} is then simulated since the readily biodegradable COD is consumed, rapidly. The SND is then mainly controlled by the consumption of slowly biodegradable COD until day 0.2 (see Figure 6.4a- OUR_{het}). Consumption of slowly biodegradable COD characterized by a tailing of OUR_{het} causes a gradual decrease in NUR_{aer} values. Shortly, at the start of aeration phase of SBR provides additional denitrification capacity when the external COD is available.

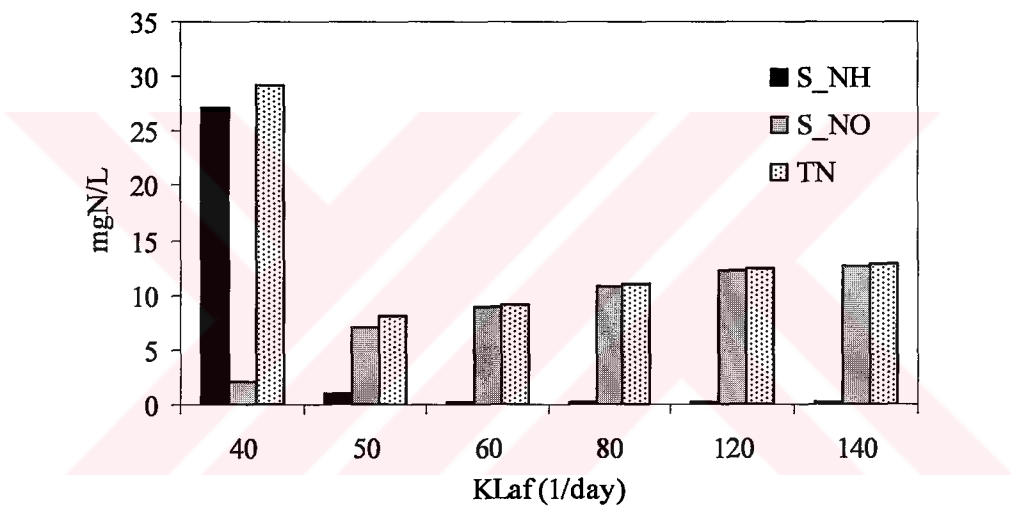


Figure 6.5 Simulation of K_{La_f} effect on effluent nitrogen components

Another simulation is carried out to visualize the effect of K_{La_f} on the effluent nitrogen components (Figure 6.5). Providing insufficient aeration below 50 day⁻¹ of K_{La_f} results in an increase of S_{NH} since the autotrophs are washed out from the system. The minimum oxygen requirement should be provided in order to allow autotrophic growth by ensuring the minimum aerobic sludge age (θ_{XA}). The minimum aerobic sludge age can be *theoretically* calculated using the equation below considering the oxygen concentration in the system (Metcalf and Eddy, 2003).

$$\frac{1}{\theta_{XA}} = \hat{\mu}_A \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_O}{K_{OA} + S_O} - b_A \quad (6.10)$$

However, the calculation of the minimum aerobic sludge age, θ_{XA} is quite difficult for the systems operated under low oxygen levels (see equation 6.10). With the aid of model simulations the minimum oxygenation corresponds to the K_{La_f} values in the range of 40-50 day⁻¹ to sustain sufficient autotrophic growth. In addition, the total effluent nitrogen level increased in parallel to the increments in K_{La_f} . The difference in effluent S_{NO} concentration simulated for the K_{La_f} of 50 and 120 day⁻¹ values is around 5.0 mgN/l which is due to the simultaneous nitrification and denitrification, SND. However, the aeration provided with K_{La_f} of 50 day⁻¹ gives the minimum effluent total nitrogen concentration. The effect of SND is clearly seen for the K_{La} values in the range of 50-120 day⁻¹ according to Figure 6.5. The SND process is promoted to some extent under reduced aeration. In Figure 6.3b, relatively minimum effluent total nitrogen (TN) is obtained for $K_{La_f} = 60$ day⁻¹ since the dissolved oxygen, S_O level is kept steadily around 0.5 mgO₂/l depending on OUR level. Hence, the dissolved oxygen set-point control may be necessary in order to maximize the nitrogen removal efficiency via SND (see Chapter 8). However, sufficient mixing should be provided in order to keep the mixed liquor in suspension when the aeration control is implemented.

6.5 Conclusions

An appropriate selection of aerator capacity for SBR systems is crucial in terms of satisfying the biological oxygen and mixing requirements. The theoretical calculations for oxygen requirement of SBR should be controlled via model simulations since the oxygen requirement is not uniformly distributed along the aeration phase. This situation may alter the total nitrogen removal efficiency of the system providing low dissolved oxygen levels at the start of the phase. The system can tolerate lower oxygen transfer rates compared to biological oxygen requirement.

Aside from the wastewater characteristics and operational conditions of SBRs, lower K_{La_f} values increase the total nitrogen removal performance via stimulating the simultaneous nitrification denitrification process, SND in the availability of biodegradable COD. The removal efficiency of SBRs can be increased with the

reduction of aeration to some extent. On the other hand, the minimum sludge age and mixing requirements should be taken into consideration.

The optimization of plant effluent together with the reduction of maintenance cost for aeration can be obtained by the appropriate selection and adjustment of aeration capacity with the aid of dissolved oxygen set-point control.



7 A CALIBRATION METHODOLOGY AND MODEL-BASED SYSTEMS ANALYSIS FOR SBRs REMOVING NUTRIENTS UNDER LIMITED AERATION CONDITIONS

7.1 Introduction

Sequencing batch reactors (SBR) are mainly characterized by sequential process phases of fill, react, settle, decant and idle periods that allow considerable flexibility in the design and operation in view of different biological wastewater treatment alternatives (Irvine *et al.*, 1997; Ketchum, 1997). This flexibility is provided by the unique features of SBRs which are: (a) influent and effluent flows are uncoupled by time sequencing (b) the clarification occurs in the same reactor (c) biological processes take place in a cyclic or periodic manner (d) a portion of the treated water is replaced by untreated wastewater for each cycle distinguishing the SBR process from other continuous flow type activated sludge systems (Wilderer *et al.*, 2001; Artan *et al.*, 2001). The design of an SBR for nutrient (nitrogen) removal is mainly based upon the selection of some relevant parameters (e.g. sludge age, volume exchange ratio, cycle time, SVI) as described in, for instance, the ATV guidelines (Teichgräber *et al.*, 2001) in combination with stoichiometric mass balance calculations on the denitrification potential, N_{DP} and available nitrogen, N_A (Artan *et al.*, 2001). In reality, the resulting wastewater treatment plants are mostly over-designed to sustain efficient carbon and nutrient removal under varying environmental and operating conditions. However, attention should be paid to the operating conditions, which may positively or negatively affect the overall system performance, even if the system is designed with safety margins. On the other hand, the optimization of operating parameters (e.g. aeration control) can be an asset to take advantage of simultaneous nitrogen removal together with enhanced biological

This chapter was presented at the 3rd IWA-SBR conference:

Insel, G., Sin, G., Lee, D.S. and Vanrolleghem, P.A., 2003. A calibration methodology and model-based system analysis for nutrient removing SBRs, 3rd IWA International conference on SBR, February 22-26th, Noosa, Queensland, Australia.

phosphorous removal known as ‘simultaneous nutrient removal’ (Daigger and Littleton, 2000).

An existing SBR plant may require a trustable optimization in terms of nutrient removal, but that necessitates better understanding and quantification of the biological processes occurring in each phase. A calibrated activated sludge model is a practical tool to try numerous operation scenarios within a short evaluation time when an upgrade of the SBR is considered (see Chapter 8). In this way, the effect of changes in process configuration/control and environmental factors can be simulated and appropriate measures can be taken in due course. However, model calibration requires expert knowledge on the influent wastewater characterization, on-line/off-line measurements, operating conditions and the treatment system itself. The model-based interpretation of the system than can then be attempted not only leads to better understanding of the biological processes but also provides a way of selecting the most appropriate operating variables to manipulate such as cycle times, aeration capacity *etc.*

In this respect, this paper describes a ‘calibration methodology’ for a lab-scale SBR performing simultaneous nutrient removal under limited aeration conditions. In addition, a systems analysis is performed via the investigation of individual biological process contributions to phosphate utilization, oxygen consumption and nitrogen removal by using the calibrated model.

7.2 Materials and Methods

7.2.1 SBR Operation and process control

A pilot-scale sequencing batch reactor (SBR) with a working volume of 80 L was seeded with sludge from the Ossemeersen wastewater treatment plant (Gent, Belgium) and operated for a 2-year period. The hydraulic retention time (HRT) and solids retention time (SRT) are maintained at 12 hrs and 10 days, respectively. Each cycle comprises an unaerated fill phase (60 min), aeration phase (150 min), anoxic phase (60 min), aerated phase (30 min), settling (45 min) and draw (15 min) phases. The total cycle time, C_T was set to 6 hours (4 cycles per day) with volumetric exchange ratio

(V_0/V_{Total}) of 0.5. The excess sludge is wasted from the end of the aerobic phase for each cycle. A schematic diagram of the SBR system is given in Figure 7.1.

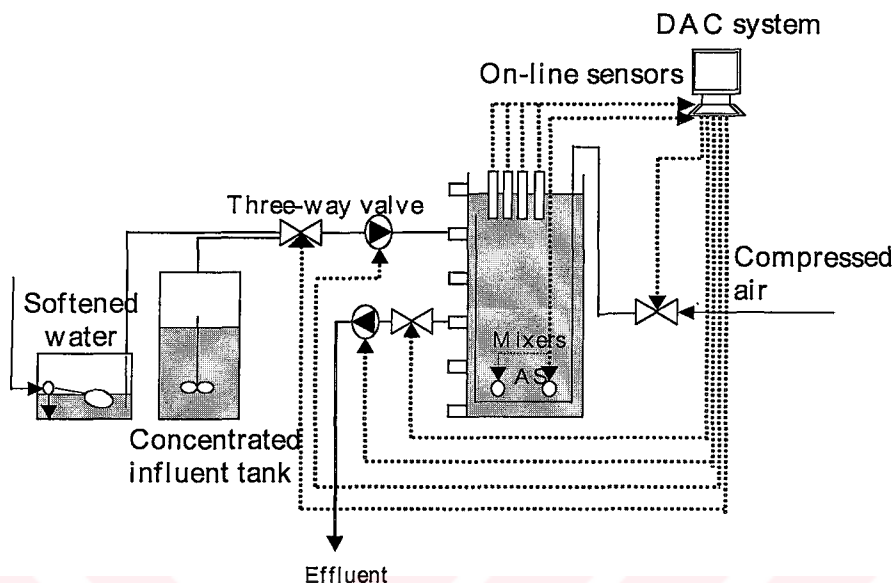


Figure 7.1 Schematic diagram of the SBR system

The controls of the duration/sequence of phases and on/off status of peristaltic pumps, mixer and air supply are automatically achieved by a LabView data acquisition and control (DAC) system. The DAC system consists of computer, interface cards, meters, transmitters and solid-state relays. Electrodes for pH, ORP (oxidation-reduction potential), DO (dissolved oxygen), temperature, weight and conductivity are installed and connected to the individual meters. The status of the reactor is displayed on the computer and the time series of the electrode signals are stored in a data log-file. The aeration is controlled by turning on-off the aeration valve. The oxygen is kept around 2 mgO₂/L with an on-off controller with 0.5 mgO₂/L dead band. Synthetic sewage representing the pre-settled domestic wastewater (Boeije *et al.*, 1998) is used as SBR influent. Based on the model, the influent wastewater characterization in terms of COD fractions, nitrogen and phosphorus components are summarized in Table 7.1. The measured output variables of ortho-phosphate, dissolved oxygen, ammonia and nitrate nitrogen were used in the calibration study. The volumetric oxygen mass transfer coefficient, K_{La} , was measured to be 255 d⁻¹. All measurements were carried out according to Standard Methods (APHA, 1998).

7.2.2 Wastewater characteristics

In the modeling studies, a modification of ASM2d (Henze *et al.*, 1999) was used by the addition of ammonification and hydrolysis of organic nitrogen processes since the influent wastewater contains soluble (0.45 μm) and particulate organic nitrogen that slowly degrade. The settling and decanting phase were characterized by a reactive point-settler model (Kazmi *et al.*, 2001). The simulations were carried out using the WEST simulation package (Vanhooren *et al.*, 2003).

Table 7.1 ASM2dN based influent wastewater characterization (adapted from Boeije *et al.* 1998)

Component	Unit	Concentration	Measurement
Total COD, COD_{tot}	mgCOD/l	411	Lab. analysis
Particulate Inert COD, X_I	mgCOD/l	18	Lab. analysis
Soluble Inert COD, S_I	mgCOD/l	18	Effluent analysis
Biodegradable COD, C_S	mgCOD/l	375	
Fermentable COD, S_F	mgCOD/l	95	Mass balance
Acetate COD, S_A	mgCOD/l	70	GC analysis
Slowly biodegradable COD, X_S	mgCOD/l	210	Mass balance
Ortho-P, $S_{\text{PO}_4\text{-P}}$	mgP/l	11	Measurement
Total Kjeldahl Nitrogen TKN	mgN/l	63	Lab. analysis
Ammonium nitrogen, $\text{NH}_4\text{-N}$	mgN/l	3	Lab. analysis
Soluble biodegradable nitrogen, S_{ND}	mgN/l	10	Mass balance
Particulate biodegradable nitrogen, X_{ND}	mgN/l	50	Mass balance

7.3 Results and Discussion

7.3.1 Measurement campaign results

On-line measurements were performed in the reactor (Figure 7.2). The nitrification end point, the consumption of nitrate due to denitrification and the phosphate release can be observed from these measurements (Spagni *et al.*, 2001). The corresponding oxygen, O_2 , filtered ortho-phosphate, $\text{PO}_4\text{-P}$, the nitrate nitrogen, $\text{NO}_3\text{-N}$, and ammonia nitrogen, $\text{NH}_4\text{-N}$, measurements are presented in Figure 7.3 and 4. The nitrite nitrogen was found to be negligible. At the beginning of the fill period, a small increase in the oxygen profile occurred because of an inherent oxygen transfer during the feeding and mixing. The gradual pH decrease under anaerobic (filling) conditions can be explained by the net

effect of (slow) phosphorus release and denitrification processes. As soon as the consumption of nitrate in the fill phase is completed (Figure 7.4), a rapid drop in pH can be observed, probably due to fermentation and phosphate release. During the first aerated period, the oxygen concentration is quite low (around 0.3 mg/l) as a result of high oxygen consumption by biomass for readily biodegradable COD degradation with fixed aeration intensity. The effect of CO₂ stripping on the pH profile seems to be higher than that of nitrification up to the mid of the aerated phase (Figure 7.2). The oxygen concentration increased up to the controlled band of 2 ± 0.5 mgO₂/L. In the following phases, it decreased to zero just after the termination of aeration (Figure 7.2-right).

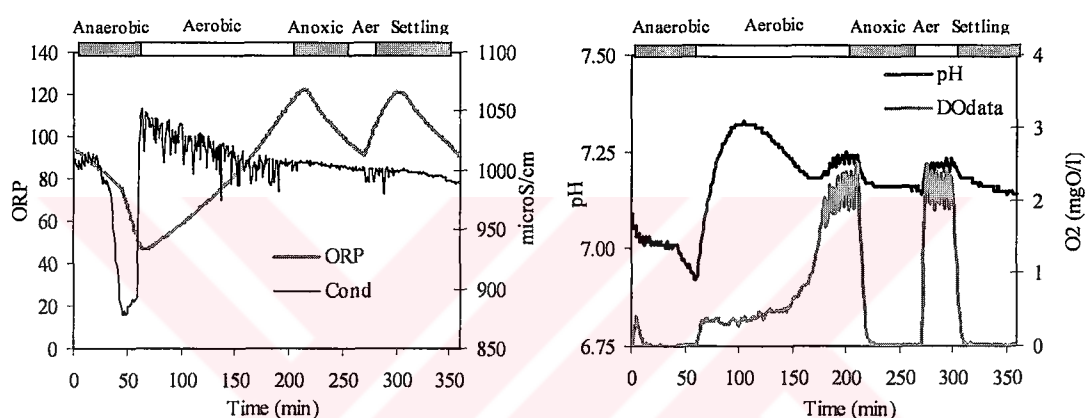


Figure 7.2 On-line measurements (left) ORP, conductivity and DO, pH (right)

The phosphate concentration increased during the fill phase because of P release (VFA uptake) and filling. Figure 7.3-right shows that the rate of phosphorus release increased as soon the nitrate was consumed. The remaining VFA was consumed with P-release (Comeau *et al.*, 1990; Kuba *et al.*, 1996). At the end of the first phase, after a steep decline, a gradual increase in the conductivity measurements can be observed after the NO₃ consumption is completed. This can be attributed to phosphorus release which liberates ions into the bulk. In the aerobic phase, the phosphate is taken up again. There is a slight increase in the phosphate concentration during the 2nd anoxic period probably because of endogenous P-release and COD turnover from the endogenous biomass.

The NH₄-N and NO₃-N profiles are quite interesting in terms of their order of magnitude at the end of the aerobic phase (Figure 7.4-left). The NO₃ generation is much higher than the observed NH₄-N consumption. This observation reveals that organic nitrogen is

transformed into $\text{NH}_4\text{-N}$ and nitrified to $\text{NO}_3\text{-N}$ directly and that, in fact, only a net $\text{NH}_4\text{-N}$ conversion rate is measured. Indeed, after the complete oxidation of $\text{NH}_4\text{-N}$, the $\text{NO}_3\text{-N}$ build-up continues until the end of the first aerobic period. So, the degradation of organic nitrogen becomes the rate-limiting step and must be incorporated in the model in such a way that it is controlled by the hydrolysis mechanism. In the 2nd aerobic period, $\text{NO}_3\text{-N}$ increased from 17 to 20 mgN/L. The organic nitrogen in the effluent water was measured analytically to be around 1.0 mgN/L which is also in agreement with the simulation result (Figure 7.4-right). It should be stressed that the total phosphate mass balance resulted in a 98% recovery confirming the exact total sludge age of the system. Within the observation period covering the calibration study, consistent long-term data with respect to effluents together with online measurements shows that the system - under constant conditions- is still at steady state.

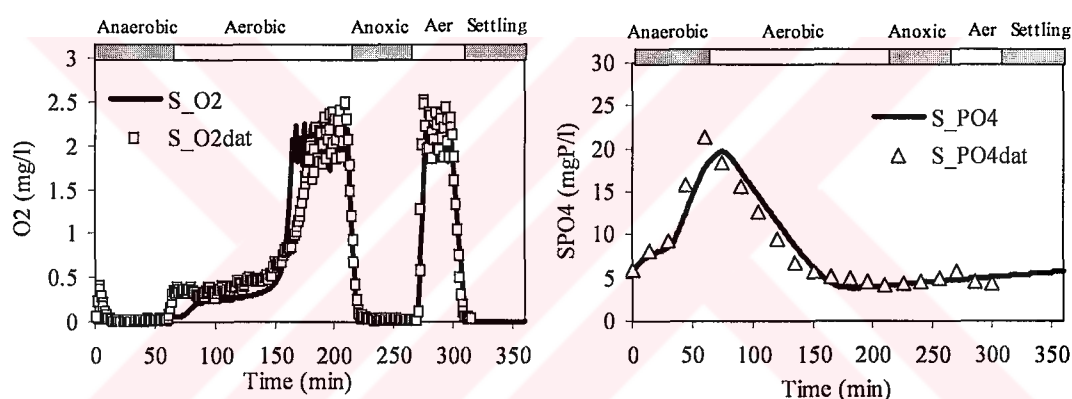


Figure 7.3 Measurements (symbols) and simulations (lines) of the dissolved oxygen (left) and phosphate (right)

7.3.2 Activated sludge model selection

The activated sludge model used was built on the basis of ASM1 and ASM2d (Henze *et al.*, 1987; 1999). According to the influent wastewater characterization, the nitrogen transformations were incorporated as an integral module (see Appendix-A, Table A1). An approach similar to ASM1 was used. The particulate nitrogen is first hydrolysed to soluble organic nitrogen, S_{ND} , and then ammonified to $\text{NH}_4\text{-N}$ by heterotrophic biomass.

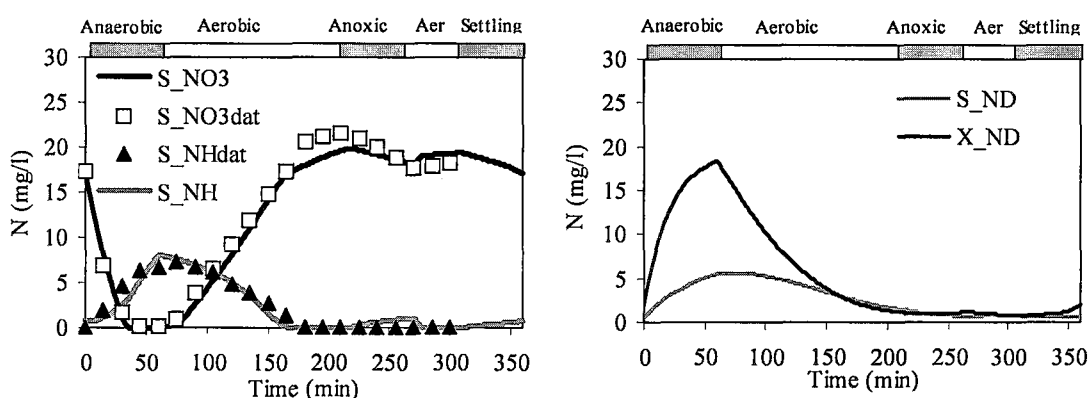


Figure 7.4 Measurements (symbols) and simulation (lines) of NH_4/NO_3 (left) soluble/particulate nitrogen (right)

The hydrolysis kinetics under anaerobic and anoxic conditions are adapted with correction factors. The kinetics and stoichiometry for autotrophs, the heterotrophs and phosphorus accumulating microorganisms are taken from the ASM2d model except for the anoxic heterotrophic yield, Y_{HNO_3} . The default values of the parameters were taken as starting point. The phosphorus components (soluble and particulate) were taken as a fraction of the influent COD fractions and model components. The conservation of the components was calculated according to Gujer and Larsen (1995).

7.3.3 Calibration methodology

A stepwise calibration methodology was developed based on long-term simulations in each iteration step (see Figure 7.5). As illustrated in Figure 7.5, a calibration methodology based on expert knowledge was constructed by introducing 4 iterative steps in the order of $\text{NH}_4\text{-N}$, O_2 , $\text{NO}_3\text{-N}$ and $\text{PO}_4\text{-P}$ profiles, respectively. For each iteration, a 30 day-simulation was carried out to ensure that the state variables gave the same trend in each cycle (“steady state”). The starting point is to obtain the proper activity of the autotrophs to generate $\text{NO}_3\text{-N}$. In the first long-term simulation with the default parameter values, the autotrophs were washed out from the system. As a result, the nitrogen half saturation coefficient for autotrophs, K_{NHaut} , was decreased because of the low ammonia concentration in the aerobic phase. Next, the maximum growth rate for autotrophs, $\hat{\mu}_A$, had to be increased in order to sustain autotrophic growth. Later on, the oxygen half saturation constants for autotrophs, K_{NHaut} , and heterotrophs, K_{NH} , were

changed to promote heterotrophic growth. In addition, the half saturation constant for hydrolysis, K_X , was included in the calibration to get better fitting of the O_2 profile (Figure 7.3-left). It should be noted here that each iteration step comprises the preceeding steps to maintain good NH_4 -N, O_2 , NO_3 -N and PO_4 -P fits.

In the third step, the anoxic yield was adjusted (0.58 mgCOD/cellCOD) in order to increase the denitrification potential and fit the measured nitrate concentrations. In the literature, the anoxic yield was also reported to be lower than the aerobic yield coefficient (Muller *et al.*, 2003; Orhon *et al.*, 1996). The slope of nitrate during the fill phase was well achieved by the calibration of the heterotrophic lysis rate, b_H . The MLVSS component could be added to Figure 7.5, but no additional calibration effort was needed for this case. It was measured and simulated around 2000 mg/l. The simulated soluble, S_{ND} , and particulate nitrogen, X_{ND} , profiles are illustrated in Figure 7.4-right. Finally, the fourth step deals with the calibration of the kinetic constants for the PAOs. The maximum acetate uptake rate of the PAO's, q_{PHA} , had to be increased in order to have them compete successfully with ordinary heterotrophs during the fill phase in the presence of NO_3 -N. The reason is that high NO_3 -N concentrations during the first 30 minutes of the fill phase caused a high denitrification rate, which consumes VFA before the true anaerobic period begins.

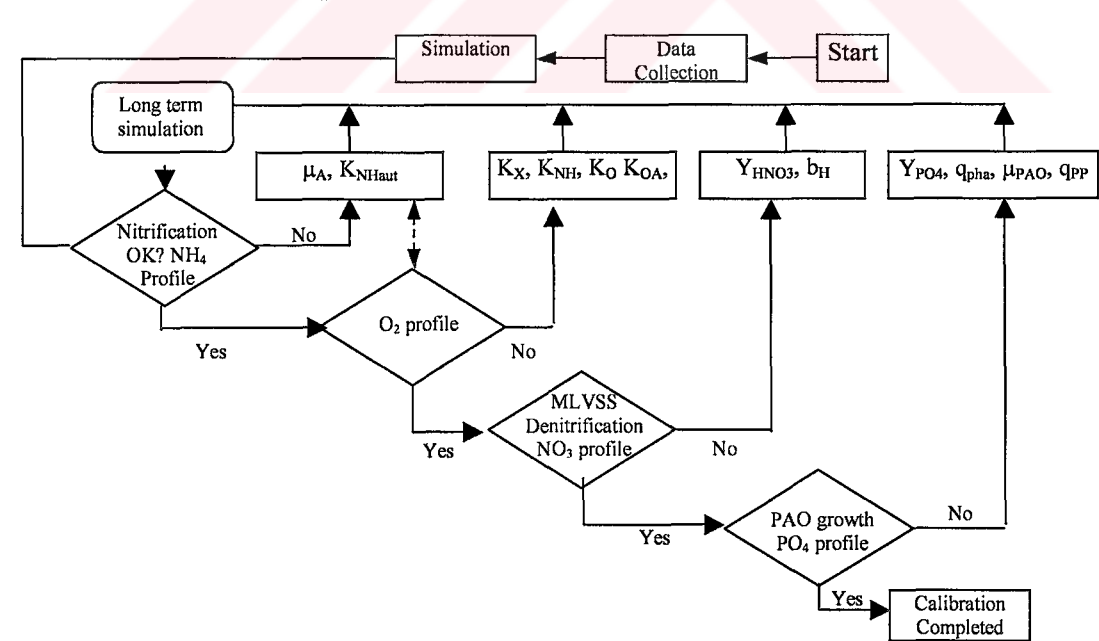


Figure 7.5 Calibration methodology for the ASM2dN model

Table 7.2 Summary of the calibrated ASM2dN parameters

Parameter	Unit	Default	Calibrated
<i>Heterotrophs, X_H</i>			
Anoxic heterotrophic yield, Y_{HNO_3}	mgCOD/mgcellCOD	0.63	0.58
Endogenous decay rate for heterotrophs, b_H	day ⁻¹	0.4	0.45
Half saturation constant for hydrolysis, K_X	mgCOD/mgcellCOD	0.1	0.045
Saturation/Inhibition coefficient for O ₂ , K_O	mgO ₂ /l	0.1	0.06
<i>Phosphorus Accumulating Organisms, X_{PAO}</i>			
Half saturation constant for ammonia (heterotrophs), K_{NH}	mgN/l	0.05	0.01
Yield coefficient for phosphate release, Y_{PO_4}	mgP/mgCOD	0.4	0.38
Rate constant for storage of PHA, q_{PHA}	gCOD/gPP.d	3.0	6.0
Maximum phosphorus storage rate, q_{PP}	gP/gcellCOD.d	1.5	1.3
Maximum growth rate for PAOs, μ_{PAO}	day ⁻¹	1.0	1.8
<i>Autotrophs, X_A</i>			
Maximum growth rate for autotrophs, $\hat{\mu}_A$	day ⁻¹	1.0	1.5
Saturation coefficient for O ₂ (autotrophs), K_{OA}	mgO/l	0.5	0.07
Half saturation constant for ammonia (autotrophs), K_{NHA}	mgN/l	1.0	0.2

In order to determine the ratio of anoxic/aerobic P uptake ratio (η_{NO_3PAO}) anaerobic-aerobic and anaerobic-anoxic phosphate uptake tests were carried out according to Brdjanovic *et al.* (1999) (results not shown). The ratio of η_{NO_3PAO} was found to be around 0.6, which is in conformity with the proposed default value in ASM2d (0.6). The yield for phosphate release, Y_{PO_4} , had to be decreased to fit the fill-phase PO₄-P profile. As stated in the ASM2d model, the storage compound, X_{PHA} , is consumed by two simultaneous processes, i.e. the phosphate uptake and the growth of PAOs. During calibration, the concentration of X_{PAOs} was increased by adjusting the maximum growth rate of PAOs, $\hat{\mu}_{PAO}$, to a higher value. Meanwhile, to achieve steeper slope and also to reach the constant PO₄ concentration at the end of the aerobic phase, the maximum phosphate uptake rate, q_{PP} , was increased (Figure 7.2-left). The calibration task was terminated when the simulated profiles were closest to all measured data (see Figure 7.2-4). The values of the calibrated parameters together with their default values are listed in Table 7.2.

7.3.4 System analysis

Using the calibrated model, the trajectories of the process rates were drawn to visualize the contribution of each process to the overall SBR behaviour. It is obvious from Figure 7.6-left that the P-release rate after the mid of the fill phase is 2.5 times higher (21 mgP/l.h) than that at the beginning of the phase (7.5 mgP/l.h) because of the removal of NO₃-N. This continues until the external carbon source is consumed completely after

around 100 min and the oxygen concentration increases. The nitrate production rate (NPR) immediately increased when aeration is turned on. The rate dropped from 13 mgN/l.h to around 5 mgN/l.h when it became hydrolysis limited.

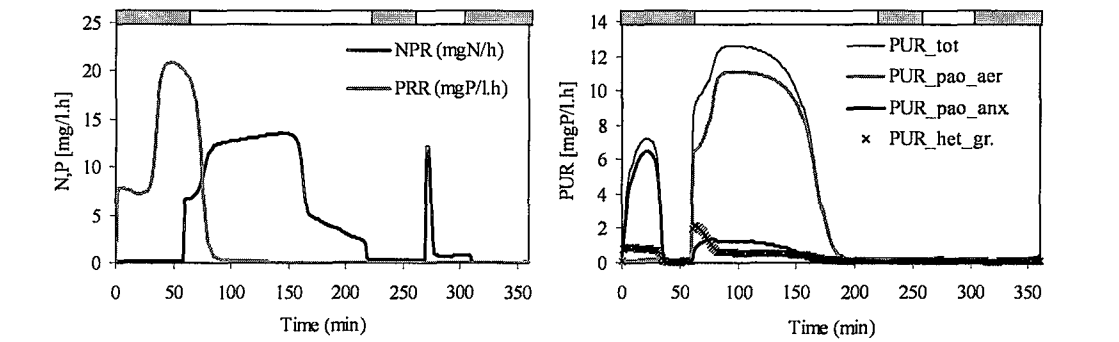


Figure 7.6 Nitrate production, P-release (left) and segments of phosphate utilization rate (right)

The simulation for the total phosphate uptake rate, PUR, reveals that the maximum contribution pertains to the aerobic phosphate uptake by the PAOs (73% of the overall P uptake) initially exhibiting an uptake rate of 11 mgP/l.h (Figure 7.6-right). As can be observed from Figure 7.6-right and Figure 7.7, P-release, anoxic P-uptake and VFA storage took place simultaneously. It is important to mention here that 19% of the removed P is taken up by the PAOs anoxically during the fill phase (12%). In the aerobic phase 7% of P is removed (Figure 7.8). The rate of the anoxic P uptake at the start of the aerobic phase was simulated to be around 1.4 mgP/l.h. The P uptake via heterotrophic growth only covers 8% of the overall P-removal (growth of nitrifiers is neglected).

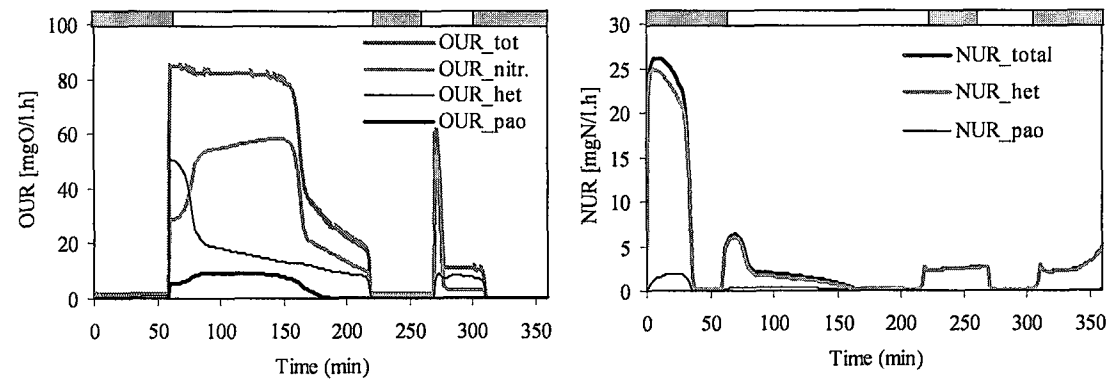


Figure 7.7. OUR and NUR contributions in a SBR cycle

According to the simulation results, the distribution of denitrified nitrogen over each of the phases can be summarized as follows: (a) 61% of total denitification took place in the first phase (fill phase), (b) 17% was denitrified under aerobic conditions due to simultaneous nitrification-denitrification (Munch *et al.*, 1996), (c) 10% denitrification was achieved in the 2nd anoxic period and (d) 10% denitrification in the settling phase. The simulation based calculations showed that 22 mg/L NO₃-N was denitrified in one cycle which is comparable with the denitrification potential calculation performed according to Artan *et al.* (2001) which led to a value of 18 mgN/l. This difference can be explained as follows. First, it should be acknowledged that the 22 mg/L does not regard the denitrification potential used by the PAOs. Another point is the additional denitrification in the aerobic phase due to low oxygen levels. This is not considered in the stoichiometric calculation. The nitrate utilization rate, NUR, is mainly governed by ordinary heterotrophic activity, i.e. 89% of the total denitrified nitrogen is used up by these microorganisms. Only 11% is consumed in denitrifying PAO activity (Figure 7.7-right).

The maximum total oxygen uptake rate, OUR, is around 82 mgO₂/l.h until 150 min (nitrification end point) and is governed by the oxygen transfer capacity. Within the aerobic phase, the maximum oxygen uptake rates for the autotrophs, heterotrophs and PAOs are around 50, 50 and 10 mgO₂/l.h, respectively. However these maximum rates are reached in different periods of the aerobic phase (see Figure 7.7). The distribution of cumulative oxygen consumptions over the processes is given in Figure 7.8-right. The autotrophic biomass accounts for 63% of the total oxygen consumption of the system. The ordinary heterotrophs only consume 29%.

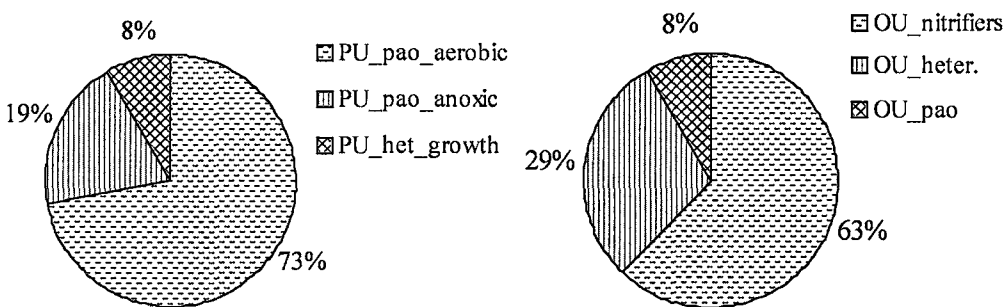


Figure 7.8 The phosphate and oxygen utilization in one SBR cycle

7.4 Conclusion

A systematic model calibration methodology was applied successfully to a lab-scale SBR exhibiting simultaneous nitrification-denitrification together with biological phosphorus removal, the so-called 'simultaneous nutrient removal'. The biological processes described in the model were found to occur simultaneously under limited aeration conditions. A low oxygen transfer inherently differentiates the system behaviour from systems under traditional design calculations. As a result, the oxygen transfer should strictly be incorporated in the calibration of biological nutrient removal to visualize the individual contributions of each process. From this point of view, models may serve as practical tools to evaluate alternatives for the optimization of SBR's. The stepwise calibration methodology applied here is necessary for an effective selection of the relevant parameters to be calibrated.

The systems analysis performed with the calibrated model clearly illustrated that the denitrification at the start of the aerobic phase and during the settling phase has a considerable contribution to the overall denitrification capacity of the system and also affects biological phosphate removal. It therefore warrants further study.

8 OPTIMAL BUT ROBUST N & P REMOVAL IN SBRs: A MODEL-BASED SYSTEMATIC STUDY OF OPERATION SCENARIOS

8.1 Introduction

Sequencing batch reactor (SBR) technology for nutrient removal has received worldwide attention from the wastewater treatment community in view of the ever-stricter demands on effluent discharge quality (Wilderer *et al.*, 2001). Both nitrogen and phosphorous removal from wastewaters have been demonstrated successfully at lab-scale and full-scale installations (Manning and Irvin, 1985; Furumai *et al.*, 1999; Keller *et al.*, 2001; Wilderer *et al.*, 2001; Demoulin *et al.*, 2001)

Being flexible to operate, a myriad of operation strategies have been developed to optimize nutrient removal performance in SBRs (Wilderer *et al.*, 2001). The operational strategies have been usually tested experimentally at lab-scale (Manning and Irving, 1985; Lin and Jing, 2001; Hvala *et al.*, 2001). Increasingly, mathematical models (e.g. ASM1 for N-removal and ASM2d for N and P-removal) have been used for developing and testing optimal operation strategies for biological N and P removal (Demuyne *et al.*, 1994; Hvala *et al.*, 2001; Artan *et al.*, 2002a). The main parameters that have been demonstrated in the above-mentioned studies to impose a major effect on the N and P removal capacity of the SBRs until now are the step-feed of the influent (Hvala *et al.*, 2001; Lin and Ying, 2001), intermittent aeration (Hanhan *et al.*, 2003; Demuyne *et al.*, 1994; Demoulin *et al.*, 2001; Lin and Tsang, 1989), oxygen set-point in the aerobic react-phase to regulate the extent of simultaneous nitrification and denitrification (Munch *et al.*, 1996; Artan *et al.*, 2002a) in the SBR as discussed in Chapter 6 and length of anaerobic, aerobic and anoxic phases (Wilderer *et al.*, 2001; Artan *et al.*, 2002a).

The objective of this study is to develop a systematic approach to determine the best operation strategy for the optimization of the N and P removal performance of the

Main parts of this chapter were presented at the 3rd IWA-SBR conference:

Sin, G., Insel, G., Lee, D.S. and Vanrolleghem, P.A., 2004. Optimal but robust N and P removal in SBRs: A model-based systematic study of operational scenarios, 3rd IWA International conference on SBR, February 22-26th, Noosa, Queensland, Australia.

SBR technology. The methodology is based on using a grid of scenarios to simulate the effect of different degrees of freedom on the SBR system. The scenarios, i.e. the operation strategies formulated using realistic combinations of the significant degrees of freedom tested so far elsewhere, are simulated using the ASM2dN model developed and calibrated in Chapter 7. Criteria for the selection of the best scenario are proposed based on not only the effluent quality but also the robustness against deviations of the modelled reality (Vanrolleghem and Gillot, 2002). Finally, the systematic approach has been applied to a lab-scale SBR. Particular attention is given to the oxygen set-point in the aerobic react phase and the sludge age on the overall performance of the SBR system.

8.2 Materials and Methods

8.2.1 Simulation platform

A lab-scale sequencing batch reactor (SBR) with a working volume of 80 L was seeded with sludge from the Ossemeersen WWTP (Ghent, Belgium). It is operated in a 6 h cycle mode, each cycle consisting of 60 min fill/anaerobic, 150 min aerobic, 60 min anoxic, 30 min aerobic and 60 settling/draw phases. A synthetic sewage is used as SBR influent, which was shown to mimic a real pre-settled domestic wastewater. The detailed description of the SBR is given in Chapter 7.2.1. Simulations were performed using WEST (Hemmis, Belgium) a dedicated software for the modelling of WWTP that contains a scenario analysis module (Vanhooren *et al.*, 2003).

8.2.2 A systematic methodology for the optimization of SBR systems

The model-based optimization of the lab-scale SBR is performed following the methodology described in Figure 8.1. The first step is the definition of the objective of the optimization study. This will determine the required calibration accuracy and serve as the main criterion in selecting the optimal operation strategy for the system. The second step is the description of the system including the definition of the degrees of freedom and constraints of the system, which will determine the framework of the optimization.

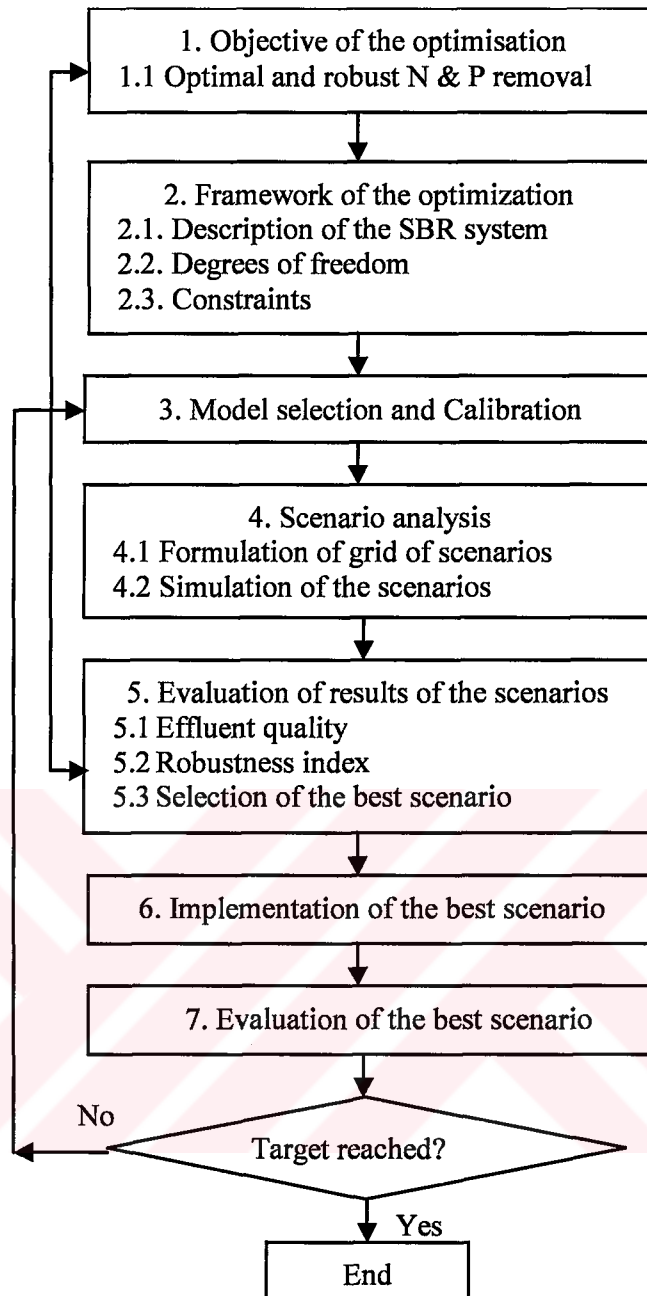


Figure 8.1 A systematic methodology for the model-based optimization of SBR systems

This is followed by the model selection and calibration step to obtain a realistic model-based description of the SBR system. Following this step, i.e. step 4, a grid of scenarios based on the above degrees of freedom and constraints is formulated and simulated using the calibrated model. The results of the scenarios are evaluated in the following step, i.e. step 5. The analysis of the results is expected to provide in-depth insight into the operation scheme of the SBR system. In this step, the optimal scenario is chosen considering the objective of the optimization. Two criteria are

proposed for this purpose: the effluent quality and the robustness of the system to deviations of the modelled system (Vanrolleghem and Gillot, 2002). Afterwards, the best scenario should be implemented to the SBR system. The last step i.e. step 7 is to check if the objective of the optimization is reached. To this aim, a measurement campaign should be carried out after the SBR system reaches a new steady-state. If the SBR performance under the newly implemented operation conditions is not satisfactory, the procedure should be iterated starting from step 3.

8.3 Results and Discussion

8.3.1 Application of the systematic methodology to a Lab-scale SBR

8.3.1.1 Objective of the optimization

In this study, the objective of the optimization is to find an optimal and robust SBR operation scenario that achieves the best possible effluent quality with respect to N and P removal under given physical boundary and influent characteristics.

8.3.1.2 Framework for the SBR optimization: degrees of freedoms and constraints

Being flexible systems to operate, SBR systems offer a large number of operation-variables to be optimized. Ideally, all possible operation variables should be used in the optimization of the SBR system. However, the number of the degrees of freedom that can be selected must be limited due to the resulting too high computational demand (In this study, simulation of one scenario takes on average 25 min with a 1GHz Pentium III processor). In this study, based on a survey of the relevant literature (see Section 8.1) and a preliminary model-based analysis of the system (see Chapter 7.3.4), the following degrees of freedoms were identified and used for the SBR optimization:

- (1) Oxygen set-point (S_{O-sp}) in the aerobic react phase,
- (2) Length of the anaerobic phase (T_{ANB}),
- (3) Length of the reaction (aerobic and anoxic) phase (T_R i.e. $T_{AER} + T_{ANX}$),
- (4) Step-feed of the influent organic load ($V_{step-feed}$) and

(5) Intermittent aeration frequency (IAF), which is explained below.

The constraints of the optimization study stem from several reasons including the lower and upper boundaries of the degrees of freedoms, the physical boundary of the SBR (e.g. maximum volume of the SBR, influent pump capacity etc.), and the priorities of the objective of the optimization. In this study, the solids retention time, SRT (10 d), hydraulic retention time, HRT (12 h), the volumetric exchange ratio, i.e. the ratio of the fill volume to the maximum volume of the reactor (0.5), and the total cycle time (360 min) are fixed. Further, the mass transfer coefficient for oxygen (K_{La}) is fixed to a sufficiently high value (500 d^{-1}) to ensure the oxygen set-point can be maintained effectively with on/off control. The last aerobic react phase is fixed to 30 min to strip the nitrogen gas entrapped in the flocs and to polish the effluent prior to discharge to the receiving water. The minimum anaerobic time is set to 60 min based on preliminary simulation results with the SBR model. The length of the settling/draw phase is also fixed to its design value (60 min) as this incorporates a safety margin to provide sufficient settling time in case of a sludge bulking event.

8.3.1.3 Model selection and calibration

From the dynamic ammonium and nitrate trends in the SBR, it was observed that the degradation of organic nitrogen (i.e. hydrolysis and ammonification) is the rate limiting-step in the over-all nitrogen turnover in the SBR (Chapter 7). This was probably due to the high fraction of organic nitrogen present in the influent (ca. 95%), which is not typical for domestic wastewaters for which ASM2d is valid. As a result, the ASM2d model had to be extended with a hydrolysis process for the entrapped organic nitrogen (ASM1) to adequately describe the dynamic N and P trends in the SBR (see Annex A-Table A1). The calibration of the so-called ASM2dN model is given in Chapter 7.3.3.

8.3.1.4 Scenario analysis: formulation and simulation of grid of scenarios

A grid of scenarios considering the degrees of freedom and the constraints of the system mentioned above was formulated as a full-factorial experimental design (Table 8.1). The intermittent aeration frequency (IAF) (Table 8.1) refers to the number of aerobic and anoxic sequences/sub-phases during the reaction phase excluding the last aerobic period. For instance, IAF 2 means that there are 2

aerobic and 2 anoxic (in total 4) sub-phases in the react phase (see Figure 8.2B). In the implementation of the intermittent aeration for the SBR model (see Figure 8.2.B), the length of the total aerobic react phase (T_{AER}) is divided equally by the number of aeration sub-phases, i.e. 1, 2, 4 and 8. For instance, when the aeration frequency is equal to 2, the length of each aerobic sequence is equal to the length of the total aerobic react phase divided by 2, i.e. $T_{AER}/2$. In the same way, the length of the anoxic sequence is equal to the total length of the anoxic-react phase (T_{ANX}) by 2, i.e. $T_{ANX}/2$. Further, the step-feed volume is partitioned equally between the anoxic sequences except for the IAF 8 where some of the sub-phases do not receive any influent COD.

The amount of influent fed to the anaerobic phase is calculated straightforwardly by subtracting the step-feed volume from the total fill volume ($V_{fill} - V_{step-feed}$). Moreover, the filling time of the SBR cycle depends on the influent feed volume (the influent pump flowrate is fixed to $0.96 \text{ m}^3/\text{d}$). Therefore the filling time is 60 min, 52.5 min and 45 min for 40 L, 35 L and 30 L influent volumes respectively. The length of the anaerobic phase (T_{ANB}) is chosen to range between 60 and 80 minutes. The aerobic period of the reaction phase (T_{AER}) (excluding the last aerobic phase) ranges from 130 to 150 minutes. Note that the sum of the lengths of anaerobic (T_{ANB}), aerobic (T_{AER}) and the anoxic (T_{ANX}) phases is constrained to 270 minutes which means that the length of the anoxic phase (T_{ANX}) is also varying for each combination of aerobic and anaerobic durations.

Table 8.1 The grid of scenarios to simulate the effect of key degrees of freedom on the SBR system

Scenario	Degrees of freedom (d.f.)				Total No. Scenarios
	$S_{O-sp} \text{ (mgO}_2/\text{l)}$	$V_{step-feed} \text{ (L)}$	$T_{ANB} \text{ (min)}$	$T_{AER} \text{ (min)}$	
1	[0.2, 0.4, 0.6, 0.8, 1,2]	[0,5,10]	[60,70,80]	[130,140,150]	162
2	[0.2, 0.4, 0.6, 0.8, 1,2]	[0,5,10]	[60,70,80]	[130,140,150]	162
4	[0.2, 0.4, 0.6, 0.8, 1,2]	[0,5,10]	[60,70,80]	[130,140,150]	162
8	[0.2, 0.4, 0.6, 0.8, 1,2]	[0,5,10]	[60,70,80]	[130,140,150]	162

The combination of these degrees of freedom under the above-mentioned constraints results in 648 scenarios, which is expected to be sufficient to provide

significant insight into the optimal operational scheme for the SBR system. In this way, the optimal scenario of the SBR operation can be searched using the predefined criteria.

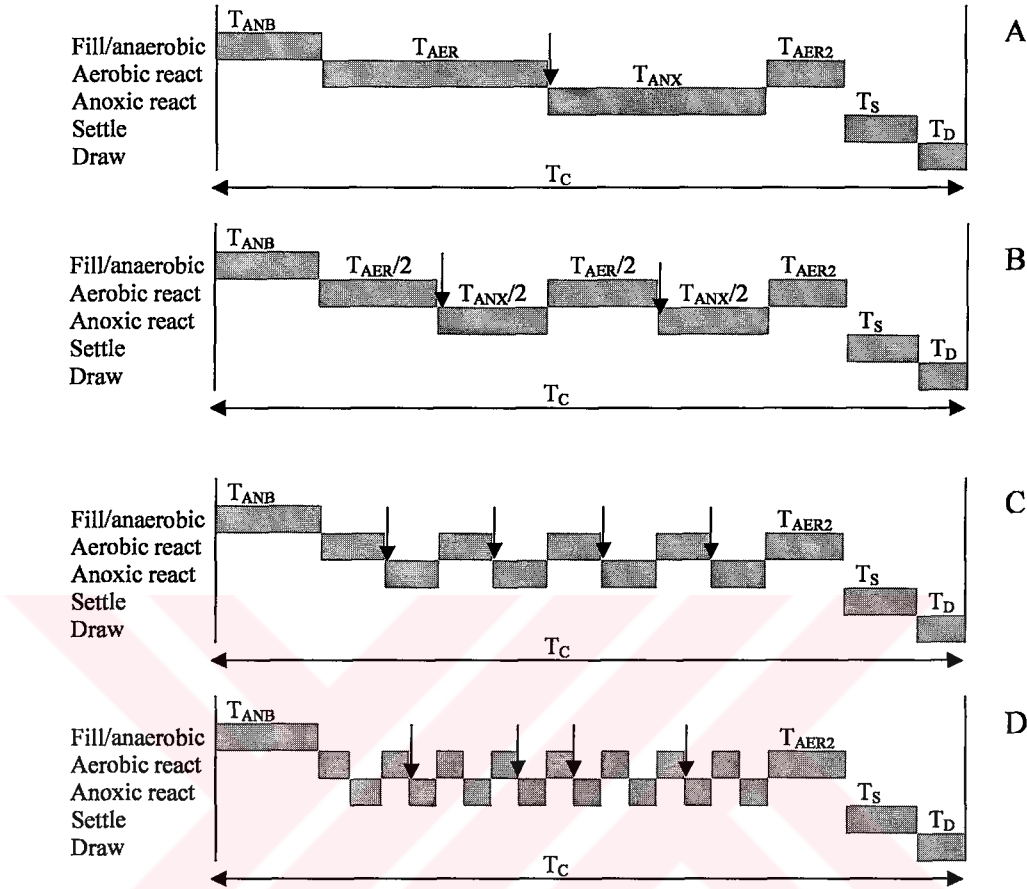


Figure 8.2 Implementation of IAF with step-feed options to anoxic sub-phases. The arrow indicates the step feed instants. SBR with IAF 1 (A), IAF 2 (B) IAF 4 (C) and IAF 8 (D).

8.3.2 Evaluation of the scenario analysis results

Effluent quality: The grid of scenarios presented in Table 8.1 is simulated for 30 days, equal to 3 times the system SRT. The steady-state results of the SBR system in each scenario are then recorded, resulting in a huge amount of data. The scenarios are compared in order to find the best scenario according to the predefined criteria, which are the minimum concentrations of NH_4 , NO_3 and PO_4 in the effluent (Table 8.2). Note that total nitrogen (TN) is the sum of NH_4 and NO_3 in the effluent.

The scenario analysis results (SCA) indicate that the best system performance for either N or P-removal are obtained under different operating conditions. The best system performance for N can provide additional 10.62 mg N/l removal (see Table 8.2 with IAF 8) which means a 57% improvement (nitrogen removal) compared to the existing performance. On the other hand, the best P-removal performance is obtained under IAF1 providing additional 4.73 mgP/l removal, which means an 83% improvement in the existing P-removal performance. Moreover, in all of the best scenarios the effluent total nitrogen contains not only nitrate but also ammonium nitrogen. In this regard, the correct definition of the objective function is crucial. In this study, the objective was set to improve the N removal defined as the sum of NH_4 and NO_3 in the effluent.

Table 8.2 Summary of the scenario analysis results: the best scenario in each category

Scenarios ID	T_{ANB}	T_{AER}	T_{ANX}	$V_{\text{Step-feed}}$	$S_{\text{O_sp}}$	$\text{NH}_{4\text{eff}}$	$\text{NO}_{3\text{eff}}$	$\text{PO}_{4\text{eff}}$	TN_{eff}
	min	min	min	L	mgO_2/l	mgN/l	mgN/l	mgP/l	mgN/l
Reference	60	150	60	0	2	0.73	17.10	5.7	17.83
IAF 1	60	130	80	10	0.4	2.50	8.26	0.97	10.76
IAF 2	60	130	80	10	0.4	2.04	7.88	1.04	9.93
IAF 4	60	130	80	10	0.4	1.70	6.67	1.47	8.38
IAF 8	60	130	80	10	0.4	1.88	5.84	1.03	7.72

The scenario analysis results (Table 8.2) are the result of the sum-up effect of all the evaluated degrees of freedom on the system. Since the number of degrees of freedom is relatively high (i.e. 5), it becomes difficult to distinguish exclusively and quantitatively the effect of each degree of freedom on the overall system performance. The following general remarks are observed from the detailed analysis of the scenario analysis data (unpublished):

- ✓ Increasing the T_{ANB} improves the P-removal efficiency, however, the N-removal performance decreases. This favours conditions for phosphorous accumulating organisms (PAOs) to effectively utilise the VFA generated during the anaerobic phase (Wilderer *et al.*, 2001).

- ✓ Increasing the T_{AER} slightly improves the performance of the nitrification process. However, this parameter has a negative effect on denitrification process (Artan *et al.*, 2002a).
- ✓ The S_{O-sp} appeared to be the most critical parameter in determining the overall behaviour of the system. A detailed discussion is provided below.
- ✓ The step-feed option has a considerable positive effect on the denitrification process. This parameter is essential in improving the denitrification capacity of the system (Hvala *et al.*, 2001; Lin and Ying, 2001).
- ✓ Increasing the intermittent aeration frequency in general has a positive effect on the nutrient (N & P) removal capacity of the system (Demuyne *et al.*, 1994)

In general, the results of the optimization study (Table 8.2) demonstrate that during the filling phase there is a strong competition between PAOs and denitrifiers for the influent COD (particularly VFA), which is in agreement with several studies (Manning and Irvin, 1985; Wilderer *et al.*, 2001; Hvala *et al.*, 2001; Lin and Ying, 2001). To improve P removal in SBRs, the fraction of influent COD utilised by PAOs should be increased during the filling phase. This can be achieved by providing sufficient anaerobic time and decreasing the initial NO_3 concentration present at the beginning of the filling phase. Hence, improving N removal in the SBR is not only useful in itself but also enhances P-removal. In this respect the following actions are useful to consider:

- (1) step-feed of the influent,
- (2) maintain oxygen limited conditions during the aerobic react phase to increase simultaneous nitrification and denitrification (SND) capacity of the system (see below),
- (3) high intermittent aeration frequency during react phase and
- (4) optimize the length of aerobic and anoxic sub-phases during the react phase.

The systematic methodology presented here significantly facilitates the efforts to find the optimal combination of the above-mentioned parameters to achieve both optimal N and P removal in SBR systems.

Robustness analysis of the best scenarios: The robustness index (RI) introduced by Vanrolleghem and Gillot (2002) is used to assess/measure the robustness of each

scenario against a change in the system operation conditions. The sensitivity of the SBR under different scenarios was determined by applying the following manipulations:

- (1) 10 % decrease in the sludge age (SRT),
- (2) 10% increase in the hydraulic loading rate,
- (3) 10% decrease in the organic (COD) loading rate and
- (4) 33% decrease in the temperature (from 15 to 10 °C). The temperature effect on the system performance was modelled using the Arrhenius equation.

Table 8.3 Sensitivity analysis and robustness index of the best scenarios (see text for explanation)

Parameters (θ)	Reference		IAF1		IAF2		IAF4		IAF8	
	TN	PO ₄	TN	PO ₄	TN	PO ₄	TN	PO ₄	TN	PO ₄
1. SRT (-10%)	0.11	0.56	-0.10	0.56	0.00	-0.07	0.05	0.18	0.05	-0.02
2. HRT (+10%)	-0.04	-0.37	-0.07	0.47	-0.08	-0.01	-0.06	0.26	-0.10	0.02
3. COD load (-10%)	0.09	0.79	0.03	0.53	0.22	0.32	0.40	0.81	0.46	0.82
4. Temp. (-33%)	0.13	0.67	2.45	12.10	3.33	7.07	1.22	-0.31	4.17	5.99
Robustness index (RI)*	9.52	1.36	0.81	0.16	0.60	0.28	1.48	1.62	0.47	0.33

$$* RI = \left(\sqrt{\frac{1}{p} \sum_{i=1}^p S_i^2} \right)^{-1} \quad \text{where } S_i = \frac{dCost}{d\theta_i} \cdot \frac{\Delta\theta_i}{Cost} \quad i=1..p \quad \text{and } Cost = [TN, PO_4]$$

Table 8.3 provides the relative sensitivities S_i (calculation, see Table footer) of the effluent TN and PO₄ concentration with respect to a change in each operating condition/parameter (defined in the parameter column). The magnitude of the relative sensitivity indicates how strong the resulting effect of a change in a parameter on the SBR system is. The sensitivity analysis of the SBR showed that decreasing the SRT of the system has a negative (although only small) effect, while increasing the hydraulic loading rate has mainly a dilution effect on the effluent N and P concentrations. Further, decreasing the influent COD load resulted in higher concentrations of N and P in the effluent. On the other hand, the temperature induced a sharp decrease in the performance of the SBR, almost leading to system failure.

Based on the comparison of the RI (Table 8.3), the reference system appeared to be the most robust with respect to N-removal, followed by the best scenario under IAF4. From a P-removal point of view, however, the SBR system is most robust

under the best IAF4 scenario followed by the reference system. However, the robustness index does not indicate the goodness of a scenario with respect to effluent quality, it only indicates how stable (good or bad) the performance is under process changes (Vanrolleghem and Gillot, 2002). The robustness of the system is particularly low when the system delivers its best effluent quality, see e.g. IAF1, IAF2 and IAF8 in Table 8.3. This implies that the optimized SBR is forced to operate close to its limit under the above-mentioned scenarios. Hence, a small deviation in the input to the system leads to drastic deviations in the performance of the system, even up to system failure where biological N and P removal is no longer achieved. From this perspective, it can be said that the robustness index of a scenario indicates how the SBR system is forced to operate close to its limits/edge and therefore how fragile it becomes against a deviation in the input to the system. This provides significant information, particularly for wastewater treatment plants operated under dynamic input conditions, since the effluent quality should be ensured not for short-term (optimal) but for long-term (variable) operation.

Selection of the best scenario for implementation: The objective of the optimization study is to optimize the operation of the SBR in such a way that the best effluent quality can be obtained. Obviously, one of the criteria to decide for the best scenario is the effluent quality in each scenario. However, the effluent quality standards (e.g. EC Directives, 91/271/EEC) usually require the treatment plant to deliver the effluent quality over a certain period of the operational time (e.g. 95%). From this perspective, the stability of the system becomes significant and should be considered equally in the final decision. Based on the effluent quality (Table 8.2) and robustness index of the best scenarios (Table 8.3), the SBR operation under IAF4 appeared to be the best scenario to provide effluent quality below discharge standards accompanied with good system stability. Under this scenario, the existing SBR performance for the N and P removal is improved by 54% and 74% respectively. In real, the best scenario has been implemented and the SBR performance is expected to reach a new steady-state soon.

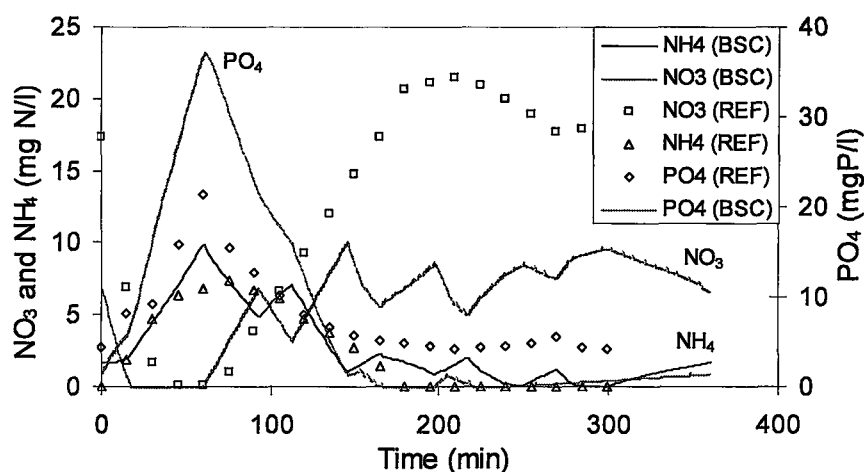


Figure 8.3 N and P-removal dynamics under the best scenario (BSC) obtained in IAF4 in comparison with the reference (REF) system

In this optimization study, a fixed length of aerobic and anoxic sequences is assumed to reduce the number of scenarios required for the optimization. It is clear that the optimization of the SBR system should also consider the variable length of the aerobic/anoxic sequences, particularly for SBRs subjected to dynamic input conditions. Moreover, the settling properties of activated sludge are not incorporated in the state-of-the-art activated sludge models such as ASM2dN (Chapter 7; Annex A, Table A1). Hence, it is not possible to predict the behaviour of activated sludge during the settling phase under different operating conditions. Ideally, this should be a third criterion to consider during the selection of the best scenario.

8.3.3 Effect of the oxygen set-point and length of the aerobic react phase

An important outcome of the scenario analysis is the fact that the system delivers the best effluent quality (both for N and P criteria) under oxygen-limited conditions (see Table 8.2). A set-of simulations (224 in total) were carried out to understand the effect of the oxygen set-point on the nitrification and denitrification processes in the SBR system. A grid of scenarios was constructed around a vector of oxygen set-points and a vector of aerobic react phase times. The simulation results obtained under the best IAF4 scenario are shown in Figure 8.4. Similar trends are observed in the ammonium and nitrate profiles obtained under the best scenarios with IAF1, IAF2 and IAF8 (Mura, 2003).

The simulation results demonstrated that a linear relationship exists between the

oxygen set-point or the length of the aerobic react phase (i.e. aerobic SRT) and the effluent nitrogen concentrations (see Figure 8.4). A certain nitrate concentration (8 mgN/l) can be obtained under different oxygen set- points and aerobic react time (see Figure 8.4B). This linear relationship can be explained by the changing extent of simultaneous nitrification and denitrification (SND) occurring during the reaction phase of the SBR as discussed in Chapter 6. Based on the simulation results, it is strongly advised to consider the oxygen set-point in the design of SBRs and probably also for other types of wastewater treatment plants.

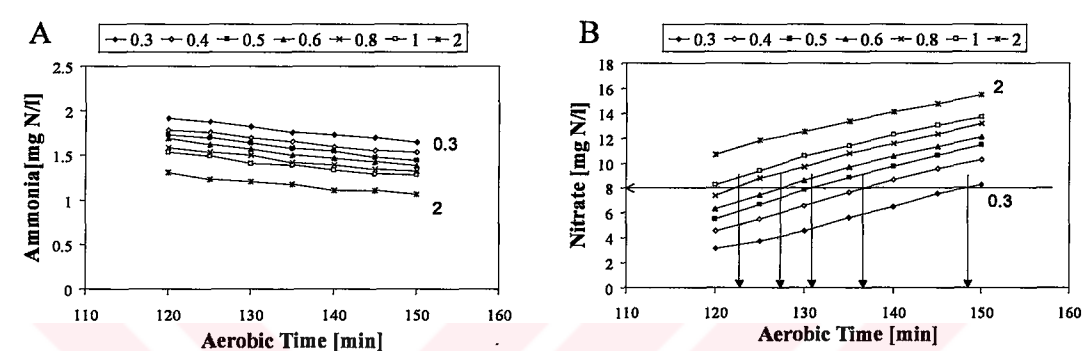


Figure 8.4 Trend of ammonium (A) and nitrate (B) as function of oxygen set-point under different lengths of aerobic react phase for the SBR operation with IAF4. Arrows indicate combinations of oxygen set-points and aerobic-time corresponding to 8-mgN/l nitrate in the effluent (B).

8.3.4 Effect of sludge age on the SBR performance and stability

In the previous sections, the scenario analysis is performed under a fixed sludge age equal to the sludge age of the reference system, i.e. 10 days. The question “What is the response of the SBR system under different sludge ages with respect to both effluent quality and robustness criteria?” is addressed in detail in this section to complement the optimization study carried out at the fixed sludge age of 10 days.

For the simulations presented in this section, the length of the anaerobic phase, the amount of step-feed and the length of the aerobic-react phase were fixed to the values obtained from the best scenarios under the different intermittent aeration frequencies (see Table 8.2). The effect of sludge age on the SBR performance is investigated under different oxygen set-points, since the oxygen set-point is found to be one of the most critical operating parameters of the SBR. In this way, the

response of the SBR system is simulated for each point in the following operation domain: a grid of sludge ages (SRT) – 8, 10, 12, 14, 16, 18, 20, 22, 24, 25 days, versus oxygen set-point – 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1, 2 mgO₂/l. This results in 240 simulations in total (i.e. including 3 different categories of intermittent aeration frequency, IAF), which is expected to be sufficient to predict the trend in the behavior of the SBR system as a function of SRT and oxygen concentration.

8.3.4.1 Effect of sludge age on effluent quality

The effluent quality results as function of SRT and oxygen set-point are shown in 3-D graphs in Figure 8.5. In these 3-D graphs, the x-axis corresponds to the oxygen set-point, the y-axis corresponds to the sludge age of the SBR system and the z-axis corresponds either to the effluent TN (equal to the sum of NH₄-N and NO₃-N in the effluent) (see Figure 8.5-left) or to the effluent PO₄-P concentrations respectively (see Figure 8.5-right). The effluent quality of the SBR system as function of sludge age has a particular behaviour dictated by the specific conditions/operating variables of the system (see Figure 8.5). However, the following general conclusions can be deduced from a detailed analysis of the effluent quality results (data not shown explicitly):

1. Below a critical oxygen set-point (in this case 0.2 mg/l), the nitrifiers are washed-out and there is no P-uptake, i.e. a system failure occurs with respect to N and P removal.
2. The P-removal is observed to be optimal for sludge ages around 10-12 days depending on the oxygen set-point in the system (see Figure 8.5 right-A). This is in accordance with experimental results shown elsewhere (Henze *et al.*, 2002; Rodrigo *et al.*, 1996; Smolders, 1995). An increase in the SRT of the SBR is observed to have a slight negative effect on the effluent P removal. This might be explained by the amount of storage polymers in the PAOs (X_{PHA}) (Smolders *et al.*, 1995). Since the substrate flux to the system is constant, the concentration of the storage polymers (fixed yield) will be diluted as the concentration of biomass kept in the system increases (i.e. increasing SRT). Consequently, the P-uptake in the aerobic/anoxic phase will be relatively lower due to decreased level of X_{PHA} in the PAOs.

3. Decreased oxygen set-points have a positive effect on the effluent P concentrations. This is most probably an indirect effect of the reduced effluent TN concentrations.
4. The effluent TN concentrations are observed to decrease parallel to an increase in SRT. Moreover, decreasing oxygen set-points have a remarkable effect on reducing effluent TN concentrations (see Figure 8.5-left). This was discussed in detail in the preceding section. Oxygen limited operation of SBR has shown to considerably improve the N-removal under all different operating SRTs and intermittent aeration frequencies (see Figure 8.5-left). This confirms/supports the findings that a lower oxygen concentration enhances simultaneous nitrification and denitrification processes as discussed in Chapter 6.
5. Increasing the intermittent aeration frequency (from 2 to 8 see Figure 8.5-left) has a positive effect both on N and P removal. This is in accordance with the experimental results shown elsewhere (Hvala *et al.*, 2001; Demuyne *et al.*, 1994; Lin and Jing, 2001).

8.3.4.2 Effect of sludge age on the robustness of the SBR system

The robustness index (RI) or stability of the SBR system under each operating condition are shown in 3-D graphs in Figure 8.6. The z-axis in Figure 8.6 corresponds to either the RI of the SBR system towards effluent TN (see Figure 8.6-left) or to the RI of the SBR system towards effluent $\text{PO}_4\text{-P}$ concentrations (see Figure 8.6-right). It is important to note that the magnitude of the RI shown in Figure 8.6 is meaningful only for comparison purposes. The trend of the robustness index (RI) of the SBR as a function of sludge age has a particular behavior, which is dictated by the specific conditions of the system. However, the following general conclusions can be deduced from the robustness analysis: The stability of SBR system has a non-linear trend as function of the system SRT, DO and intermittent aeration frequency. Moreover, the robustness of the system is different for N and P removal (see Figure 8.6). The trend of RI related to phosphate is clearly increasing (robustness increases parallel to the increase in sludge age) as shown in Figure 8.6-right. The trend of RI related to TN on the other hand can be said to be decreasing parallel to a decreasing SRT, with a few exceptions (see Figure 8.6-left).

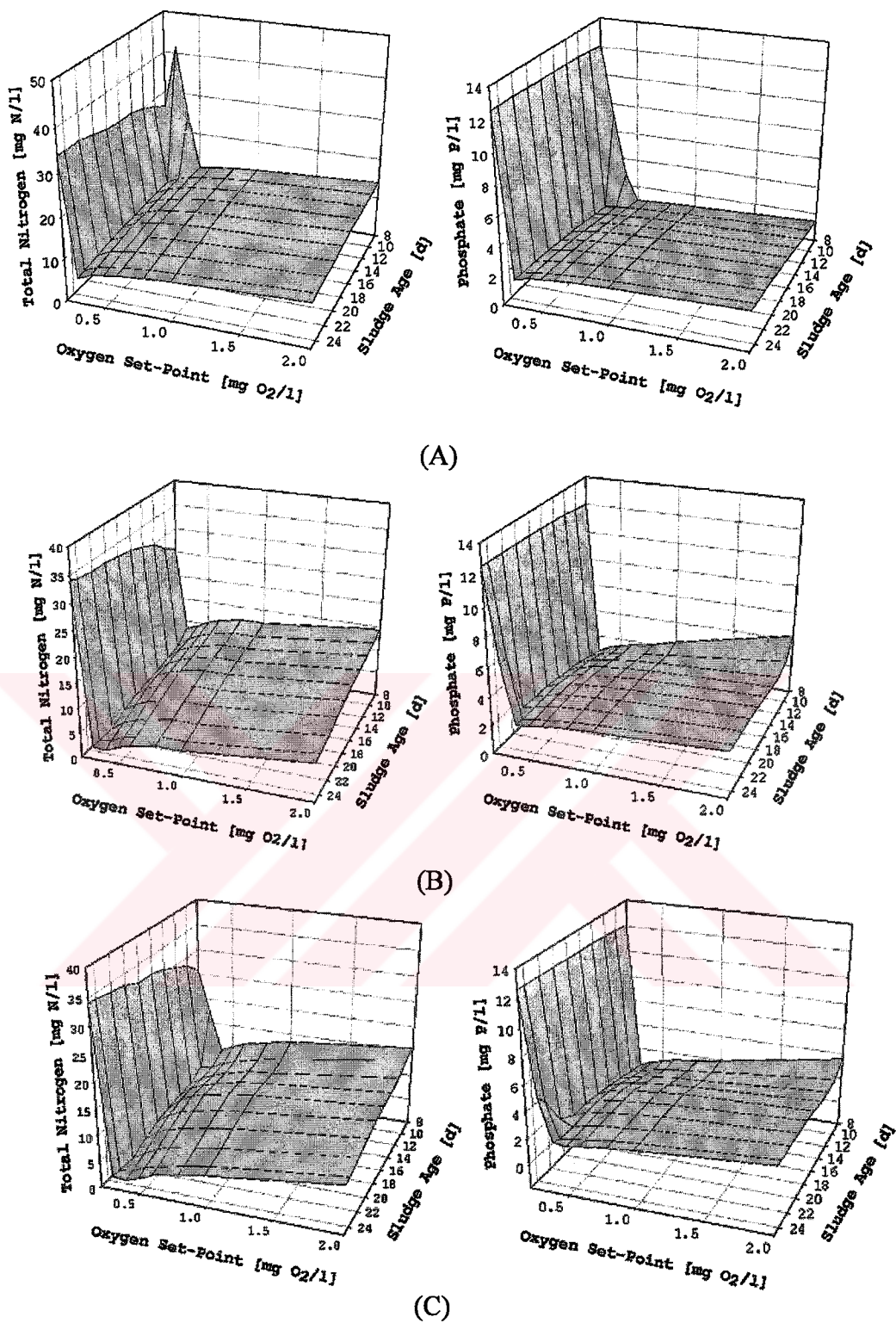
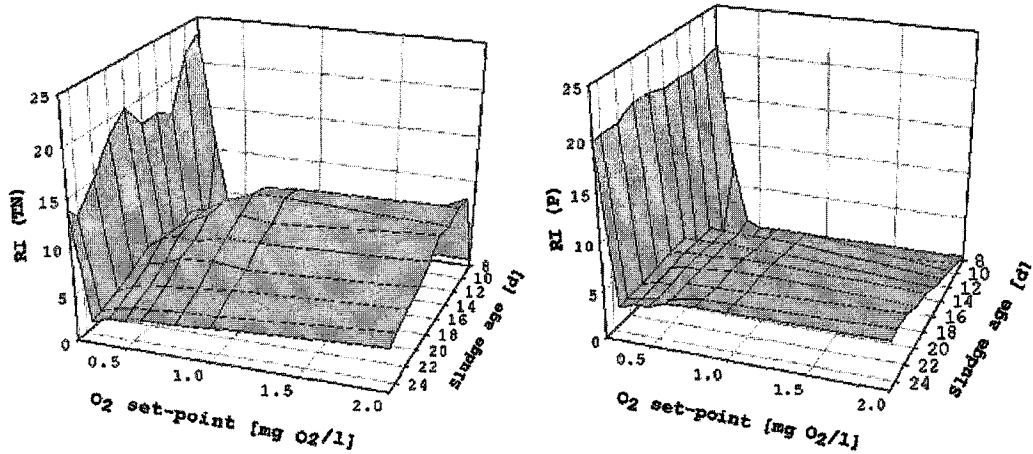
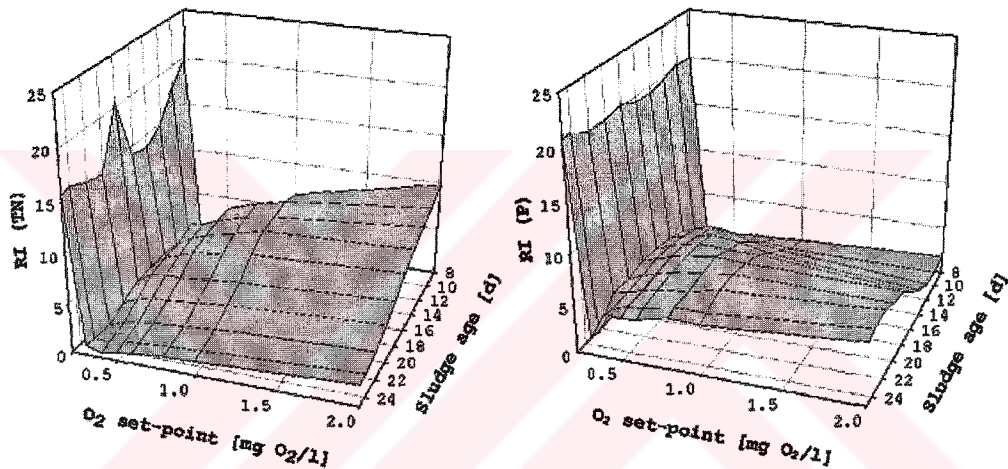


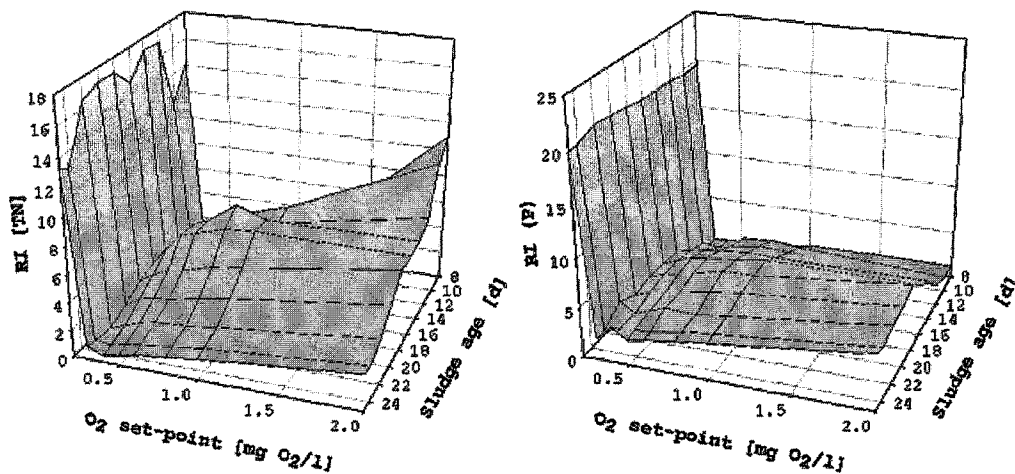
Figure 8.5 SBR performance with respect to effluent TN (left-hand) and P concentrations (right-hand) as a function of sludge age under different oxygen set points: IAF2 (A) IAF4 (B) and IAF8 (C).



(A)



(B)



(C)

Figure 8.6 Stability/robustness of the SBR system with respect to TN (left-hand) and P removal (right-hand) as a function of sludge age under different oxygen set points: IAF2 (A) IAF4 (B) and IAF8 (C).

1. The robustness of the SBR (both for TN and P) is observed to increase parallel to an increase in oxygen concentration (see Figure 8.6). It is a common characteristic observed in each intermittent aeration category (IAF2, IAF4 and IAF8). An exception should be made for the scenarios with oxygen set-point equal to 0.2 mg/l. In this case, although the robustness of the system is at its maximum (see Figure 8.6), the effluent quality is worse (see Figure 8.5). This special case means that for this operation mode, the response of the SBR with respect to effluent quality cannot be altered (either in negative or positive way) resulting in maximum robustness index values.
2. A detailed analysis of the components of the robustness index (results not shown) showed that the temperature has the biggest influence on the nitrification performance of the SBR. The phosphate removal performance, on the other hand, is very sensitive towards a change in the COD load (Grady *et al.*, 1999).
3. The effect of the hydraulic retention time on the overall system performance is, however, observed to be minimal. The temperature effect on nitrification is well compensated by either increasing the oxygen set-point in the system or equivalently increasing the sludge age of the system as discussed in Chapter 5 and 6 (see e.g. left hand side of Figure 8.5). This is expected since increasing the oxygen set-point (see above) indirectly increases the aerobic SRT of the SBR.

The stability of nitrogen removal is particularly regulated by the temperature variation in the system. For phosphate removal, on the other hand, it is the change in influent COD that plays an important role. Variation of the hydraulic retention time does not affect the stability of the system considerably.

Comparing the effluent quality (Figure 8.5) and the robustness index (Figure 8.6) in the SBR system under different operating conditions (particularly as a function of SRT and oxygen) shows that the robustness of the SBR system is decreasing parallel to the improvement in the effluent quality.

This was also observed in the preceding section mentioned above and was observed in Vanrolleghem and Gilliot (2002) too. This supports the above-mentioned argument that optimization of the SBR system to obtain improved effluent quality asks for operating the SBR system close to its limits. Furthermore, it means that optimized SBR operation asks to sacrifice robustness thereby making the SBR operation fragile against external disturbances. This aspect is particularly significant for the full-scale optimization of biological systems, which are exposed to dynamic variations and uncertainties in the input to the system. As such robustness analysis of the different operation scenarios should be part of the decision making process.

8.4 Conclusions

In the first part of this research (see Chapter 7), a systematic approach (methodology) for the optimization of SBRs using mechanistic models is developed and evaluated at a lab-scale SBR in view of an improvement of effluent N and P discharges.

Based on a compromise between the effluent quality and the robustness of the SBR operation, the best scenario for SBR optimization is found out to be a step-feed with 4 intermittent aeration sub-phases during the react phase. Under this scenario, it is possible to improve the current N and P removal performance of the SBR by 54% and 74% respectively.

In the second part of this study, the model-based study of the effect of SRTs and oxygen set-point on the SBR performance and stability were performed. The results showed that:

- ✧ N-removal improves parallel to increasing SRT. Moreover, oxygen-limited operation of SBR remarkably enhances the effluent N (see Chapter 6).
- ✧ P-removal is optimal around 10-12 days depending on the oxygen set-points whereas increasing SRTs have slightly negative effect on P-removal. Similar to N-removal, a decreasing oxygen concentration in the system improves effluent-P quality.

Under all different SRTs and oxygen set-points, there is an inverse correlation between effluent quality and robustness of the system. In other words, improving N and P removal of the system decreases the stability of the system. This is most probably caused by the fact that the SBR system is pushed to its limits for improving N and P removal, which makes the system less stable against external disturbances.



9 EVALUATION OF NUTRIENT REMOVAL PERFORMANCE FOR AN ORBAL PLANT USING ASM2d MODEL

9.1 Introduction

In recent years, nutrient removal gained more importance in order to prevent eutrophication of receiving waters. As a solution, different plant configurations can be used for the design of wastewater treatment plants to achieve nutrient removal from domestic wastewaters. From an engineering point of view, the reliability of the treatment plant is important to meet nutrient discharge limits at all times. Extended aeration systems are associated with plants for small communities where reliability and simplicity of the operation are of prime importance (Grady *et al.*, 1999, Orhon and Artan, 1994, Randall *et al.*, 1992). The applicability of the system is good, because less sludge is to be disposed of, no further treatment is needed for the sludge, it maintains good effluent quality and allows flexibility and simplicity for the plant operators. However, an increase in the total volume (etc. for an upgrade) by addition of aerobic or anoxic reactors increases the investment and operational/maintenance costs.

An Orbal plant is a type of extended aeration activated sludge plants, which claims to achieve simultaneous nitrification and denitrification in a single reactor, offering reduced costs. Generally, three or four channels are recommended for design as shown in Figure 9.1-left (Drews *et al.*, 1972, 1973). The simultaneous nitrification and denitrification in the outer loop that receives the influent wastewater give an overall denitrification performance of 80% operated under moderate sludge ages in order to suppress the growth of microorganisms causing bulking and settling problems (Daigger and Littleton, 2000).

This chapter was presented at *WEFTEC 2003 Conference*:

Insel, G., Russell, D., Beck, B. and Vanrolleghem, P.A., 2003. Evaluation of Nutrient Removal Performance for an Orbal[®] Plant Using the ASM2d Model, *WEFTEC 2003: 76th Annual Technical Exhibition and Conference*, October 11-15, 2003, Los Angeles, California, U.S.A.

In Orbal systems, the outer loop is designed to be the largest channel used for simultaneous nitrification-denitrification and combine the advantages of completely mixed and plug flow reactors in one bioreactor (Smith, 1996). Step-feed in terms of return activated sludge (RAS) and influent wastewater can be used in the optimization of the plant (Applegate *et al.*, 1980).

In the literature, different hydraulic layouts were considered for the Orbal plants. A tracer test was conducted for an Orbal plant by Burrows *et al.* (1999). It was concluded from the residence time distribution results that the outer channel could be regarded as two CSTR in series, however, while the middle and inner channels could be configured as single CSTRs. On the contrary, Cinar *et al.* (1998), Daigger and Littleton (2000) considered the outer channel as 6 reactors in series but the other channels as individual CSTRs, as well.

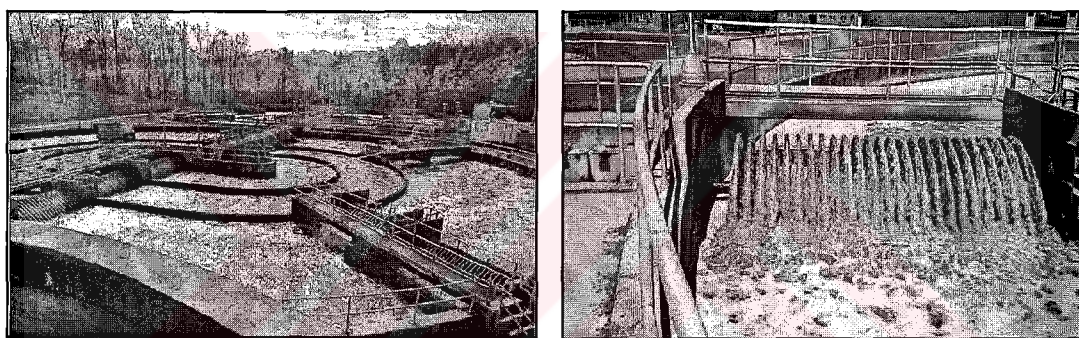


Figure 9.1 Pictures of biological reactor and vertical disc aerators (Liu, 2000)

Aeration is provided by a number of perforated discs installed perpendicular to the rotating shaft. The discs are partially immersed in the mixed liquor and rotated around their horizontal axes (see Figure 9.1-right). The main feature for the operation strategy is that the Orbal plants are operated under oxygen deficit conditions (around 0.1-0.75mgO₂/l) promoting the simultaneous nitrification and denitrification together with carbon and biological phosphorus removal (DeSilva and Rittman, 2001, Daigger and Littleton, 2000, Bertanza, 1997, Applegate *et al.*, 1980, Drews *et al.*, 1972). Simultaneous nitrification and denitrification is achieved by supplying oxygen to all channels by mechanical disc aerators (Figure 9.1-right). The actual oxygen demand of the outer loop might be as high as 75% of the total system, the aeration discs allocated for the channel supply only 30-60% of the oxygen requirements. The dissolved oxygen

in the middle loop varies depending upon the organic loading. The last (inner) channel works as a polishing mode to remove the remaining COD and ammonia (U.S Filter/Envirex, 2002). For simultaneous nitrification-denitrification, it was suggested that the dissolved oxygen concentration around 0.5 is suitable to achieve a nitrification rate equal to the denitrification rate (Munch *et al.*, 1996).

It was hypothesized that three general mechanisms are responsible for simultaneous biological nutrient removal. These are (a) bioreactor mixing patterns that allow the anoxic and anaerobic zones necessary for biological nutrient removal (b) anoxic and anaerobic zones within the flocs and (c) the presence of novel microorganisms in the system (Littleton *et al.*, 2002, Daigger and Littleton, 2000, Applegate *et al.*, 1980). The removal efficiency for carbon, nitrogen and phosphorus removal is reported to be in a wide range depending upon the operation strategy, plant configuration, wastewater strength and environmental factors (i.e. temperature). It was stated that the plants operated under low oxygen concentration up to 90-95% nitrogen removal could be attained (Pochana and Keller, 1999, Rittman and Langeland, 1985). The largest denitrification was attained at a COD/TKN ratio of 6.4 under 0.18 mg/l oxygen concentration in the bulk liquid (DeSilva and Rittman, 2001). Drews *et al.* (1972) reported that the removal efficiency of COD in the range of 78.1%-88.9%. By keeping the dissolved oxygen concentration below 1.0 mg/l, the total nitrogen removal efficiency was in the range of 65.6%-86.3% with elevated ammonia concentrations in the effluent around 5-8 mg NH₄-N/l without achieving EBPR.

A model-based process analysis of an Orbal plant carried out by Daigger and Littleton (2000) via ASM1 simulation showed that the oxygen limited conditions without internal recycle from inner channel to outer channel exerted a minimum effluent nitrate concentration due to the fact that the oxygen carry over through the outer channel probably disturbed the simultaneous biological nutrient removal in outer ring. Depending upon the variation in the organic loading (55%-132%) and the sludge ages (8-33 days), the removal efficiencies for total phosphorus removal efficiency were calculated in the range of 61%-95%. The total nitrogen removal was calculated to be around 85-90% (Daigger and Littleton, 2000). Applegate *et al.* (1980) compared the extended aeration and the step feed operation mode (by diverting a portion of inflow to

the second channel) for a full-scale Orbal plant. The removal efficiency for total nitrogen is increased from 76% up to 91%. Enhanced biological phosphorus removal, EBPR has been observed in aerated bioreactors without anaerobic zones prior to aerobic or anoxic reactors (Cinar *et al.*, 1998, Applegate, 1980). For this, the anaerobic zones formed inside the flocs and/or vertical or horizontal flow patterns in the outer channel may promote the phosphorus release resulting in an overall biological phosphorus removal (Daigger and Littleton, 2000). On the contrary, it was also suggested that the influent total phosphorus concentrations are often low so that phosphorus removal may simply be due to biomass synthesis (Daigger and Littleton, 2000). Regarding the EBPR modelling, Cinar *et al.* (1998) was unable to model using the steady state ASM2 model because the anaerobic conditions that are necessary for PHA storage could not be obtained. The simulations using ASM2 with 3 CSTR-in-series representing the Orbal also could not yield PAO growth (Littleton *et al.*, 2002, Cinar *et al.*, 1998).

In this study, the behavior of the Georgia/Athens Orbal plant was investigated under dynamic loadings with respect to its nitrogen and phosphorus removal using the ASM2d model (Henze *et al.*, 1999). The first step is to calibrate the model using steady state simulations. In the second step, the behavior of the plant under dynamic loading is investigated.

9.2 Materials and Methods

9.2.1 WWTP definition

The Orbal plant under study is located in Georgia, Athens treating the wastewater of 50000 PE. The layout used in the calibration consists of a bioreactor and 4 final clarifiers (1 spare for rain events). The biological reactor is composed of three concentrically arranged closed loop bioreactors (see Figure 9.2-left). Influent wastewater first enters the outer loop and passes through the middle, inner reactor and the final clarifier, respectively. The plant can be operated as a step-feed plant and/or the return sludge can be diverted to the inner rings depending upon the operating strategy. As can be seen from in Figure 9.2-left, the influent wastewater and return activated sludge,

RAS, are fed only to the outer loop without any step feed pattern for the calibration period. The overall plant capacity is 20328 m³/day (5.37 MG/day) on average.

The total volume of the biological reactor is 12553 m³ consisting of outer, middle and the inner rings with the volumes of 8665 m³ (69% of total volume), 2544 m³ (20%) and 1344 m³ (11%), respectively. The surface area for each circular final clarifier is 448 m² with 4.8 m in height (Figure 9.2-right). The hydraulic retention time (HRT) and the sludge age of the system is 18 hrs and 9-10 days, respectively. The mixed liquor concentration in the aerobic reactor is kept around 3000-3500 mg/l and the reactor is operated under low oxygen for the simultaneous nitrification-denitrification. Oxygen transfer is provided with surface disc aerators and all loops have disc aerators mounted on a rotor providing the recirculation of mixed liquor within the reactor. Each rotor has 24 aeration discs (see Figure 9.1-right). Depending upon oxygen requirement and operation the number and the spans between discs, speed and the immersion depth can be adjusted as appropriate. So, this feature gives considerable flexibility in terms of oxygen transfer. The velocity in the channel is in the range of 0.28-0.35 m/sec (0.3 m/sec in average) by keeping the mixed liquor in suspension.

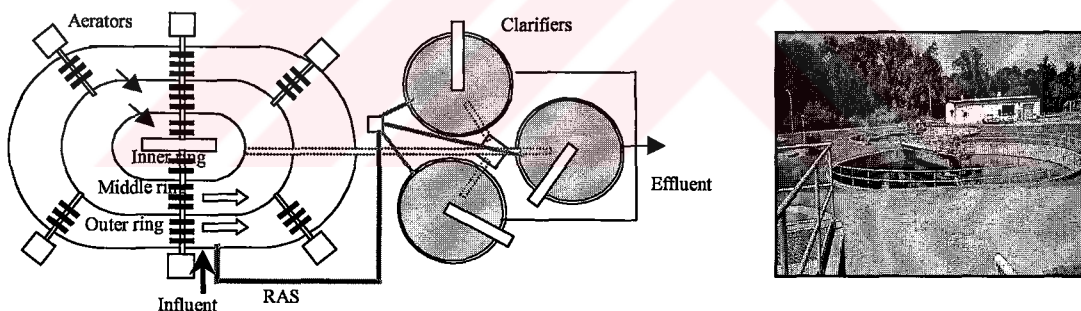


Figure 9.2 The plant layout for the simulated plant (left) and clarifier (right)

9.2.2 Measurement campaign data and calibration

In the course of measuring campaign, the influent flow rate, return activated sludge, RAS, waste activated sludge, WAS flow rate, 0.2 micron-filtered TOC, total filtered organic nitrogen, filtered ammonia nitrogen, orthophosphate, dissolved oxygen concentration in the channels and the sludge blanket level were measured in every 15 minutes with Environmental Process Control Laboratory, EPCL manufactured by Capital Controls-Minworth Systems Ltd. (Liu, 2000). The measuring campaign data for

the Athens/Orbal plant was obtained from Liu (2000). The reader should consult to Liu (2000) for more information about the analytical methods, data collection and the hardware facilities used in the measuring campaign. The experimental results are shown in the results and discussion section.

The influent wastewater characterization in terms of COD fractions used in the dynamic calibration was generated according to the filtered TOC measurements. The ratio of COD_{tot}/TOC ratio was adopted as 3.1 according to Metcalf and Eddy (2003) and Servais *et al.* (1999). The average percentages for the COD fractions were adopted from Henze *et al.* (1999). The flux based average wastewater characterization and the COD fractionations are given in Table 9.1. The BIOMATH calibration protocol (Vanrolleghem *et al.*, 2003) was applied for the calibration of the plant using the existing plant data. As a first step, simple layout composed of 3 reactors in series was used for the preliminary simulations. All simulations were performed in the modelling and simulation software WEST (Vanhooren *et al.*, 2003).

Table 9.1 Flux based average influent wastewater characterization

Component	Unit	Concentration	% of total COD
Total COD, COD_{tot}	mgCOD/l	404	
Biochemical Oxygen Demand, BOD_5	mgO ₂ /l	159	
Total inert COD, C_I	mgCOD/l	174	43
Particulate Inert COD, X_I	mgCOD/l	150*	37
Soluble Inert COD, S_I	mgCOD/l	24	5
Biodegradable COD, C_S	mgCOD/l	230	57
Fermentable COD, S_F	mgCOD/l	60	14
Acetate, S_A	mgCOD/l	30	7
Slowly Biodegradable COD, X_S	mgCOD/l	140	32
Ortho-P, S_{PO4-P}	mgP/l	1.8	
Total Phosphate, TP	mgP/l	5.3	
Ammonium, NH_4-N	mgN/l	12	
Total Kjeldahl Nitrogen TKN	mgN/l	22.4	
TSS (calculated from COD)	mgSS/l	217	
COD_{tot}/TKN (BOD_5/TKN)		18 (7.1)	
COD_{tot}/TP (BOD_5/TP)		76 (30)	
C_S/TKN		10	
C_S/TP		43	

*calibrated in order to fit the MLSS

The growth of PAOs could not be sustained because they were unable to compete with other heterotrophs. As a result, PAOs were completely washed out at the end of the simulation even though the parameters pertaining to PAOs were changed (Cinar *et al.*, 1998, Littleton *et al.*, 2002). In order to improve the PAO growth in the system the plant

layout shown in Figure 9.3 was introduced to WEST (Vanhooren *et al.*, 2003). The outer, middle and the inner ring are represented by 6, 4 and 2 CSTRs in series based on the reactor geometry. The volumes of each reactor for the outer, middle and inner ring are 1444, 636 and 672 m³, respectively. As stated above, three out of 4 clarifiers were operational during the measurement campaign period. Because three of the clarifiers were under identical conditions, a simple clarifier with a non-reactive 20 layered settling model (Takács *et al.*, 1991) was assigned for the simulation of the sludge blanket in the clarifier. The overall surface area, A and the water height, H_s in this clarifier are 1345m² and 4.8 m, respectively. The flow rates for the influent underflow and the sludge wastage rates were introduced in WEST as input-log files. The flow rate of the influent, return activated sludge (RAS) and activated sludge (WAS) used in the simulations are illustrated in Figure 9.4.

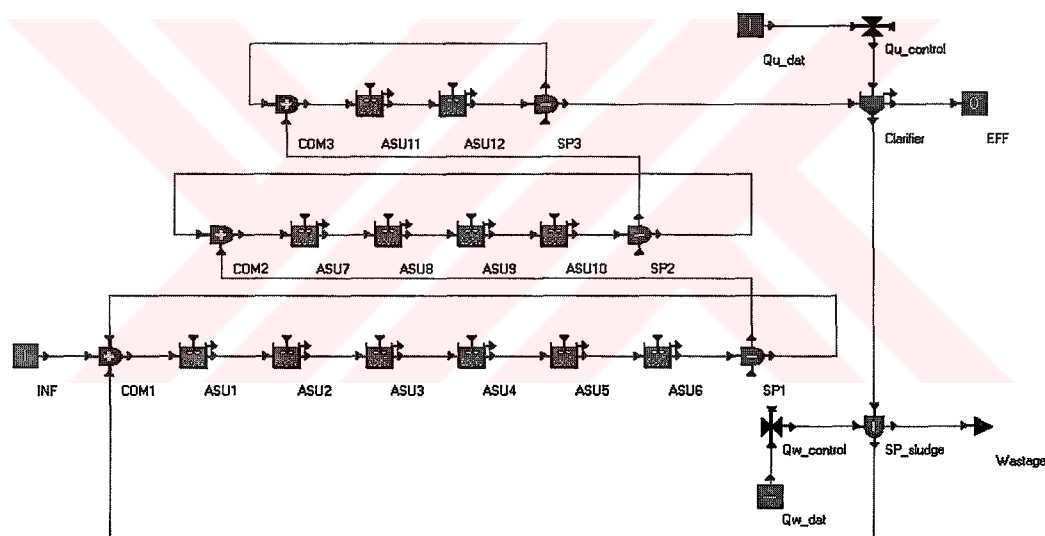


Figure 9.3 Implementation of plant layout in WEST

A steady state influent file was used for the preliminary simulations in order obtain an appropriate biomass composition that would be a starting point for the dynamic calibration. The ASM2d model was selected for this calibration issue. In order to reflect the wastewater plant performance under steady state average measurement outputs were considered during the steady state calibration. A manual iterative estimation method was used until an appropriate initial biomass composition was obtained. It should be stressed

here that the manual iterative method was only terminated when the same values were found considering all measurement outputs for the steady state and dynamic calibration, as well. The scheme of the calibration approach is illustrated in Figure 9.5. The steady state simulation relates to a 50 days period so that all the components reached their steady state values. The most sensitive parameters with respect to the measurements outputs were selected for adjustment.

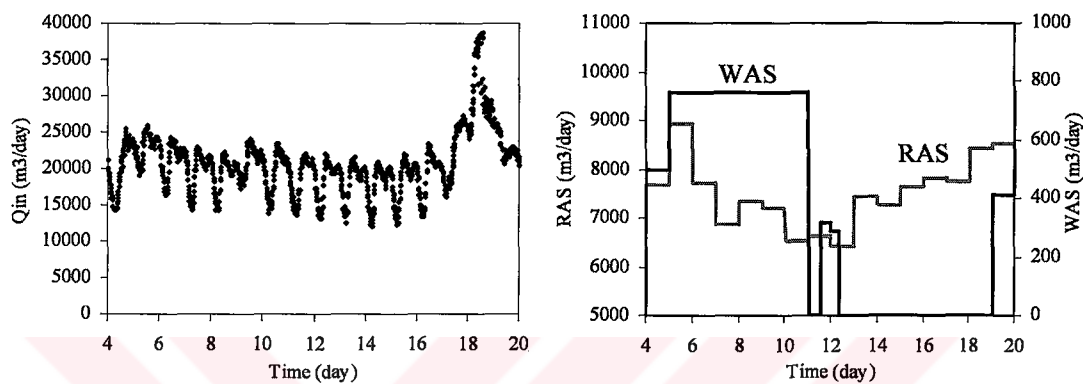


Figure 9.4 Influent flow rate (left), RAS and WAS flow rates (right)

9.3 Results and Discussion

The steady state simulation not only reflects the overall treatment capacity of a plant but also approximates the appropriate biomass composition of the mixed liquor which is a crucial factor for the calibration and the estimation of the parameters (Vanrolleghem *et al.*, 2003). The reason is that an inappropriate determination of the sludge composition causes bias in the other calibrated parameter values. The results of the steady state simulation based on flux and concentrations are shown in Table 9.2 and Table 9.3. It can be inferred from Table 9.2 that the removal efficiency for TKN and TP is around 77% and 94%, respectively. Simultaneous nitrification and denitrification provided a removal of 42% of the total daily influent TKN load was removed by simultaneous nitrification and denitrification. The remaining 35% is entrapped in the sludge and used as a nutrient. The removal efficiency of total nitrogen removal of the plant is in compliance with the counterparts in the literature of which were reported in the range of 65.6%-86.3%.

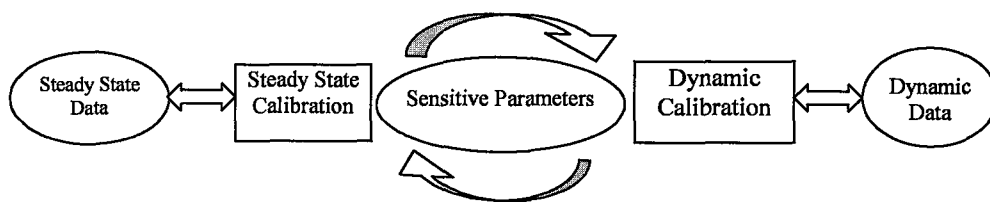


Figure 9.5 Schematic representation of the calibration methodology

The first step in the calibration study was to fit the solid mass balance over the treatment plant. The sludge age of the system was calculated to be around 10 days from the phosphate balance that is in agreement with the information provided from plant operators. In order to fit the sludge concentration in the reactor and maintain 3000-3500 mg MLSS/l in the middle ring, the particulate inert COD fraction in the influent was calibrated during steady state calibration. According to the value in Table 9.1, the X_I fraction was found to be comparably higher. Figure 9.6 shows the measured and the simulated MLSS concentrations in the middle ring. It is obvious that, till day 18, the model captured the trend of MLSS in the reactor successfully. The difference between the measurement and simulation is the operational changes in the process by the plant operators.

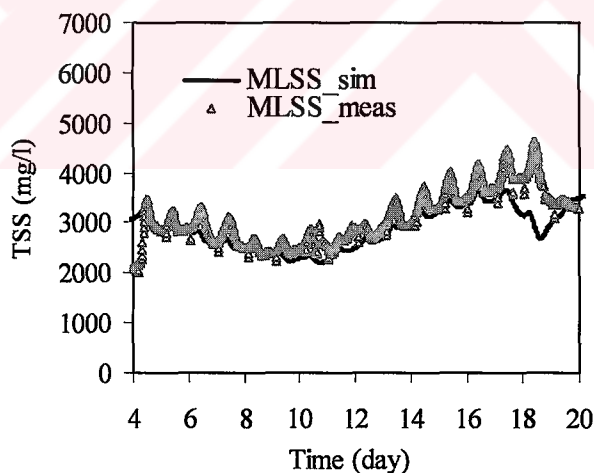


Figure 9.6 MLSS profiles in middle ring

For instance, at day 18 the mixed liquor is diverted into the middle channel because of the storm event reported. Insufficient information on the changes in flowrate and made the system difficult to calibrate in terms of sludge blanket in the clarifier. It should be noted here that the sludge wastage is not constant during the calibration period that was

also included in the model. The ridges on the MLSS profile were also captured to some extent by the model because the reactor received a much higher TSS load during the morning and afternoon time when the flow rate increased. In the steady state calibration the measured and simulated ammonia concentrations in the effluent are 4.4 and 4.8 mgN/L, respectively. The reported effluent ammonium nitrogen concentrations are typically around 5-8 mgN/l in the effluent (Drews *et al.*, 1972, Drews and Greeff, 1973, Applegate, 1980). The phosphorus removal efficiency of the plant was found to be closer to the upper limit of the range 61%-95% (Daigger and Littleton, 2000, Cinar *et al.*, 1998, Applegate, 1980). The measured and simulated effluent phosphate concentrations are 0.6 and 0.3 mgP/L for steady state simulation.

A higher phosphorus removal efficiency was attained since the NO₃ concentration is nearly zero in the outer ring leading to the anaerobic condition necessary for PAOs (Comeau *et al.*, 1986, Ekama and Wentzel, 1999, Kern-Jespersen and Henze, 1993, Kuba *et al.*, 1994).

Table 9.2 Simulated steady state plant performance

Component	Influent kg/day	Effluent kg/day	Removed kg/day	Removal %
Flowrate	20328*	19878*		
TSS load	4411	198	4213	96
COD load	8944	485	8459	95
TKN load	450	105	345	77
			191**	42**
TP load	108	6	103	94

*units in m³/day, ** removed by simultaneous nitrification and denitrification

The calibrated ASM2d parameters are visualized in Table 9.3 together with their default values (Henze *et al.*, 1999). Calibration study revealed that the most sensitive process on the oxygen budget is found to be the hydrolysis process. In the ASM2d report, the anaerobic hydrolysis reduction factor, η_{fe} is recommended to be 0.4 as a default value. According to the calibration results carried out by Satoh *et al.* (2000), a lumped parameter group $\eta_{fe}k_h$ was estimated to be 0.35 where η_{fe} is 0.2. The hydrolysis rates were reported to be much higher for NDBEPR than for ND systems (Clayton *et al.*, 1991). Another statement on the hydrolysis is that the hydrolysis rate is independent from electron acceptor conditions (Gujer *et al.*, 1999, Mino *et al.*, 1995b, Goel *et al.*,

1998). However, the hydrolysis rates were also reported to be dependent on the electron acceptor conditions (Sözen *et al.*, 1998, Henze *et al.* 1987, 1999, Maurer and Gujer, 1994, Henze and Mladenovski, 1991).

Table 9.3 Parameters used in the calibration for ASM2d

Parameters	Symbol	Unit	Default*	Calibrated**
Biological parameters				
Autotrophs, X_{AUT}				
Maximum growth rate for X_{AUT}	μ_{Amax}	day ⁻¹	1.0	0.70
Half saturation constant of O ₂ for X_{AUT}	$K_{O AUT}$	mgO/l	0.5	0.10
Heterotrophs, X_H				
Half saturation constant of O ₂ for X_H	K_O	mgO/l	0.2	0.13
Anaerobic hydrolysis reduction factor	η_{fe}	-	0.4	0.35
Phosphorus Accumulating Organisms, X_{PAOs}				
Maximum storage rate for PHA	q_{PHA}	day ⁻¹	3.0	2.20
Poly-P requirement per PHA stored	Y_{PO4}	gP/gCOD	0.4	0.36
Rate for lysis of X_{PAOs} X_{PP} X_{PHA}	b_{PAOs} , b_{PP} , b_{PHA}	day ⁻¹	0.2	0.08
Saturation coefficient for phosphorus in storage of X_{PP}	K_{PS}	mgP/l	0.2	0.50
Settling parameters				
Maximum theoretical settling velocity	v_0	m/day	-	680

*@ 20°C ** @ 17°C

The anaerobic hydrolysis reduction factor, η_{fe} was experimentally found in the range of 0.8-1.0 (Mino *et al.*, 1995) and it was reported that, depending on the rate and the configuration, the η_{fe} has a crucial role on the phosphorus release concomitantly, the X_{PAOs} , X_{PP} and effluent phosphate concentrations in the bulk liquid (Larrea *et al.*, 2002, Ekama and Wentzel, 1999, Carucci *et al.*, 1999b). The slowly biodegradable COD degradation is a very important issue with respect to the realistic modelling of activated sludge systems because it is primarily responsible for the attainment of realistic space-time dependent electron acceptor profiles (Maurer and Gujer, 1994, Bidstrup and Grady, 1988). To keep it simple, only the anaerobic hydrolysis reduction factor was changed from 0.4 to 0.35.

The yield coefficient for Poly-P requirement per PHA stored, Y_{PO4} was decreased to 0.36 mPO₄/mgCOD to lower the peaks during the morning and afternoon (under high COD loadings). The second issue is that the pH in the outer reactor is around 6.7 resulting in a lower phosphate release as discussed by Smolders *et al.* (1994a) and Filipe and Daigger (1999). It was shown that the energy generated from the observed phosphate release at low pH is not enough to convert acetate to acetylCoA, so the

glycogen metabolism is more pronounced. The value of this parameter shows a wide variation in the literature with a range of 0.4-1.4 (P/C) by Wentzel *et al.*(1985). The studies carried out by Filipe *et al.*, 2001, Romansky *et al.* (1997) and Smolders *et al.* (1994a) showed the effect of different pH on phosphorus release. A decrease in pH resulted in a decrease in released phosphate under anaerobic conditions. So, the calibrated value of the Y_{PO4} is in concert with the results of Smolders *et al.* (1994).

The oxygen saturation constant for heterotrophs, K_O was decreased from 0.2 to 0.13 mgO₂/l in order to increase the activity of the heterotrophs and PAOs under oxygen limited conditions. The K_O varies significantly depending on the model structure, biomass type and mixing patterns in bioreactors (Orhon and Artan, 1994). Lau *et al.* (1984) reported a value of K_O varying from 0.01 mgO₂/l for filamentous bacteria, to 0.15 mgO₂/l for floc-forming bacteria. According to the literature, the value of K_O is reported to be 0.002 mgO₂/l in the general model of Dold and Marais (1986), 0.2 mgO₂/l by Larrea *et al.* (2002) and De la Sota *et al.* (1994), 0.7 mgO/l for a SND (EBPR) modeled by Meijer *et al.* (2001), 0.5 mgO₂/l in the full scale modelling studies of Wichern *et al.* (2001) and 0.15 mgO₂/l by Carucci *et al.* (1999). In addition, Meijer *et al.* (2001) stressed the relationship between the K_O and the influent slowly biodegradable COD fraction, X_S . The effluent nitrate concentration is highly dependent on the oxygen saturation constant, K_O . Lowering the K_O value together with the $X_S/(X_S+X_I)$ ratio resulted in the increase of the nitrate concentration because of limited denitrification capacity. In IAWPRC (ASM1, ASM2d, ASM3) models, a value of 0.2 mgO₂/l is suggested.

The half saturation oxygen constant for autotrophs was reported in wide range of 0.002-2.0 mgO₂/l (U.S. EPA, 1975, Dold and Marais, 1986). On top of that, after an adaptation period, low oxygen concentration was found to have an influence on the cell aggregation where the establishment of smaller aggregates exerted low oxygen affinity constants in an aerated reactor (Park and Noguera, 2002). The value of the maximum autotrophic growth rate, μ_{AUT} and the half saturation constant for ammonium were reported in a wide range of 0.25-1.23 day⁻¹ and 0.06-5.6 mgN/l (Cinar *et al.*, 1998, Dold, 2002, Stenstrom and Podushka, 1980, Sözen *et al.*, 1996, Daigger and Nolasco, 1995, Copp and Murphy, 1995). The maximum growth rate for autotrophs was reported in the range

of $0.66\text{--}78\text{ day}^{-1}$ under low oxygen levels (Hanaki *et al.*, 1990). Under low oxygen levels, the nitrification process was activated by decreasing the K_{OAUT} during the steady state calibration.

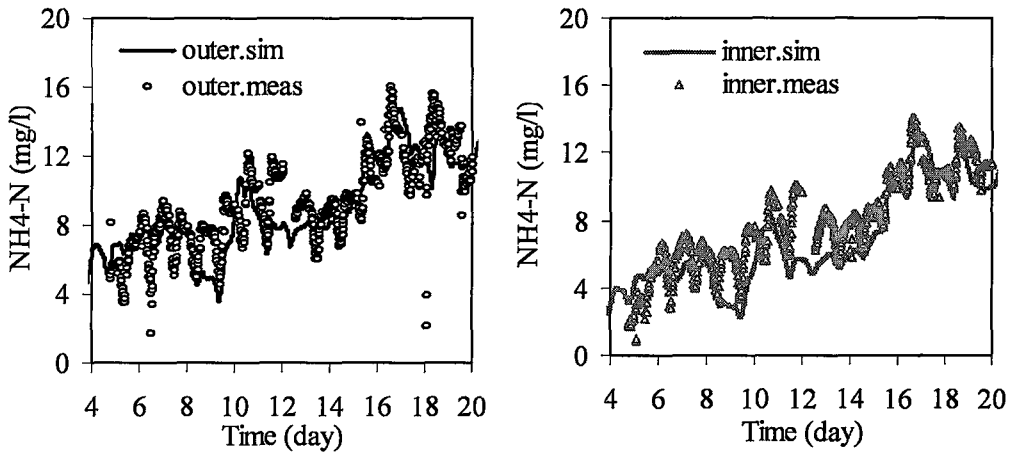


Figure 9.7 $\text{NH}_4\text{-N}$ profile in outer and inner rings

The maximum growth rate for nitrifiers was calibrated under dynamic conditions. The results show that the rate was adversely influenced by low oxygen concentrations and/or slightly lower pH values (Orhon and Artan, 1994). The μ_{Amax} and K_{Oaut} were fine-tuned separately with the aid of the calibration method (Figure 9.5) using the steady state and dynamic data. The μ_{Amax} and K_{OAUT} were adjusted to 0.7 day^{-1} and $0.10\text{ mgO}_2/\text{l}$ respectively. The values are in the range of their reported bounds. The activity of nitrite oxidizers was strongly limited at $0.5\text{ mgO}_2/\text{l}$ and nitrite can be accumulated up to 60 mgN/l (Hanaki *et al.*, 1990). However, nitrite concentrations were negligible in the measuring campaign data.

The values of the q_{PHA} in the literature vary between $3.0\text{--}8.0\text{ gCOD/gCODd}$ (Siegrist *et al.*, 2002, Cinar *et al.*, 1998, Daigger and Nolasco, 1995, Wentzel *et al.*, 1989). The maximum storage rate for PHA, q_{PHA} was assigned to $2.2\text{ gCOD/gcellCOD.d}$ also falling in the range of $2.0\text{--}3.0$ suggested in Henze *et al.* (1999). The steady state calibration studies of Cinar *et al.* (1998) for oxidation ditches showed that EBPR could only be attained by setting the q_{PHA} to 8.0 gCOD/gCODd using the ASM2 model. Otherwise, X_{PAOs} could not compete with the ordinary heterotrophs and finally washed out from the system because of the fact that they could not build up their PHA pool for biomass

growth and Poly-P storage. This may have been due to the over estimation of the denitrification capacity of ordinary heterotrophic biomass.

The lysis rates for X_{PAO} , X_{PHA} and X_{PP} were adjusted to 0.08day^{-1} since the PAOs were washed out from the system. This adjustment in this parameter provided for a relatively constant PAO concentration in the bioreactor. Also, the PHA pool could be efficiently used by PAOs under dynamic loadings. Similar observations and calibration results were also reported for values around 0.12day^{-1} suggested by Siegrist *et al.* (1999) and 0.14day^{-1} by Cinar *et al.* (1998). The hypothesis is that the PAOs slow down their endogenous metabolism in order to compete with other heterotrophs under low oxygen/nitrate concentrations (Cinar *et al.*, 1998, Randall *et al.*, 1992). Another reason could be predation by protozoan activity that exists mainly under aerobic conditions (van Loosdrecht and Henze, 1999, Tijhuis *et al.*, 1993). The saturation coefficient for phosphorus uptake, K_{PS} was increased to 0.5 which allowed to keep the P fluctuations smoother under dynamic conditions. Figure 9.7 shows that there is an increase in the effluent ammonia concentration because of the suppressed growth due to the oxygen limitation. The autotrophic biomass concentration, X_{AUT} was simulated to be around 15 mg COD/l and showed a decrease towards 10 mgCOD/l during that period because of oxygen limitation and excessive sludge wastage (see Figure 9.11). It was difficult to calculate the minimum sludge age for autotrophic biomass because of oxygen-limited conditions.

Generally, the oxygen concentrations were simulated to be below 0.2-0.5 mgO₂/l depending upon the organic loadings. During the time interval between 8-12 days, an increase in the oxygen level concomitant to NO₃ peaks can be observed in Figure 9.8, Figure 9.9. In reality, the most probable reason is the decrease in the biodegradable COD load causing an oxygen increase or increase in the aeration capacity. As a result, the activity of autotrophs increased under non-limited oxygen conditions. In addition, the aeration capacities of the disc aerator system in all reactors were kept constant despite some minor changes done by plant operators during the calibration period. In spite of these uncertainties, a fairly good fit was attained on the ammonia, the nitrate and the phosphate measurement outputs.

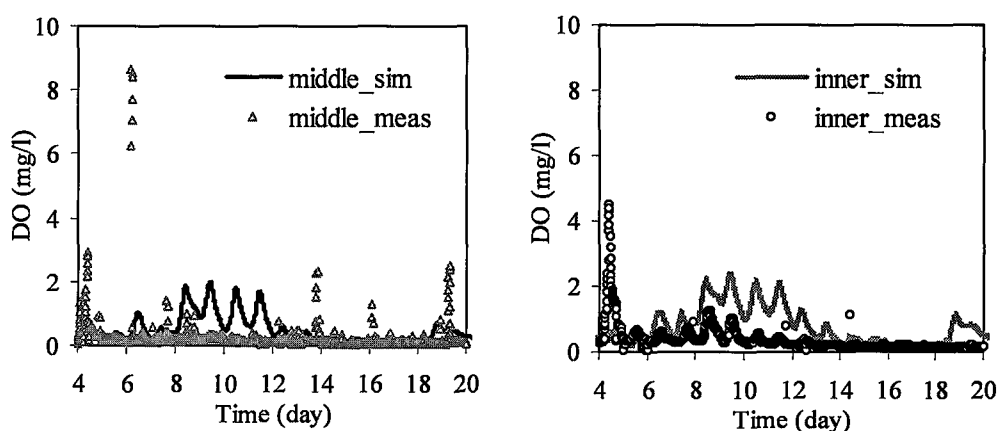


Figure 9.8 Dissolved oxygen in middle and inner rings

The filtered phosphate concentrations in the effluent stayed below 1.0 mgP/l during the measurement period. However, Figure 9.10 reflects the phosphorus in the middle ring and in the clarifier. According to the figure, the effluent phosphorus slightly increased and fluctuated until day 12. On the following days, obviously, the removal efficiency again recovered. In addition to that, these fluctuations in the profile are quite visible because of the variations in the incoming organic loading during the day. Depending on that situation, the internal storage polymer, PHA was also found to be varying over time. The exhaustion of the PHA pool also causes phosphorus release due to endogenous decay metabolism. Shortly, two marginal situations could be observed along the day period (a) depending upon the influent COD load, PAOs could release phosphorus in the absence of electron acceptors. This situation inevitably occurs if aeration is not sufficient under elevated organic loadings, (b) phosphorus release can also occur if no PHA pool is available for phosphorus uptake. In the literature, the reason of the phosphate peaks were attributed to the temporal imbalance between P-release and uptake by Isaacs *et al.* (1995) or the depletion of internally storage pool due to the excessive aeration and/or low organic loading (Brdjanovic *et al.*, 1998b, Temmink *et al.*, 1996).

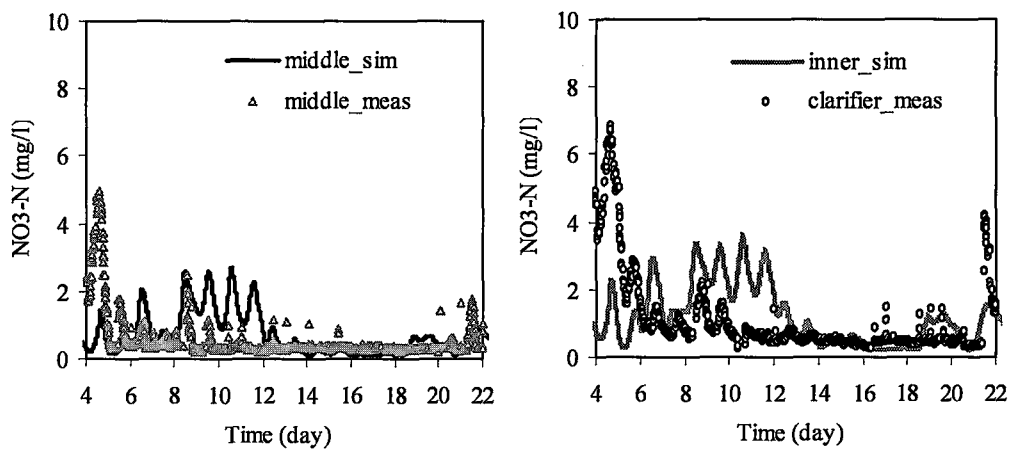


Figure 9.9 Nitrate nitrogen profile in middle and inner rings

Another point is the difference between the simulated and measured phosphate profiles in the clarifier. The difference may be attributed to a “secondary release of phosphorus” in the final clarifier since the nitrate and the oxygen levels are very low. Wouters-Wasiak *et al.* (1996) stated that the secondary phosphate release occurs at low rates (0.2-0.4 mgP/gVSS.h) when the nitrate concentration is below 0.5 mgN/l in the absence of oxygen, as well.

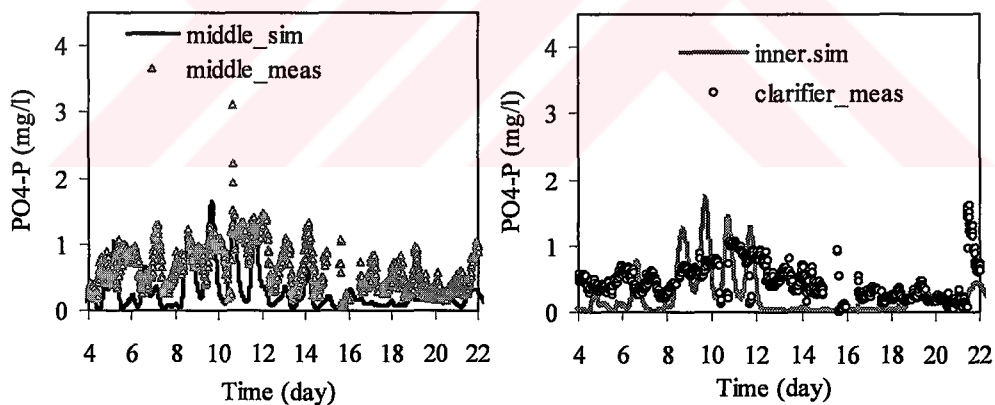


Figure 9.10 Phosphate profiles in middle and inner rings

The exhaustion of the PHA pool also makes PAOs to release phosphorus into the bulk liquid to derive energy for their maintenance (Siegrist *et al.*, 1999). The adjustment of the aeration and sludge wastage can be the solution to maintain the storage material at some degree during these starvation periods (Miyake and Morgenroth, 2002). Recovery time needed for phosphorus removal can be decreased in that manner. Considering the

dual storage phenomena, it was suggested that the glycogen cannot replace PHB for phosphate uptake under aerobic conditions and it is only used for maintenance (Brdjanovic *et al.*, 1998b). The trajectories of the simulation pertaining to the biomass components are illustrated in Figure 9.11.

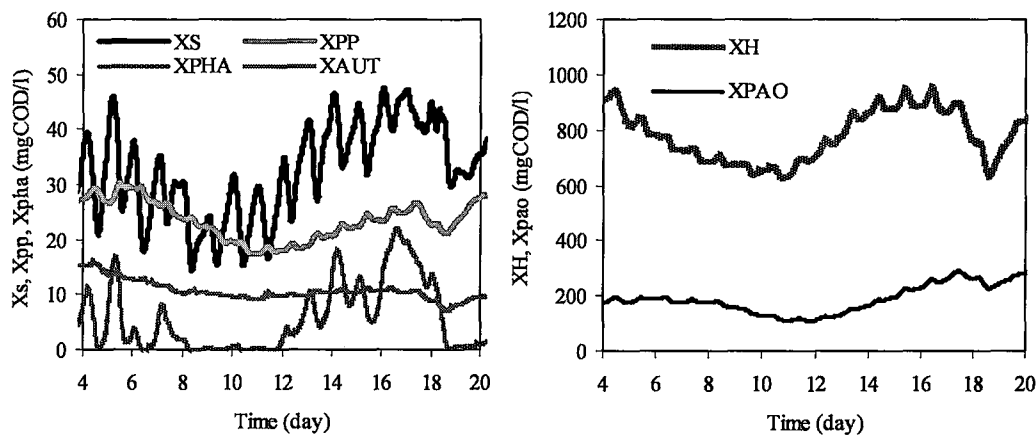


Figure 9.11 Simulated biomass composition (middle ring)

Finally, a non-reactive Takacs *et al.* (1991) settling model with 20 layers was used to simulate the sludge blanket and concentrations in the clarifier. The theoretical settling velocity, V_0 was set to 680 m/day in order to allow faster settling in the clarifier and keep the sludge blanket at low levels ($H_S < 1\text{m}$). Figure 9.12-left reflects the measured and the simulated sludge blankets in the clarifier. The simulation for the period between 4-18 days successfully predicted the sludge blanket. However, as seen in the figure, the model overestimates the sludge blanket height at 18th days. Diversion of the flow into the middle ring could explain the experimentally obtained sludge blanket at 18th days. Sludge concentration profile measured on day 10 showed a good agreement with the experimental sludge concentration profile along the depth of the clarifier (Figure 9.12-right).

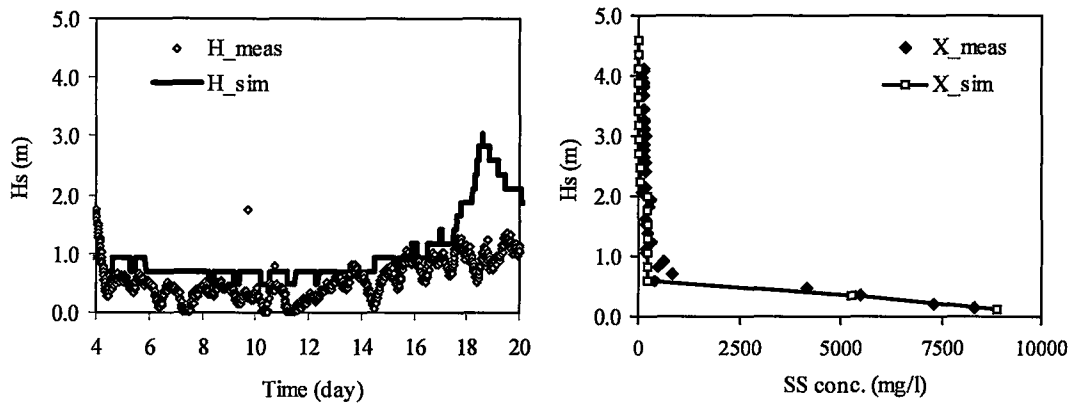


Figure 9.12 Sludge blanket height, H_s (left) and sludge concentration profile (right) in the clarifier (at day: 10)

It should also be noted here that during the rain event some measures had been taken by the plant operators in order to prevent sludge lost from the clarifier which were not very well documented. As a result, it was difficult to conclude and model the effect of low organic loading in last days. The gradual decline in the biomass components during the first 12 days is due to the excessive sludge wastage. In the following period the recovery (increase in concentration) in all components was simulated and the trends of all components are identical. These results also agree with the phosphorus removal recovery stated above. The concentration of PHA was found to be instable. As previously discussed and concluded from the simulations, the recovery of the PHA pool is highly dependent on the COD load and the aeration capacity of the plant.

9.4 Conclusions

The influent wastewater characterization in terms of COD fractionation plays a crucial role in modelling. For instance, uncertainty in the slowly biodegradable COD caused oxygen elevations in the reactors. As a result all processes depending on oxygen concentration (i.e. P release, nitrification, denitrification) are adversely affected by this fact. So, the hydrolysis mechanism plays an important role not only on the oxygen levels and COD source in the reactors but also on the effluent nutrient concentrations. The measurement outputs were found to be very sensitive to the treatment plant operational parameters. A successful calibration is highly dependent on better understanding of the

system in terms of process changes. Otherwise, it causes biased estimation and/or misleading conclusions in the model calibration.

The EBPR mechanism in simultaneous nitrification-denitrification, SND was found to be instable in terms of the storage polymer pool. During daytime, the variation in the COD load may result in P release. On the other hand, the exhaustion of this storage polymer also leads to P release because of endogenous metabolism. This should be investigated further. The system operated under low oxygen levels and under varying input load suffered from oxygen limitation, as a result, nitrification failure. In addition, insufficient aeration and excessive sludge wastage resulted in nitrification loss during the measuring campaign period. With efficient control of aeration, nitrification can be improved. However, EBPR should be taken care of then, because of nitrate will build up in the outer ring. So, the sludge wastage and the aeration control are necessary for stable operation of SND systems.

The changes in the plant operations should be well defined in order to represent them in the simulation. This would be a part of the verification of the model. Otherwise, it is impossible to calibrate or verify the model and/or to interpret the measurement results. A successful model calibration necessitates collection of ample information about the real situation in the plant.

10 DYNAMIC MODEL CALIBRATION FOR AN INTERMITTENTLY AERATED CARROUSEL TYPE ACTIVATED SLUDGE PLANT: EVALUATION OF THE LONG-TERM PREDICTION PERFORMANCE OF A CALIBRATED MODEL

10.1 Introduction

Since the promulgation of the EU Directives (91/271/EEC) regarding strict discharge standards for nitrogen and phosphorus, especially in sensitive areas, appropriate design and plant optimization issues are gaining more importance. Activated sludge plants are the most commonly used technology for removing organic carbon and nutrients (N, P) from domestic and/or industrial wastewaters to meet the discharge criteria. In general, a number of process alternatives have been proposed. Among these alternatives, carousel type systems are associated with plants for small communities, where stability and simplicity of operation are of prime importance in the absence of primary clarification (Grady *et al.*, 1999; Randall *et al.*, 1992). The stability of treatment efficiency, especially with regard to nutrient removal, is often difficult to achieve due to the complex characteristics of biological processes.

The features that distinguish carousel type systems from other conventional activated sludge plants are (a) it is operated with high sludge age, (b) it has a simplified flow diagram and (c) it possesses channel (plug) flow characteristics. The system provides not only well-stabilized sludge but also flexible operation (i.e. aeration control) alternatives under dynamic conditions. In order to provide phosphorus removal and to prevent excessive growth of filamentous microorganisms, anoxic or anaerobic selectors are introduced prior to the aerobic/anoxic reactors. Another option can be the intermittent feeding or aeration of the mixed liquor (Grady *et al.*, 1999; Randall *et al.*, 1992).

The optimization of the operation of an activated sludge plant using a model-based approach necessitates successful and reliable calibration of the dynamic mathematical

models. In literature, many mathematical models have been used to describe the biological processes. The models concerning carbon and nitrogen removal are described by ASM1 and ASM3 (Gujer *et al.*, 1999). Enhanced Biological Phosphorus Removal (EBPR) together with carbon and nitrogen removal are described by other models (Wentzel *et al.*, 1992; Henze *et al.*, 1995,1999; Barker and Dold, 1997). Metabolic models for EBPR were also proposed which include the maintenance of biomass as a separate process (Smolders *et al.*, 1994; Murnleitner *et al.*, 1997; Filipe and Daigger, 1998).

Several studies have been conducted concerning the calibration of the Enhanced Biological Phosphorus Removal (EBPR) type activated sludge plants, as described by the ASM2 and ASM2d models (Cinar *et al.*, 1998; Carrette *et al.*, 2001; Makinia *et al.*, 2002). From a modelling point of view, the data collection with regard to influent wastewater, environmental influences (i.e. temperature changes) together with biomass characterization play a crucial role to increase the reliability of the model that will be used for retrofitting or process optimization. On top of that, difficulties in the calibration of the treatment plant are encountered very often because of the limitations in available plant information and the over-parameterized (too complex) structure of the mathematical models (Ayasa *et al.*, 1995; Weijers and Vanrolleghem, 1997; Brun *et al.*, 2002; Reichert and Vanrolleghem, 2001). Consequently, prior to the calibration, a measuring campaign should be designed in order to collect informative data from the treatment plant (see Chapter 1).

In literature, several calibration protocols have been proposed namely STOWA protocol (Hulsbeek *et al.*, 2002), HSG guidelines (Langergraber *et al.*, 2003a) and BIOMATH protocol (Vanrolleghem *et al.*, 2003; Chapter 1). The STOWA protocol is tailored for the SIMBA simulation software and based on extensive experience obtained from dynamic modelling of over 100 activated sludge treatment plants in the Netherlands (Hulsbeek *et al.*, 2002). The HSG guidelines (Langergraber *et al.*, 2003), on the other hand, summarize the experience of university members from Germany, Austria and Switzerland with the simulation of dynamic activated sludge models. The BIOMATH calibration protocol is based upon the work of Petersen *et al.* (2002) with dynamic modelling of WWTPs in Belgium and extended in Chapter 1 for general applications.

The above-mentioned calibration protocols have a common target: to provide a standardized approach for the calibration of dynamic activated sludge models and thereby to facilitate the application of dynamic models into practice. Subsequently, it is hoped that the standardized approach will improve the calibration accuracy and provide a basis for quality control/reliability check and comparisons between different calibration studies (Hulsbeek *et al.*, 2002; Langergraber *et al.*, 2003). These protocols differ in their approaches to reach this common target. The STOWA protocol proposes a physical-chemical method combined with BOD measurements for the characterization of influent wastewater (Hulsbeek *et al.*, 2002) and it provides a detailed and step-by-step approach for the implementation of a calibration study. The HSG guidelines, on the other hand, focus more on the systematic and detailed documentation of the calibration study rather than providing a detailed procedure on how to calibrate a mathematical model (Langergraber *et al.*, 2003). Finally, in the BIOMATH protocol, a dynamic calibration procedure based on interactive modules is proposed which aims to obtain a minimum effort and cost-effective calibration. To this aim, the calibration procedure was made flexible and interactive where different choices are provided to the user corresponding to different levels of calibration accuracy. Moreover, the Optimal Experimental Design (OED) concept is incorporated at different levels of the calibration procedure in order to provide a cost-effective and information rich experimental designs. In this study, the BIOMATH calibration protocol is applied/followed to ascertain a standard approach for calibrating the activated sludge model in this study it is ASM2d.

An important step in modelling is the validation step, which is a long disputed and controversial issue. In this step, the objective is to check the ability of a calibrated model to predict the behavior of a treatment plant under operating conditions (drastically or gradually) different than the calibration period. On the other hand, there is no general agreement on how to validate a model for dynamic activated sludge treatment plants in the above-mentioned calibration protocols (i.e. concerning data collection frequency, period and duration etc.).

From a model-validation point of view, a significant question arises as to what extent/how long a calibrated and/or validated model does indeed represent/predict the behavior of a treatment plant. In other words, what is the evolution/fate of a calibrated

model in time in view of its prediction performance? This aspect of modelling is particularly important in order to ascertain the reliability of a model in view of its long term applicability/performance to simulate the behavior of the complex WWTP systems before full-scale implementation purposes e.g. process upgrade, optimization, control or design purposes. To this aim, this study focuses on the evolution of a calibrated model in time. In other words, the validity of a calibrated model is monitored over a long-term with separate and dedicated measurement campaigns to understand and therefore assess the need for re-calibration of the model.

The objective of this study is tested at a municipal wastewater treatment plant located in Noord Brabant, the Netherlands (Haaren WWTP). A mathematical model (ASM2d), which was calibrated with the measurement campaign (MC1) data performed 3 years ago (Insel *et al.*, 2003b), is used. A new measurement campaign (MC2) following the BIOMATH protocol (Chapter 1) is performed for this study to collect information rich dynamic data for validation and/or re-calibration of the Haaren WWTP. It is important to note that the operation strategy of the Haaren WWTP remained the same over the last three years but that influent dynamics were naturally different over past 3 years. The modeling work is structured as follows: First the results of the new measurement campaign (MC2) are given in comparison with the first measurement campaign (MC1). This is followed by the comparison of the predictions/simulations of the model calibrated on the basis of the treatment plant dynamics obtained in the first measurement campaign (MC1) (Insel *et al.*, 2003b). Then, the calibrated model is simulated with the new input dynamics obtained from the second measurement campaign (MC2) and the simulation results are compared to the treatment plant performance obtained in the second measurement campaign (MC2). In other words, the validity of the model is evaluated. That means that the long-term prediction ability of the calibrated model (in other words the fit of the calibrated model to the second measurement campaign (MC2) designed 3 years later) is evaluated and the issue of re-calibration of the model is addressed. Finally, the model is re-calibrated and the simulation results are compared to the performance of WWTP in the second measurement campaign (MC2). Last, the recalibrated model is used to understand in depth the dynamic nutrient removal performance in the Haaren WWTP.

10.2 Materials and Methods

10.2.1 Wastewater treatment plant definition

The treatment plant under study is located near Haaren, Noord-Brabant, the Netherlands. The activated sludge plant is a carousel type plant receiving the wastewater of 50000 PE. The average daily influent flow rate of the plant was recorded to be 6500 m³/day (the average of 4 days during the measurement campaign). An anaerobic selector is present prior to the carousel tank in order to prevent sludge bulking (see Figure 10.1). The carousel plant consists of one anaerobic reactor, 2 carousels and 6 clarifiers. The carousel reactors are operated in parallel and basically the system has two lanes after the anaerobic selector. In case of high hydraulic loadings, the influent flow bypasses the anaerobic selector and is equally distributed to the carousels.

Four out of 6 clarifiers are operational under average daily flow loading. The sludge recycle is controlled in order to avoid sludge overflow from the weirs of the clarifiers. During average daily flow loading 4 recycle pumps are activated and the sludge recycle is controlled with these pumps according to manual SVI measurements. The total maximum capacity of the recycle pumps is 600 m³/h under heavy rain events. The volumes for the anaerobic compartment (1), carousels (2) and the clarifiers (4), are given in total as 1400 m³, 10000 m³ and 2460 m³ respectively. The operational SRT of the system is around 22 days. The overall hydraulic retention time of the system is 1.8 days.

10.2.2 Operation/Control Strategy

The dissolved oxygen concentration is simultaneously controlled in both carousels. The control strategy is different for day and night operation. During the day period, the 2 aerators in each carousel are manipulated to keep the dissolved oxygen concentrations in the range between 0.9 mg/l and 1.2 mg/l.

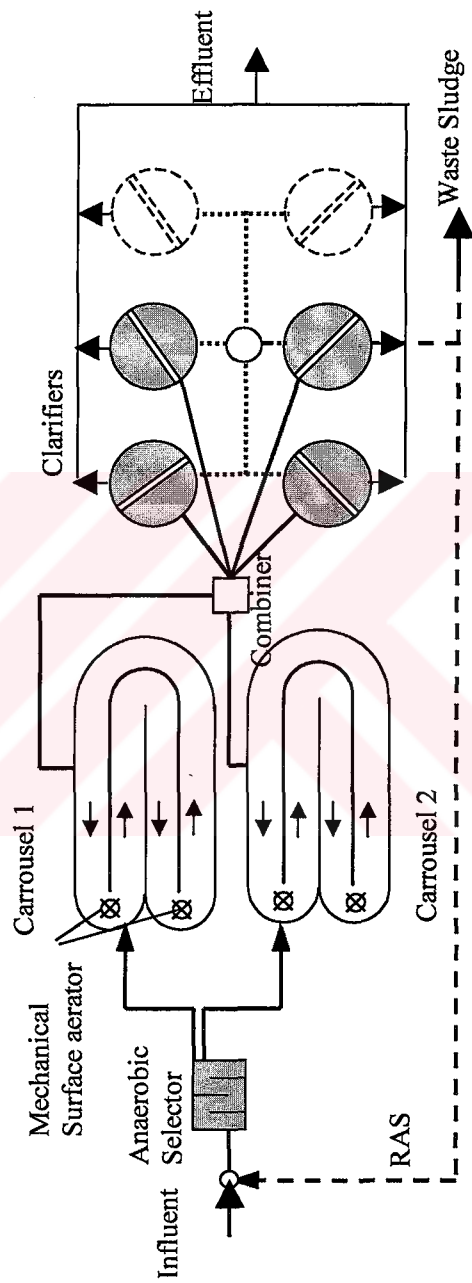
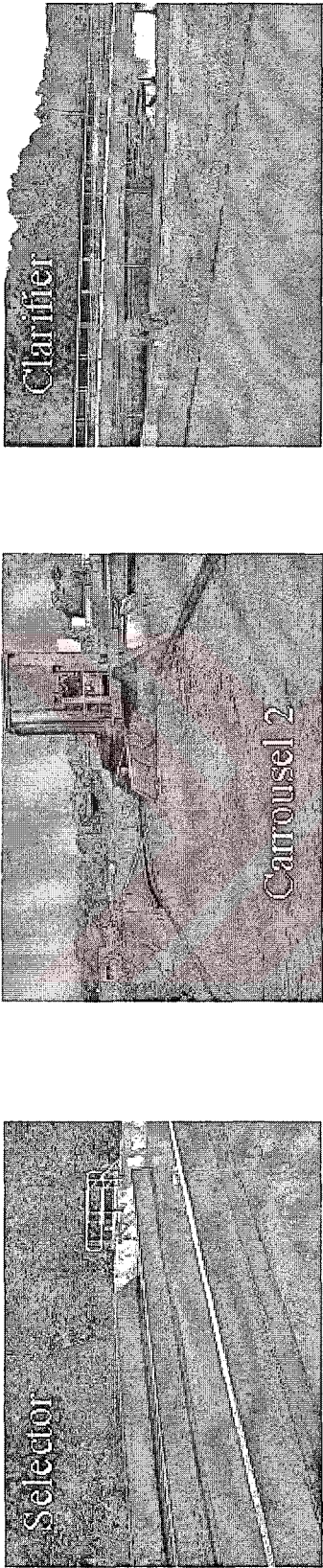


Figure 10.1 Pictures and schematic diagram of activated sludge plant

In the course of the night period, the carrousel is operated as an alternating plant by turning the aeration on/off in so-called intermittent aeration to stimulate denitrification. In this alternating aeration period, the total cycle time, T_C is set to 110 minutes. The aeration is shut off during 80 minutes and turned on for 30 minutes. In each 30 minutes aeration period, the aerators are operated as during the day period and the dissolved oxygen is controlled in the range of 0.9-1.2 mgO₂/l. It should be noted that during the intermittent aeration one of the aerators was kept at its maximum level (low O₂ transfer) for keeping the MLSS in suspension. The average internal mixed liquor recycle rate in the carrousel is calculated as 635,040 m³/day which is 108 times the influent flow rate leading to a typical flow velocity of 0.3 m/s. The average sludge recirculation rate (Q_R) through the anaerobic selector is calculated as 8434 m³/day.

10.2.3 Measurement campaigns

In the framework of this study, dynamic plant data obtained from 2 different measurement campaigns were used in order to check the success of the prediction of the model as mentioned above. In the first measurement campaign (MC1), an intensive rain event happened just before the first measurement campaign (see Figure 10.2), which does not reflect the real plant efficiency under daily average loading (Insel *et al.*, 2003b). In this respect, the second measurement campaign (MC2) was conducted under dry weather conditions. It is used as a validation data set for the calibrated model (Insel *et al.*, 2003b) to give an idea on the real average removal efficiency without any external disturbances. Both measurement campaigns were performed in the summer period.

10.2.3.1 First measurement campaign (Insel *et al.*, 2003b)

The measurement campaign data comprises the dissolved oxygen (DO), NO₃-N (both on-line); effluent ortho-phosphate and TSS concentrations (lab analyses) in the carrousel for a period starting from 17/07/2000 till 25/07/2000 corresponding to day 7 and 14, respectively. The total/filtered (0.45µm) COD, VFA, BOD_u, total/filtered TKN, NH₄-N, total/filtered phosphate and TSS measurements were performed with a grab sampling interval of 4 hrs during the measurement campaign period. The temperature of the mixed liquor was reported in the range of 17.2-19.2 °C. The average wastewater and COD

characteristics used for the steady state analysis are given in Table 10.1. The nitrate and the oxygen concentrations were measured in Carrousel 1 with a sampling interval of 15 and 5 minutes, respectively. The ortho-phosphate analyses were performed every day from the effluent weir of the clarifier. The daily samples for filtered phosphate samples were taken from the effluent.

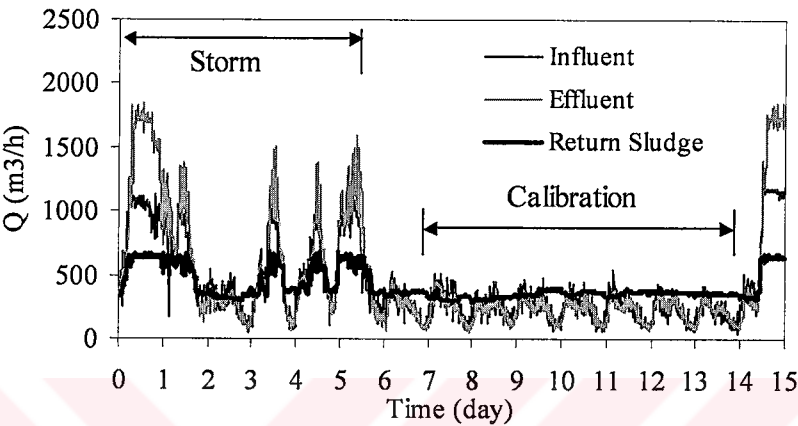


Figure 10.2 Influent, effluent and RAS flow-rates in the 1st Measurement Campaign (Insel *et al.*, 2003b)

10.2.3.2 Second measurement campaign (MC2)

The MC2 data comprise on-line DO, NO₃-N and NH₄-N measurements; ortho-phosphate from the selector and the effluent of the plant for 4 days starting from 16th to 19th June 2003. In addition, the total/filtered (0.45µm) COD, VFA, BOD_u, total/filtered TKN, NH₄-N, total/filtered phosphate and TSS measurements for influent wastewater characterization were also measured from the grab samples taken at different frequencies and locations (see below) during the measurement campaign period. The temperature of the mixed liquor was around 19 °C. The average influent wastewater characterization, which was used for the steady state analysis is given in Table 10.1 in the results section below. In addition, flow-rates of the influent, RAS and WAS were also collected from the SCADA system (see Figure 10.3) and quality of the flow data was checked and improved (see Annex B). No sludge blanket was observed during the course of the measurement campaign.

The measurement campaign was designed based on expert knowledge and system analysis (Vanrolleghem *et al.*, 2003; Chapter 1). However, the application of OED as a tool for designing the optimal measurement campaign should be considered for the future studies in order to save cost and time associated with measurement campaigns (Chapter 1). The following sampling frequency and measurements were performed between 16/07/2003 and 19/07/2003:

Influent to the selector: 4-hours flow proportional composite samples were taken automatically every 4 hours (in total 6 samples/day) for the analysis of influent COD, COD_{filtered}, TKN, TKN_{filt}, TP, PO₄³⁻, TSS and VSS. Grab samples were also taken two times a day from the influent for the analysis of BOD, COD (for determination of biodegradable fraction of COD i.e. influent BOD_u/COD_{tot} ratio), VFA (for the determination of VFA/COD ratio) and NO₃. All the grab samples except for the BOD were filtered in-situ and preserved according to the Standard Methods (APHA, 1995).

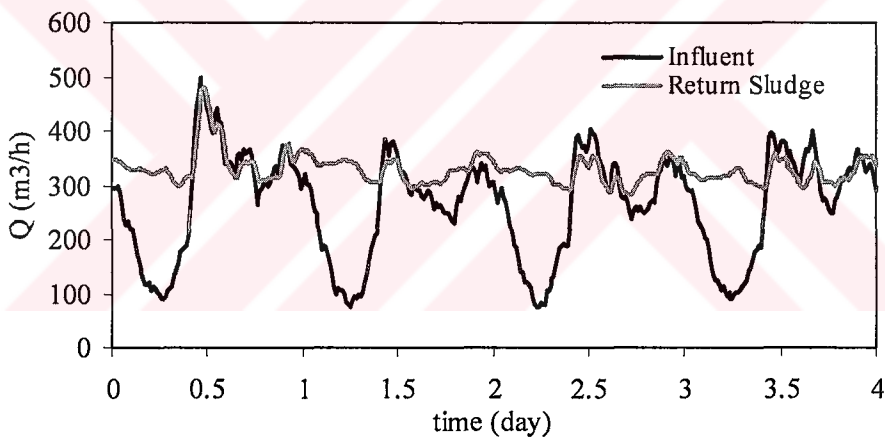


Figure 10.3 Influent, effluent and sludge recycle flowrate in the 2nd Measurement Campaign

Selector: Two grab samples per day from the first compartment of the selector and two grab samples a day from the output compartment of the selector were taken and manually filtered in situ. These grab samples were used for the analysis of NO₃-N, PO₄³⁻ and VFA in the selector.

Carrousel: 3 grab samples were taken per day and manually filtered for the analysis of PO₄³⁻ and 1 sample per day was taken for the analysis of the COD, TKN, TP (used for

determination of the TKN/COD and TP/COD content of the MLSS), MLSS and MLVSS. Moreover, online ammonium and nitrate sensors were positioned next to each other in the 8th compartment of the carrousel (see Figure 10.5) for the online measurements at 15 minutes interval. One on-line DO sensor, positioned in the middle of the carrousel (6th compartment), provides data every 5 minutes.

Return activated sludge (RAS): One sample was taken manually per day for the analysis of TP and MLSS (used for the mass balance and to check the system SRT). In addition, one sample was also taken every day from the waste activated sludge line for the analysis of TP and to calculate the actual sludge age of the system.

Effluent: 8 hours flow proportional composite samples were automatically taken everyday for the analysis of effluent TSS, COD, TKN, NH₄ and NO₃. One grab sample was also taken every day for the measurement of effluent BOD, COD (for the effluent BOD/COD ratio) and TP (needed to check the system SRT).

In addition, on June 18th 2003 the frequency of the grab samples in the influent, selector and carrousel was doubled (from 2 to 4 samples per day). The reason was simply to monitor the fast dynamics (if any) in the system with grab samples. The sample preservation, transport and analysis were all performed according to Standard Methods and/or Dutch standards unless otherwise mentioned. For the filtering, 0.45µm nylon filters (Millipore) were used. VFA analyses were performed using gas chromatography. The BOD measurements were performed with WTW-OxiTop.

10.2.4 Calibration methodology

The calibration of the activated sludge plant comprises three main steps (see Chapter 1). These are (a) *simple steady state calibration* (b) *steady state calibration* and (c) *dynamic calibration* steps. According to the proposed method, the first step concerns the *simple steady state calibration* after gathering the necessary information about the plant. This step mainly deals with the overall sludge balance over the system. In general, the aim is to obtain and maintain the measured sludge concentration with the simulations. In the simplified layout that is used for this calibration step (Figure 10.4), S1 and S2 delineate the two sections of the selector (an anoxic and an anaerobic zone) with a total volume of

1400 m³. Compartments C1 (Aerobic) and C2 (Anoxic) represent the carrousel with a total volume of 10000 m³. It should be noted here that the DO controllers are not modelled at this stage. Instead, the dissolved oxygen in the aerated reactors was set to 1.2 mg/l. The final clarifier was considered as a point settler in which the solids removal efficiency is almost 100%. In this step, the sludge wastage was estimated under steady state loading (flux based average). During the *steady state calibration* and the *dynamic calibration* steps, the aim is to mimic the real activated sludge plant together with the control strategy under steady state and dynamic loadings.

It should be noted that the parameters that are influential to the biomass compositions e.g. Y_H , b_H and/or X_I were changed only during the *simple steady state* and *steady state calibration* steps. During the dynamic calibration these parameters remained unchanged. For the steady state and dynamic calibration, a more complex layout was devised to reflect the plug flow characteristics of the bioreactor (Figure 10.5).

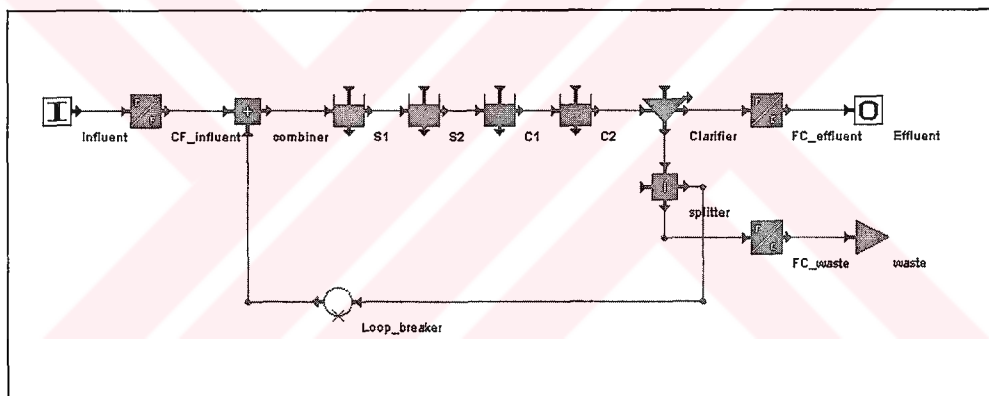


Figure 10.4 Plant layout for simple steady state calibration (WEST)

According to Abusam and Keesman (1999) the number of CSTRs in series is suggested to be limited to 10 reactors or to the minimum number needed for adequate modelling of the aeration configuration for closed loop reactors. In this respect, the anaerobic and the carrousel reactor were regarded as 4 (S1-S4) and 8 compartments in series (C1-C8), respectively based upon the plant geometry, DO measurements along the reactor and reactor geometry (Figure 10.5).

The sludge age calculation is of great importance for BNR plants because the TSS balance, active fraction of the biomass and internal storage products are highly

influenced by cell residence time (Henze *et al.*, 2002; Rodrigo *et al.*, 1996). Both authors suggest that the most appropriate sludge age for BNR plants is around 20 days. In this study, a mass balance for TP is performed using the TP measurements in the influent, effluent and WAS to verify the SRT of the system, which was found to be around 22 days (see Annex-B).

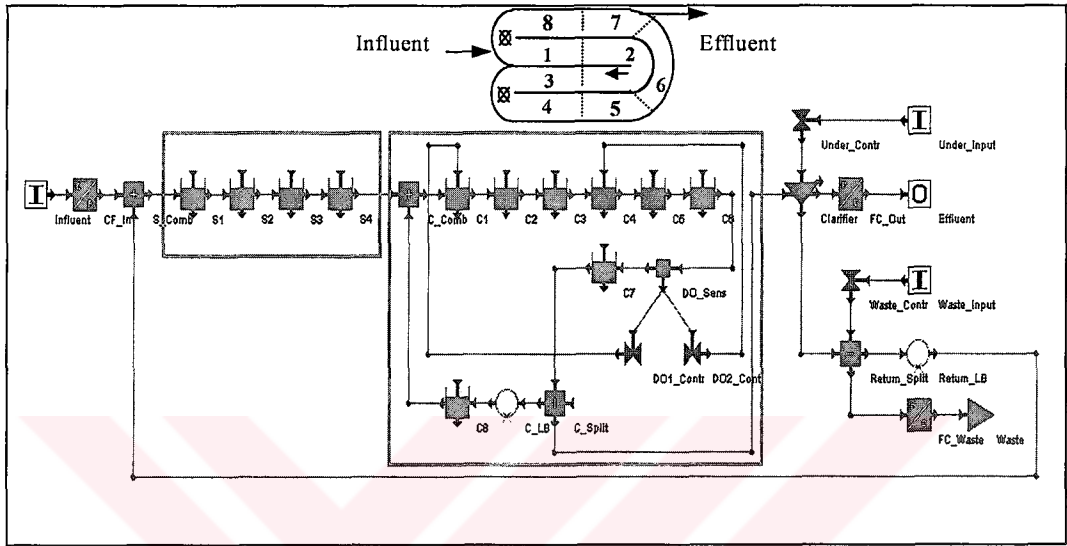


Figure 10.5. Plant layout implemented in WEST software

In the *steady state calibration*, a flux-based average steady state influent file was applied. The simulations were carried out to find out the initial biomass composition in the reactors under steady state loading that would fit the average measured N, P concentrations. This approach provides the initial values for the state variables that were then used in dynamic simulations. Dynamic simulations were carried out with the dynamic influent file. In order to mimic the smoothing effect of the final clarifier on the effluent N, P concentrations, a non-reactive mixed tank with a 2460 m³ volume was introduced after the point settler (not shown in Figure 10.5). The two identical lanes of the activated sludge plant and the clarifiers were combined together in order to decrease the computation time. The model implementation (ASM2d) and simulations were performed using a dedicated simulation package WEST (Vanhooren *et al.*, 2003).

10.3 Results And Discussion

10.3.1 The results of the second measurement campaign (MC2)

10.3.1.1 Determination of degradable fraction of influent COD

The biodegradable fraction of the influent COD was measured for the first day and second day of the measurement campaign (16-17/06/2003). The BOD was monitored for 28 days respectively and plotted together with the model-fits (see Figure 10.6). The ultimate BOD, BOD_U was estimated by fitting the following BOD model (Metcalf and Eddy, 1998; Weijers, 1999):

$$BOD_t = BOD_U (1 - e^{-kt}) \quad (\text{Eq10.1})$$

where t is time, k is the first order degradation constant and BOD_t is the BOD at any time t . The two BOD measurements indicate at least two phases (see Figure 10.6). In the first phase, the degradation rate of the organic carbon compounds is very fast suggesting that this might be the S_S fraction of the COD (e.g. VFA). This is followed by a slower degradation of the organic which might corresponds to the X_S fraction of the COD. These observations are supported by the study of Weijers (1999) where the BOD curves were analyzed using a simplified ASM1 model for aerobic conditions.

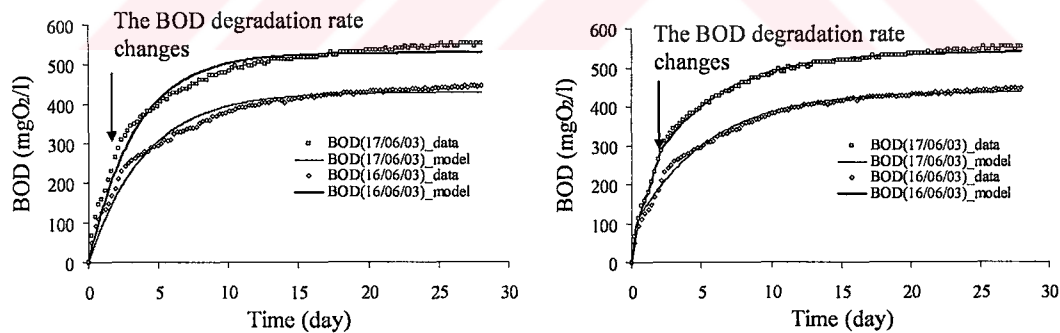


Figure 10.6 The BOD_U results of the influent grab samples taken at 16/06/2003 and 17/06/2003 respectively and the model fits (left) BOD model (Eq10.1) (right) simplified ASM1 model. Note that only every third data points of the BOD measurements is shown in the figure for the sake of clarity.

The model fit to the BOD measurements is observed to be remarkably better using the simplified ASM1 model (see Figure 10.6-right) than the traditional BOD model given in

Equation 10.1 (see Figure 10.6-left). The degradable fraction of the influent wastewater predicted by the BOD model was lower (around 6%) than the value predicted by the simplified ASM1 model. This is in contrast to the findings of Weijers (1999) where the BOD_U was clearly higher than the biodegradable COD, COD_{BD} predicted by the ASM1 model. This discrepancy between the BOD_U and COD_{BD} in this study can be attributed to the fact that the fit of the BOD model to the data (see Figure 10.6-left) was not as good as the fit of the ASM1 model (see Figure 10.6-right). It is clearly seen that the BOD_U was underestimated compared to the measurements (see Figure 10.6-left). This poor fit of the BOD model may have caused the underestimation of the BOD_U .

Table 10.1 BOD_U estimation results using BOD and simplified ASM1 models and degradable fraction (BOD_U/COD) of influent wastewater. Biodegradable COD, $COD_{DB} = S_s + X_s$

Sample	COD	BOD model			Simplified ASM1	
		BOD_U	k	BOD_U/COD	COD_{DB}	COD_{DB}/COD
	mgO ₂ /l	mgO ₂ /l	d ⁻¹		mgCOD/l	
16/06/2003	590	430	0.25	0.73	460	0.78
17/06/2003	710	530	0.3	0.75	561	0.79
Average	650	480	0.275	0.74	510	0.78

In this study, the degradable fraction of the influent COD was determined to be 76% by taking the average of the estimate of both models (BOD model and simplified ASM1, see in Table 10.1). This value is relatively high which also means that less inert COD is present in the influent compared to other WWTP calibration studies performed in the Netherlands (Roeleveld and Van Loosdrecht, 2002; Weijers, 1999).

10.3.1.2 Endogenous decay rate of the biomass

To determine the decay rate, the endogenous respiration of the biomass is monitored under continuous aeration for about 15 days in a 2 L batch reactor. As nitrification inhibitor 30 mg/l ATU was added to the batch reactor. The pH and temperature of the reactor were monitored and observed to remain relatively constant around 7.12 and 18.6 °C respectively.

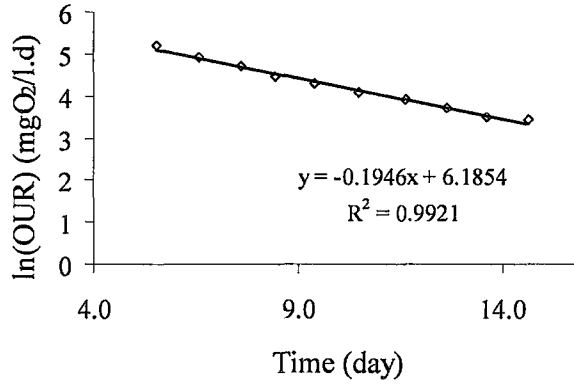


Figure 10.7 Endogenous respiration rate (OUR_{end} - ◇) of biomass over 15 days and the model-fit to the data (—). ATU (30mg/l) is added to inhibit nitrification.

The OUR measurements were started at the 5th day to ensure that the slowly degradable COD, X_S , and internal storage products of the biomass, X_{STO} , present in the mixed liquor were depleted considerably. The experimental results and the model-fit are shown in Figure 10.7. The aerobic endogenous decay rate of the biomass b_H' was determined to be 0.195 d^{-1} which is well in the range reported in the literature (Henze *et al.*, 1995b).

The endogenous decay rate corrected for the death-regeneration model of ASM2d can be calculated straightforwardly to be 0.39 d^{-1} assuming Y_H is 0.63 and f_{XI} is 0.2 (see below). This value is very much close to the default value of the ASM2d (Henze *et al.*, 1999) hereby supporting the use of default values of ASM models in case of lack of experimental data.

$$b_H = \frac{b_H'}{1 - Y_H(1 - f_{XI})} = 0.39 \text{ d}^{-1}$$

10.3.1.3 Average influent wastewater characterization (flux-based)

The average influent wastewater composition (flux-based) was calculated for the 1st and 2nd measurement campaigns and is given in Table 10.2. The strength of the influent wastewater in terms of total COD and TP for the 2nd calibration period is higher than that of the 1st calibration period while the TKN concentrations are almost the same (see Table 10.2). This can be attributed to the heavy rain event that took place just before the

1st measurement campaign or a change in the wastewater composition in time (Insel *et al.*, 2003b). The prediction of effluent quality of the treatment plants is highly dependent on the COD/TKN and COD/TP ratio as well as the fractionation of the COD components. As stated in Grady *et al.* (1999) and Randall *et al.* (1992), 8-10 mgVFA-COD/l is necessary for the removal of 1 mgP/l from wastewaters. It should be noted here that 6-8 mg VFA-COD is lost when 1 mgNO₃-N is recycled via the internal or sludge recycle streams through the anaerobic reactor.

Table 10.2 Influent wastewater characterization and COD characterization (flux based average)

Component	Unit	1 st Campaign	2 nd Campaign	Remark
Total COD, COD _{tot}	mgCOD/l	495	590	Measurement
Particulate Inert COD, X _I *	mgCOD/l	100	100	Mass balance
Soluble Inert COD, S _I	mgCOD/l	27	30	Effluent soluble COD concentration
Fermentable COD, S _F	mgCOD/l	25	130	Mass balance from soluble COD components
Acetate COD, S _A	mgCOD/l	95	70	GC analysis
Slowly biodegradable COD, X _S	mgCOD/l	248	250	Mass balance from particulate COD fraction
Ortho-phosphate, S _{PO4} -P	mgP/l	5	7.3	Measurement
Total phosphate, TP	mgP/l	8	12	Measurement and mass balance
Ammonium nitrogen, NH ₄ -N	mgN/l	50	48	Measurement
Total Kjeldahl nitrogen, TKN	mgN/l	63	66	Measurement
Soluble organic nitrogen	mgN/l	NA	6	
COD _{tot} /TKN	-	7.8	8.9	-
COD _{tot} /TP	-	62	50	-

* 28-day biochemical oxygen demand average of two days

Based on the biodegradable fraction of the influent wastewater (see above), the influent COD was fractionated following the BIOMATH protocol (Chapter 1) and is given in Table 10.2. Using the fraction of the inert particulates in the influent, X_I, calculated above, the average X_I in the influent was determined to be 100 mgCOD/l (see Table 10.2). It was observed that the steady-state model prediction of the MLSS concentration using the above-determined X_I in the influent was below the measured MLSS concentration in the carrousel, which is 4750 mg/l on average during the measurement campaign. The reason of this discrepancy could be the underestimation of the influent TSS concentration, especially during the flow peaks. Another factor could be the influent slowly biodegradable COD (X_S) can be fractionated further into several sub-classes with different degradation rates *i.e.* settleable, colloidal COD fractions (Orhon *et al.*, 2002). These fractions of X_S may act as inert X_I, depending on the SRT of the treatment plant and therefore contribute to the measured MLSS concentration in the

carrousel. However, further research is needed to clarify this discrepancy.

The calculation shows that the average COD/TKN ratio for the 2nd measurement campaign is 8.9, which claims that there is more COD source available for the denitrification compared to the first one. Therefore, it is expected that the effluent NO₃–N concentration should be lower but it was not as it is discussed in detail below.

10.3.1.4 Diurnal changes in influent wastewater composition

In this section, the diurnal changes in the wastewater composition are addressed on the basis of load changes in COD, TKN and TP concentrations. As shown in Figure 10.8 (right), the loads of COD, TKN and TP reveal cyclic changes during the measurement campaign. The ratio of COD/TKN and COD/TP calculated based on corresponding fluxes are in the range of 7.5-10.5 and 40-65 respectively which falls in a confident region appropriate for an efficient biological nutrient removal (Orhon and Artan, 1994; Randall, 1992).

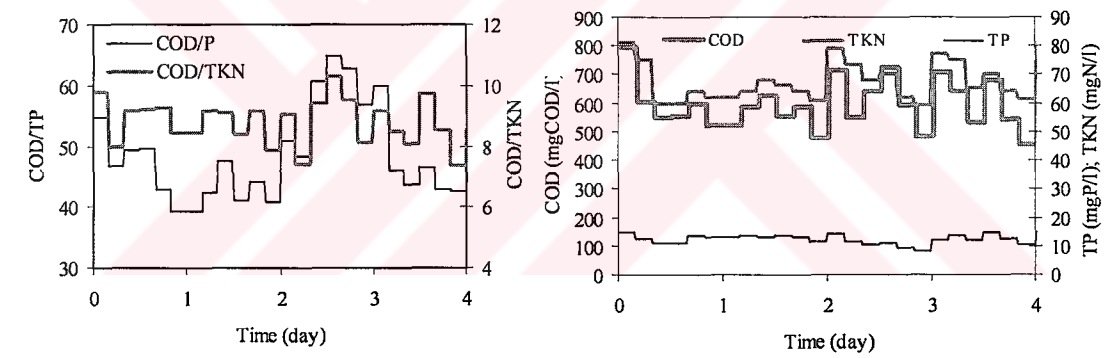


Figure 10.8 Flux-based influent COD/TKN and COD/TP ratio (left) influent COD, TKN and TP concentrations (right)

Diurnal changes in the influent wastewater composition cause variation in the organic loading rate to the treatment plant (see Figure 10.8). In this way, the activated sludge is exposed to a dynamic feed pattern, which stimulates storage phenomena (van Loosdrecht and Heijnen, 2002). In this case, it is observed that the COD/TKN and COD/TP ratio were rather low from 3:00 AM until 7:00 AM in the morning (see Figure 10.8 and Figure 10.9). On the other hand, between 8:00 to 20:00, the organic loading rate of the plant was sustained at a maximum level but it also reaches a peak load around

noontime. These changes in COD load may cause a change in the DO profile along the reactor if there is no aeration control is implemented. For instance, the anoxic fraction, $T_{\text{anox}}/T_{\text{total}}$ in the biological reactor becomes lower when the aeration is limited during the maximum COD load.

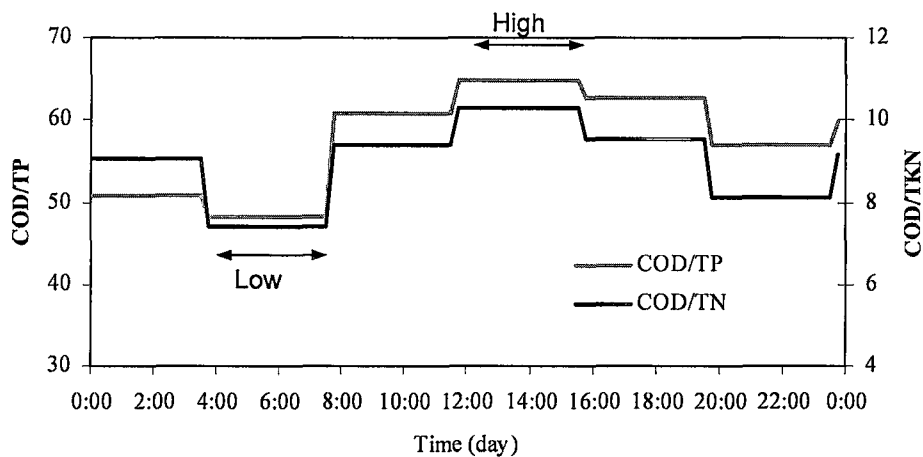


Figure 10.9 Diurnal changes in COD/TKN and COD/TP load

10.3.2 The calibrated model: Simulation Results (Insel *et al.*, 2003b)

In this section, simulation results using first campaign and obtained with the calibrated model using these first measurement campaign data are presented. The measured and simulated concentrations of nitrate, ammonia nitrogen together with effluent phosphate and dissolved oxygen in the 6th compartment of the carrousel reactor are measured as shown in Figure 10.10 and Figure 10.11. According to Figure 10.10 (left), during day-time, the nitrate can be observed to build up to 15 mgN/l. A reasonably good fit is obtained for the oxygen profile in the middle of the tank (6th reactor). The reason is that aeration is in excess and anoxic conditions cannot be generated for efficient denitrification. It should be noted that only the surface aerators provide mixing in order to keep the mixed liquor in suspension. With this model calibration, nitrification is found to be well described, but effluent phosphorus concentrations are slightly over-predicted by the model (see Figure 10.11-right).

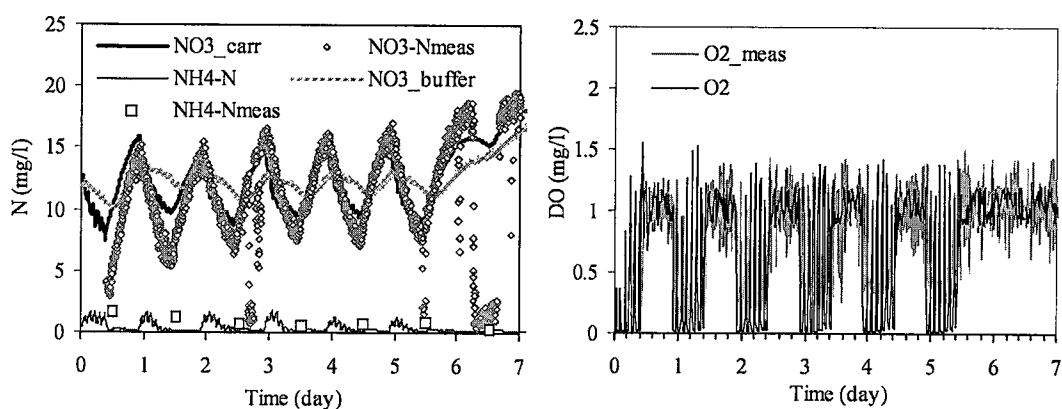


Figure 10.10 Simulated and measured nitrogen (left) and dissolved oxygen (right) (Insel *et al.*, 2003b)

Another important point is the rain event that happened just before the measurement campaign. This made the system difficult to calibrate in terms of solid balance, process stoichiometry and kinetics (Insel *et al.*, 2003b). Figure 10.11 (left) reflects the simulated and measured MLSS where excessive sludge wastage caused a large drop in the MLSS concentration in the carrousel. The calibrated parameters are given in the 1st calibration column of Table 10.3. One of the objectives was to keep the number of parameters for calibration to a minimum while getting a good fit on all measured variables.

The calibrated parameters are the anaerobic hydrolysis reduction factor, anoxic hydrolysis correction factor, the oxygen half saturation constant for heterotrophs, the endogenous decay rate for X_{PAOs} X_{PP} X_{PHA} , the half saturation constant for hydrolysis, and the half saturation constant of autotrophs for oxygen. The endogenous decay rate for PAOs was set to 0.14 day^{-1} , which is slightly lower than the default value proposed in ASM2d (0.2 day^{-1}). It was also suggested by Siegrist *et al.* (1999) that comparably reduced decay rates for PAOs could be observed under PHB limiting conditions in which the biomass is subjected to alternating electron acceptor conditions. The half saturation constant for oxygen is lowered to $0.15 \text{ mgO}_2/\text{l}$ to increase the efficiency of the aerobic processes. Consequently, the value of the half saturation constant for O_2 (X_{AUT}) is also set to $0.2 \text{ mgO}_2/\text{l}$, which is in agreement with literature values (Orhon and Artan, 1994; Stenström and Poduska; 1980).

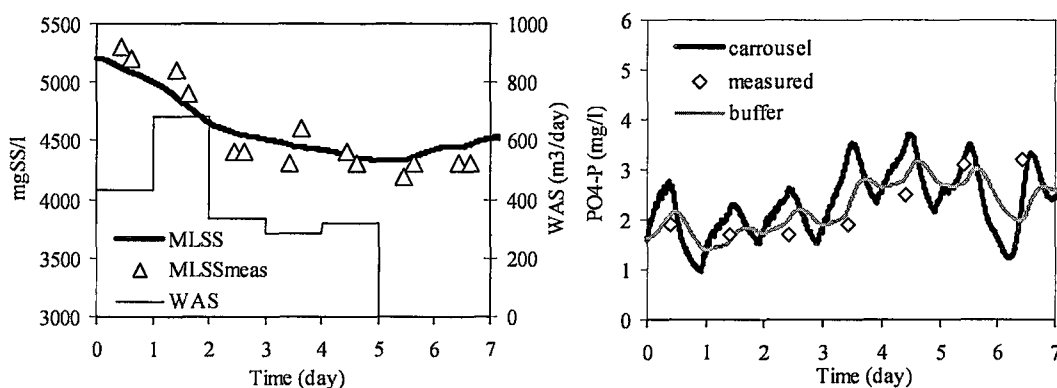


Figure 10.11 Simulated and measured MLSS (left) and effluent phosphate (right)
(Insel *et al.*, 2003b)

10.3.3 The calibrated model: validation with the Second Measurement Campaign (MC2) data

The aim of this section is to check the prediction performance of the calibrated model by using the new dynamic influent wastewater characterization (MC2) obtained under different conditions (see Figure 10.8), i.e. for the ‘validation’ of the model. Another important point is to determine the reason of a possible discrepancy between the simulations results and the measurements.

For the validation of the model, the following procedure was applied:

1. Use the calibrated model and calibrated parameters
2. Use the new operating conditions prevailing during the new measurement campaign: e.g. sludge wastage, SRT, internal recirculation rates, aeration, return sludge recycle etc.
3. Determine the initial conditions of the model: Simulate the calibrated model for long-time using the new operating parameters of the Haaren WWTP and the average influent wastewater composition obtained from MC2 (see Table 10.2).
4. Use the new input dynamics obtained during the MC2

5. Perform dynamic simulations: Use the model of step-1, the operating conditions of step-2, the initial conditions determined in step-3 and the dynamic input wastewater composition of step-4.
6. Compare the simulations with the measured dynamic trends in the treatment plant

During the validation as outlined above, the calibrated model and the parameters of the calibrated model (see Table 10.3) remained the same.

It is important to note that the calibrated model is also used to simulate longer than the duration of the measurement campaign (MC2) that covers only 4-days. The aim of extending these dynamic simulations beyond the measurement campaign duration is solely to monitor for longer period the trends in the dynamics of $\text{NH}_4\text{-N}$, $\text{NO}_3\text{-N}$ and DO measured on-line in the Haaren WWTP. To this aim, the influent wastewater composition/data collected during 4-days of the measurement campaign (MC2) were assumed to be the same and therefore repeated to the following days. For example, the same influent composition of the first and second days of the MC2 were used for simulating plant behavior on the 5th and 6th days respectively. It is clear that measurements should have been preferred instead of this assumption but the associated costs of additional measurements would be too high. It is, however, significant to stress that for these longer simulations the operating conditions such as influent flow, sludge recycle and sludge wastage rates were not assumed, but taken from the SCADA system of the Haaren WWTP.

In the second measurement campaign, additional phosphate and ammonia concentrations were measured at high frequency. It is observed that the simulated phosphate concentration in the selector reached up to around 45 mgP/l on average (see Figure 10.12-left). The simulated phosphate concentration is higher (around 15 mgP/l on average) than the measured phosphate concentration in the selector. Consequently, this resulted in a much lower simulated phosphate concentration in the effluent than the measured phosphate concentration in the effluent (see Figure 10.12-left). As shown in Figure 12 (right), a reasonable fit on the dissolved oxygen profile was observed.

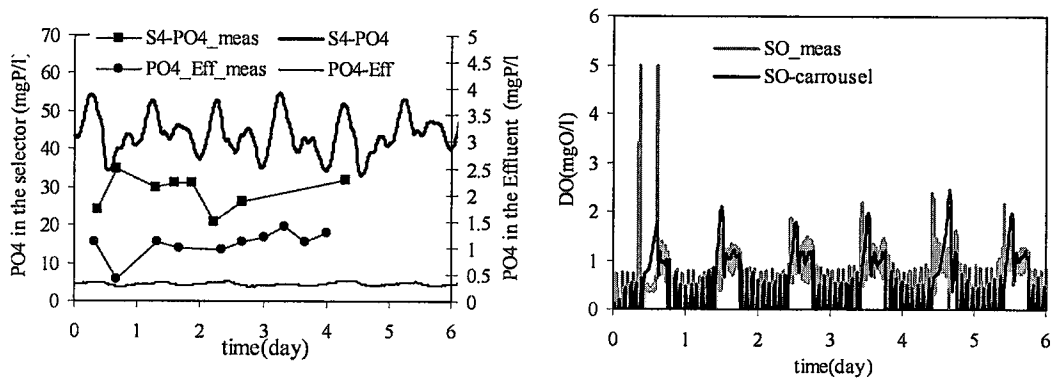


Figure 10.12 Simulated phosphate (left) and dissolved oxygen (right) concentrations

The simulated nitrate and ammonium trends are compared to the on-line measurements in the carrousel in Figure 10.13. The simulated trend of nitrate concentrations in the carrousel is observed to agree remarkably well with the nitrate measurements in the carrousel (see Figure 10.13-left). Although the calibrated model overestimates the peak in the ammonia concentrations, the predicted trend of the ammonium concentration in the carrousel is in acceptable agreement with the on-line measurements (see Figure 10.13-right).

The simulated nitrate concentrations are observed to deviate slightly from the measurements starting on the 5th and 6th days (a similar observation can also be made for ammonium concentrations on day 5 and 6). It is important to note that the influent wastewater compositions for these two days were assumed (see above). Therefore, it is very much likely that these deviations in the simulated ammonium profiles are caused by the uncertainty in the influent wastewater composition. Despite this uncertainty, however, it is also remarkable that the simulated trends in the nitrate profiles on these two days are fairly acceptable. This observation emphasizes the significance of the quality of the influent characterization as well as a need for long-term monitoring of the influent to WWTP systems.

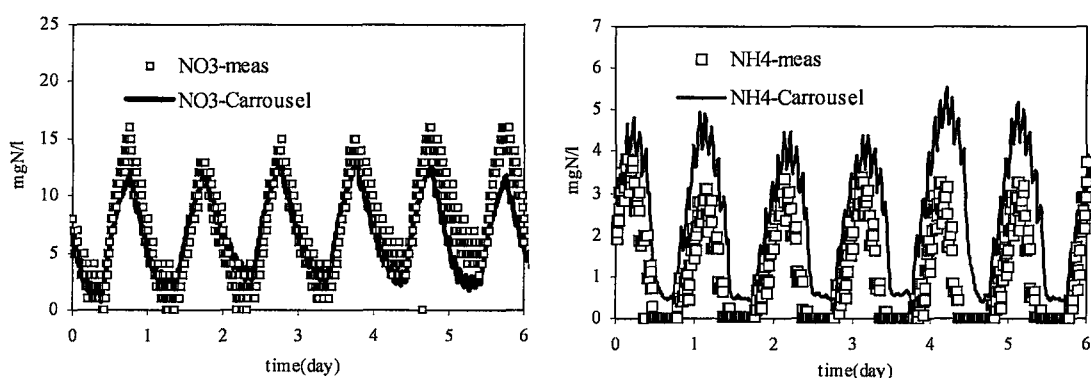


Figure 10.13 Simulated and measured nitrogen components

Two weeks of simulated MLSS concentrations in the carrousel (on average 4220 mgSS/l) are given in Figure 10.14 and compared with the daily MLSS measurements (on average 4470 mgSS/l). It is observed that there is a mismatch between the model predictions and the measurements on the first and the third days of the measurement campaign (MC2). However, the general trend observed in the MLSS dynamics in the carrousel is predicted sufficiently well by the calibrated model.

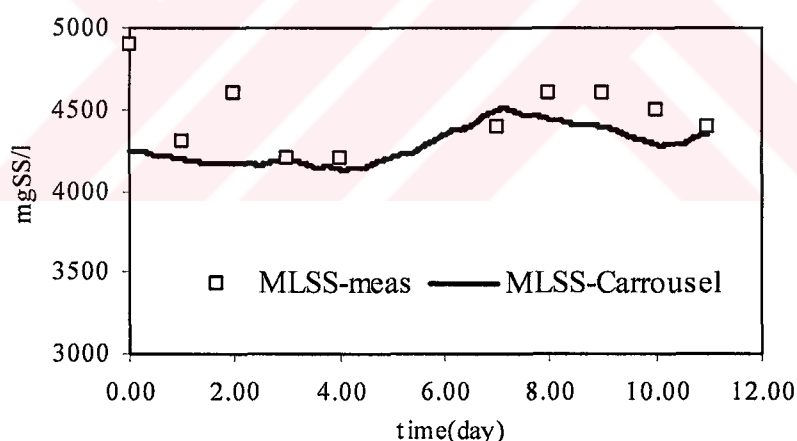


Figure 10.14 Simulated and measured MLSS concentration in the carrousel

Based on the prediction performance of the calibrated model after 3 years as presented above, it can be said that the model predicted the dynamic behavior of the Haaren WWTP remarkably well, particularly the measured MLSS, $\text{NO}_3\text{-N}$ and DO trends in the carrousel. Moreover, the calibrated model was also able to adequately simulate the trend observed in $\text{PO}_4\text{-P}$ and $\text{NH}_4\text{-N}$ concentrations but to a lesser accuracy. These outcomes

are not surprising since the model was calibrated by only considering on-line $\text{NO}_3\text{-N}$, DO and off-line MLSS measurements (see Insel *et al.*, 2003b). Overall, the validity of the model is high.

This good model validity indicates the quality of the calibrated model, itself. It also indicates the quality of the dynamic measurement campaign data used to simulate the calibrate model. The quality of the measurement campaign data can be attributed particularly to the accurate data collection and detailed influent wastewater characterization (see above). When the dynamic influent wastewater composition is not measured but assumed on day 5 and 6, the model prediction of the nitrate concentrations in the carrousel already deviates from the measurements (see Figure 10.13-right).

However, as addressed above, the off-line phosphate measurements in the selector (see Figure 10.12-left) and the ammonium concentrations in the carrousel (see Figure 10.13-left) were over-predicted by the calibrated model. In the following section, it will be attempted to improve the prediction performance of the model by fine-tuning some of the parameters. In other words, the calibrated model will be re-calibrated.

10.3.4 Recalibration of the model

The results obtained in the validation step discussed above show that the calibrated model adequately represents the dynamic behavior of the Haaren WWTP, even 3-years after the calibration period. However, there are some aspects that can be improved, particularly the ammonium concentrations in the carrousel and the phosphate concentrations in the selector. It was tried to recalibrate the model to improve the model fit to those measurements. It should be noted that the period selected for the MC2 reflects the average behavior of the plant efficiency under dry weather conditions during summer.

The calibration methodology given in Chapter 1 was applied for the recalibration. The model was recalibrated by fine-tuning the anaerobic hydrolysis reduction factor, η_{fe} , the half saturation constant for hydrolysis, K_X , and the affinity constant of autotrophs for ammonium, K_{NH} (see Table 10.3).

Table 10.3 Calibrated parameters for the first and re-calibration steps (the re-calibrated parameters are shown in *italics*)

Parameters	Symbol	Unit	Default	1 st Calibration	Recalibration
<i>Heterotrophs</i>					
Anaerobic hydrolysis reduction factor	η_{fe}	-	0.4	0.8	<i>0.2</i>
Anoxic hydrolysis correction factor	η_{NO3hyd}	-	0.6	0.8	0.8
Half saturation constant for oxygen (X_H)	K_O	mgO ₂ /l	0.2	0.15	0.15
Half saturation constant for hydrolysis	K_X	gCOD /gCOD	0.1	0.03	<i>0.1</i>
<i>Phosphorus Accumulating Organisms</i>					
Endogenous lyses rate for X_{PAOs} X_{PP} X_{PHA}	b_{PAO}	day ⁻¹	0.2	0.12	0.12
	b_{PP}			0.12	0.12
	b_{PHA}			0.12	0.12
<i>Autotrophs</i>					
Half saturation constant for O ₂ (X_{AUT})	K_{OAUT}	mgO ₂ /l	0.5	0.2	0.2
Half saturation constant for NH ₄ -N (X_{AUT})	K_{NH}	mgN/l	1	1	<i>0.5</i>

Compared to the first calibration, it is observed in the recalibration study that the anaerobic hydrolysis correction factor, η_{fe} has a large impact on the PHA pool for EBPR since it liberates readily biodegradable COD in the selector. Moreover, it directly affects the dissolved oxygen concentration in the beginning of the carrousel reactor. The anaerobic hydrolysis correction factor, η_{fe} was therefore used as a recalibration parameter. However, there is little information available about this parameter in the literature (Ekama and Wentzel, 1999; Hu *et al.*, 2003b). Similarly, the half-saturation constant for the hydrolysis process was also increased compared to the first calibration to decrease the rate of hydrolysis, which is directly affecting the availability of VFA in the selector (see Figure 10.15-left). Re-calibrating these two parameters was sufficient to improve the model fit to the phosphate measurements in the selector (see Figure 10.15-left). That consequently indicates that these two parameters can also be regarded as sensitive parameters for this calibration study. Note that these parameters were also found sensitive in Brun *et al.* (2002). Moreover, the affinity constant of autotrophs for ammonium nitrogen was also re-calibrated to improve the model fit to the ammonium measurements in the carrousel (see below).

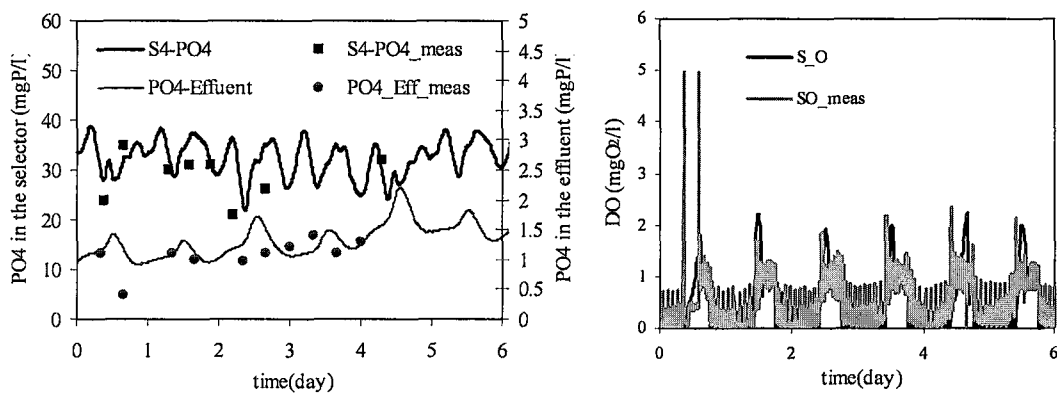


Figure 10.15 Simulated phosphate and dissolved oxygen concentrations

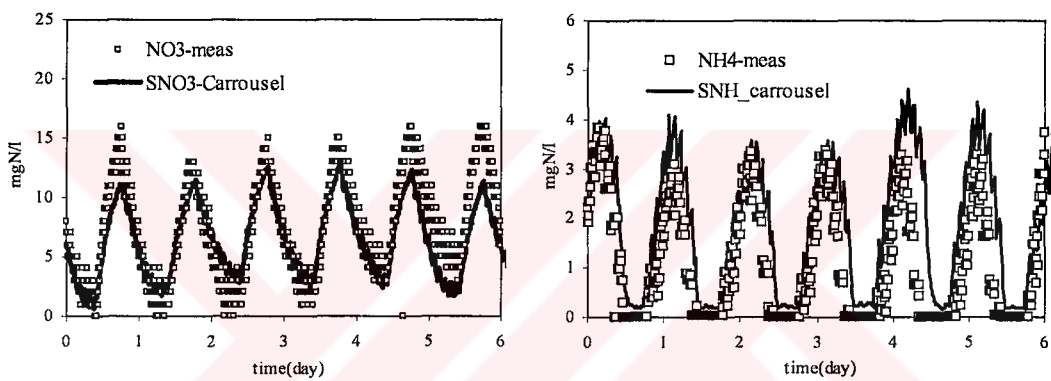


Figure 10.16 Simulated and measured nitrogen components (a) nitrate (b) ammonium.

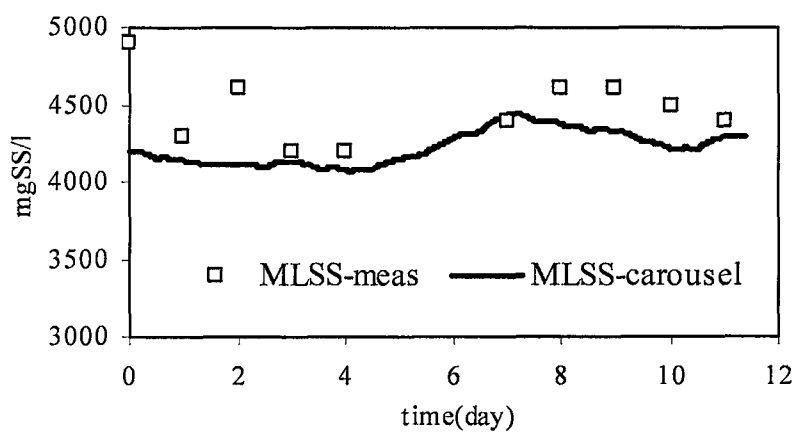


Figure 10.17 Simulated and measured MLSS concentration in the carrousel

The simulation results with the recalibrated model under dynamic loading (MC2) are compared to the measurements in Figure 10.15, Figure 10.16 and Figure 10.17. The simulated dynamics of ammonium and phosphorous in the Haaren WWTP are improved considerably by the recalibrated model by changing the above-mentioned parameters (see Figure 10.15, Figure 10.16 and Figure 10.17). At the same time, the re-calibrated model was able to simulate the trends of nitrate, oxygen and suspended solids concentrations in the carrousel as good as the first calibrated model.

It is important to also mention that during the process of re-calibration, the parameter i_{NXS} , i.e. the nitrogen fraction of slowly degradable COD, X_S , had to be increased from 0.04 mgN/mgCOD (the average calculated i_{NXS} from the influent wastewater characterization; see Annex B-Table B1) to 0.06 mgN/mgCOD. The value 0.06 mgN/mgCOD was close to the maximum of the measured i_{NXS} fractions in the influent wastewater characterization. This increase to 0.06 was required to better fit the measured total nitrogen concentration (NO_3 -N and NH_4 -N) in the carrousel and to mimic the addition nitrogen load coming from the sludge thickener. Consequently, there is a discrepancy between the measured influent characteristics and the model requirement. In this respect, it is important to point out here that the ASM2d model (Henze *et al.*, 2000) assumes a fixed parameter to describe the influent slowly degradable particulate organic nitrogen, X_{ND} , as a function of the influent X_S . However, this may not be the case in reality, as observed in this study too (see Annex B).

10.3.5 Model-based analysis of the nutrient removal in the Haaren WWTP

The recalibrated model is used here to study the main biological conversion processes in the treatment plant, which is responsible for the overall nutrient removal performance in the EBPR plants (Wentzel *et al.*, 1992).

The dynamic influent load, particularly the time when the plant is under high organic-COD loading rate, has a strong effect on the release of phosphorous in the anaerobic selector (see Figure 10.18-right). Concomitantly, cyclic phosphate fluctuations are simulated in the carrousel reactor, which in turn resulted in a more realistic prediction of phosphate in the effluent (Figure 10.15-right). It should be noted again that a mixed tank is used just after the carrousel plant in order to simulate the mixing behavior of the

clarifier. During the night period, elevated phosphate concentrations are obtained in the carrousel. However, the phosphate concentration is lowered due to the smoothing effect of the buffer tank that keeps the effluent phosphate concentration below 2.0 mgP/l during the measurement campaign period.

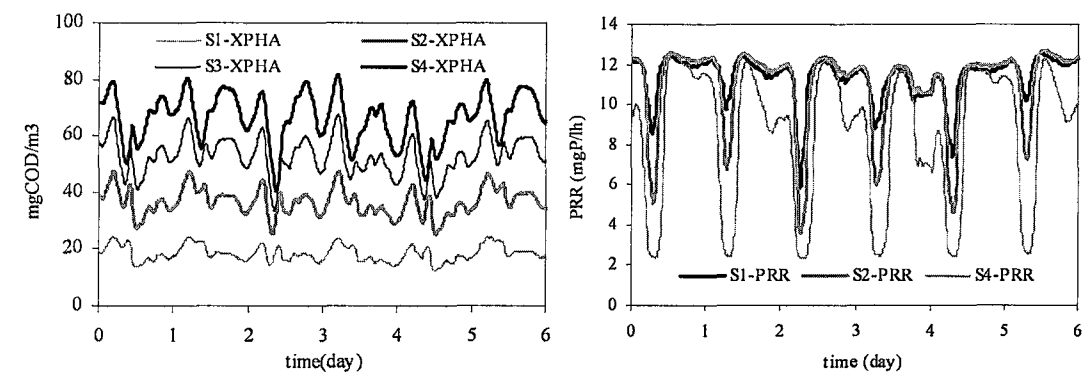


Figure 10.18 Simulations of the phosphorous release rate, PRR (right) and X_{PHA} (left) in the different sections of the selector

The X_{PHA} concentrations and the phosphate release rates (PRR) in the selector are also simulated and shown in Figure 10.18. It was observed that the X_{PHA} concentrations are increasing while moving through the 4 compartments of the selector. Moreover, these internal storage products of PAOs exhibit dynamic fluctuations throughout the selector due to the dynamic variation in the influent wastewater composition (see Figure 10.8). On the other hand, the PRR is at its maximum during the daytime when the plant is under high COD loads. But this is still not sufficient to increase the X_{PHA} level at the beginning of the selector (see Figure 10.18-right). During night time, the PRR decreased by more than half which is in agreement with the phosphate concentrations in the carrousel reactor as illustrated in Figure 10.18-right. The phosphate release rate dropped down to around 8 mgP/l.h in the last compartment in the evening.

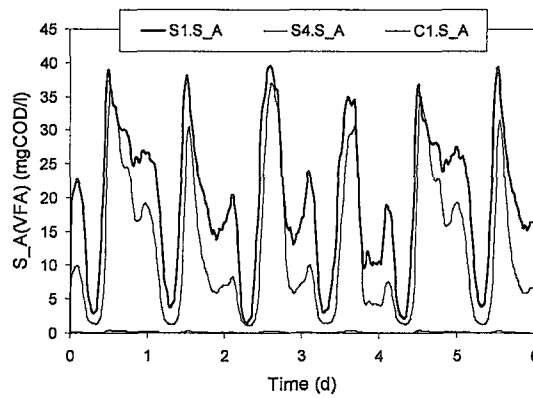


Figure 10.19 Simulation of S_A (VFA) concentrations in the selector and inlet of the carrousel

The simulations of the VFA concentration in the different compartments of the selector reveal that in the morning, high concentrations of readily biodegradable COD, S_A are still available while denitrification taking place at the head/inlet of the selector (see Figure 10.19). Meanwhile, as seen in Figure 10.18-right, the PRR is at its maximum rate of 12 mgP/l.h during daytime, clearly depending on the available VFA. Despite the fact that during night time the nitrate load is reduced under the intermittent aeration mode, the PRR drops drastically by a factor of 2-3 in the selector due to the low influent COD loading (see Figure 10.19). The same effect of the low influent COD load can be seen on the elevated phosphate concentration profile in the carrousel during night time (results not shown). It is noteworthy that the concentration of S_A in the first compartment of the carrousel is almost zero due to the rapid uptake of the readily degradable COD by the aerobic heterotrophs.

The denitrification rate calculated as the sum of the anoxic activity of heterotrophs and PAOs and expressed as nitrate uptake rate (NUR) of the biomass, reaches up to 250 gN/m³-d in the first compartment of the selector where the nitrate in the return activated sludge is reduced using the influent readily biodegradable COD (see Figure 10.20-left). The denitrification rate reduces to almost zero in the following compartments of the selector parallel to the decrease in the nitrate concentration down to zero (see Figure 10.20-left). On the other hand, the decrease in the denitrification rate favours the phosphorous release activity (PRR) of PAOs (see Figure 10.18-right). This is particularly true when the influent COD load is too low, because both processes compete

for the readily biodegradable COD in the influent, particularly for the volatile fatty acids (Wentzel *et al.*, 1992). The result of this competition also influences the internal storage products content of the PAOs (see Figure 10.18-right).

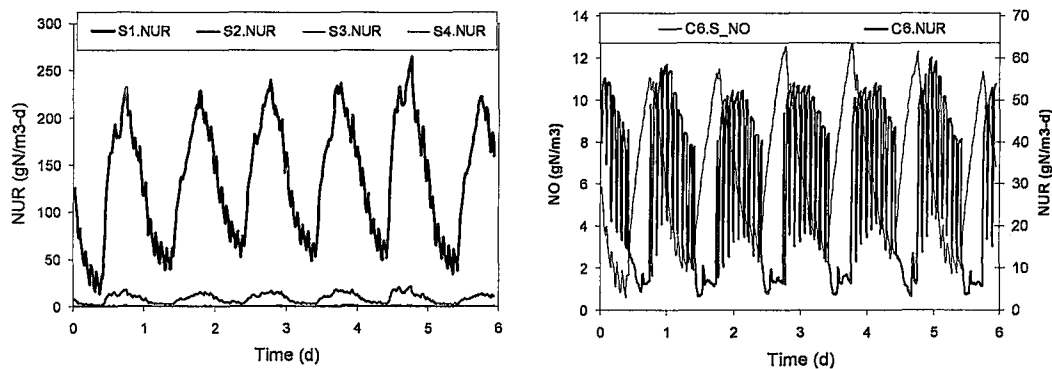


Figure 10.20 Simulations of the NUR in the selector (left) and the NUR and nitrate in the carrousel (right)

The denitrification activity in the carrousel is observed to reach up to around 60 gN/m³-d (see Figure 10.20-right). This is significantly lower than the rate achieved in the selector (see Figure 10.20-left). The reason for this difference is the limited availability of external carbon source in the carrousel (the only COD sources are the hydrolysis of X_S and endogenous processes) in contrast to the selector where fresh COD is supplied with the influent wastewater.

The nitrification activity was negligible (zero) in the selector (results not shown) as expected since there is no aeration provided in this reactor. However, the nitrification activity in the carrousel was observed to reach up to 122 gN/m³-d and 98 gN/m³-d during nighttime (alternating mode) operating modes and 82 gN/m³-d and 48 gN/m³-d during the daytime (full-aeration mode) operation at the inlet and at the end compartments of the carrousel respectively (see Figure 10.21). In both operation modes, the nitrification activity is higher at the inlet compartment of the carrousel because the oxygen concentrations are higher in this part of the carrousel and then gradually decreasing along the carrousel. These results confirm the plug-flow type behavior of the carrousel reactor when oxygen is considered (as mentioned above).

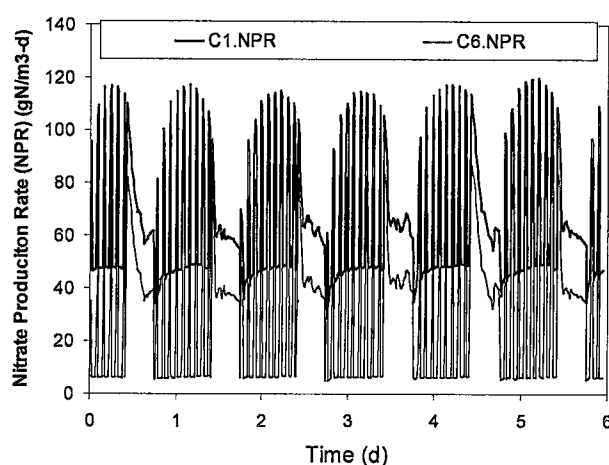


Figure 10.21 Simulations of the nitrification activity (as nitrate production rate, NPR) in the carrousel.

It is worth mentioning that the re-calibration period (dry-weather conditions) and the design of the measurement campaign itself appear to be sufficiently informative to characterize the plant behavior and reflect the overall N, P removal efficiency on a yearly basis. This is important since it was shown that a longer period with (approx. 2-3 days) is necessary for the plant to recover full EBPR capability after low organic loadings such as observed during intense rain events (Temmink *et al.* 1996; Brdjanovic *et al.*, 1998b). In this respect, it is crucial to perform a well-designed and dedicated measurement campaign when the plant is under normal loading conditions.

On top of the daily variations, the diurnal variations in the influent also induce remarkable dynamics in the ammonium, nitrate and phosphorous profiles in the Haaren WWTPs. This is because all biological activities are influenced by/depend on the influent wastewater characteristics. For example, influent dynamics are observed to cause a variation in the X_{PHA} content of the PAOs in the selector during the day as presented in Figure 10.19 (left). These variations, subsequently, cause an oscillation in the phosphorus profile in the carrousel and in the effluent. During night time operation, the nitrate concentrations throughout the carrousel are significantly decreased (see Figure 10.16). This is because the plant is operated in alternating mode by turning on/off the aeration as opposed to daytime operation where the aeration is fully on. In this way, the denitrification processes is more enhanced at night time operation (see Figure 10.19-

right). Although the nitrate concentrations are reduced, the influent COD load, particularly the readily biodegradable COD, S_s , was not sufficient to regenerate the storage pools, X_{PHA} , in the PAOs. This is also clear from the PRR simulations in Figure 10.19 (right). In this respect, it is also important to note that the plant is subjected to higher COD/TKN and COD/TP ratios during night time periods, which further favour denitrification and P-release.

10.3.6 General Discussion: The state and future perspective of model calibration

The mathematical model for Haaren WWTP which was calibrated with a set of dynamic measurement campaign data collected 3 -years ago (Insel *et al.*, 2003b) is observed to predict the recent dynamic trends of nutrients in the Haaren WWTP remarkably well. In other words, the calibrated model predictions of the Haaren WWTP were largely valid even after a long time.

Moreover, some aspects of the calibrated model, particularly the predictions of the phosphate concentration in the selector and the ammonium concentration in the carrousel, could be improved further by re-calibrating a few (in total 3) relevant parameters of the model. The re-calibration of the model was performed straightforwardly (required little effort) while these efforts resulted in considerable improvements in the prediction performance of the model.

This long-term prediction capability of the model showed that the model remained largely valid in view of representing the Haaren WWTP. This suggests that the life cycle of a calibrated model can be compatible with the life cycle of a WWTP. This particular result of the long-term model validation encourages the use of the calibrated model for further applications, e.g. optimization of operation oriented at minimizing aeration costs, optimal control of the WWTP under rain events, upgrade of WWTP and design of new WWTP etc.

The good level of model validity demonstrated in this study indicates the goodness of the calibrated model itself. Moreover, it also indicates the quality of the set of dynamic measurement campaign data used to calibrate the model. The quality of the measurement campaign data can be attributed particularly to the accurate and detailed data collection and influent wastewater characterization.

Having demonstrated the significance of the composition of the influent wastewater in relation to the model outputs, the response of the calibrated model under seasonal changes in the influent wastewater characteristics should also be considered. It is important to emphasize that the model was calibrated and validated with dynamic data collected under summer conditions. It will certainly be very valuable to evaluate the prediction performance of the calibrated model throughout the year dealing with seasonal changes (autumn, winter and spring) where remarkable differences in the influent wastewater characteristics can be expected (Henze *et al.*, 2001).

In this study, the calibration of the model as well as the design of the measurement campaign to collect information rich data about the Haaren WWTP were based on expert knowledge. It is very important to stress that this expert knowledge based calibration approach is tedious and requires considerable amount of time. A cost effective and information rich alternative approach is to use a systematic calibration procedure (Chapter 10.1):

1. Determine parameter subsets for calibration: assess the identifiable parameter combinations that can be calibrated (Ayesa *et al.*, 1995; Weijers and Vanrolleghem, 1997; Reichert and Vanrolleghem, 2001; Brun *et al.*, 2002).
2. Design the measurement campaign using Optimal Experimental Design (OED) principles to obtain information rich data about the system in view of increasing the identifiability of the model/reduce the uncertainty of the calibrated parameters.

The systematic calibration approach is especially useful when the model is over-parameterised with respect to available measurements (Weijers and Vanrolleghem, 1997; Omlin *et al.*, 2001; Reichert and Vanrolleghem, 2001; Brun *et al.*, 2002). This level of complexity of the models often leads to identifiability problems and uncertainty in the calibrated parameters (Weijers and Vanrolleghem, 1997; Alewel and Manderscheid, 1998; Omlin and Reichert, 1999; Omlin *et al.*, 2001; Reichert and Vanrolleghem, 2001). A systematic calibration approach may offer a promising solution to the above-mentioned obstacles.

10.4 Conclusion and Perspectives

In this study, it has been shown that the model, which has been calibrated with data collected 3 years before (MC1) predicts the recent dynamic behavior of the WWTP monitored with a recent measurement campaign data (MC2) remarkably well. In other words, the calibrated model predictions of the Haaren WWTP were largely valid even after a long time.

Some sub-models of the calibrated model, particularly the phosphate concentration in the selector and ammonium concentration in the carousel, were improved considerably by re-calibrating a few (in total 3) relevant parameters of the model. The re-calibration of the model was performed straightforwardly and required little effort.

This long-term prediction capability of the model suggests that the life cycle of a calibrated model is compatible with the life cycle of a WWTP (in this case, the Haaren WWTP). This in turn encourages the use of such models for further applications e.g. optimization, control of operation, upgrade or design of WWTP etc.

The influent wastewater composition is very important in relation to the quality of the model output. Since the two measurement campaigns were both performed in the summer, the model response (i.e. the prediction performance) should also be checked under seasonal changes i.e. winter, spring and autumn, to ascertain the model's validity under these conditions too.

The quality and quantity of the influent wastewater characterization is the most expensive yet the most important aspect of modelling of full-scale wastewater systems. A systematic calibration approach offers OED based measurement campaign design, which produces information rich design at a cost effective price. This approach is suggested for the future modelling exercises.

11 FINAL CONCLUSIONS AND PERSPECTIVES

In this thesis, the integrity of the related chapters within the modeling of organic carbon, nitrogen and phosphorus removal processes is provided as follows: The first chapter provided a literature review pertaining to general modeling and calibration concepts for activated sludge plants removing carbon, nitrogen and phosphorus from wastewaters. The second, third and the fourth chapters, a respirometry-based influent wastewater characterization methodology, -which is of great importance in BNR plant modeling- is proposed. In addition, expected calibration problems and pitfalls in parameter estimation using respirometry-based wastewater characterization are discussed via comparing the results of different identifiability methods. Under certain influent wastewater characteristics, the effects of environmental conditions and process configurations (i.e. temperature, aeration intensity) on process performance of biological nutrient removal (BNR) in SBRs are explained in Chapter 5, 6 and 7. After using a proposed ‘model calibration methodology’ in Chapter 7, the stability of the BNR capability of SBR system under varying environmental factors are studied in Chapter 8. The following final two chapters of this thesis (Chapter 9 and 10) summarize the effects of important processes (ie. hydrolysis) connected with the influent wastewater characterization. The prediction capability of activated sludge model is discussed for a full-scale treatment plant within certain a time span of 3 years. Within the framework of this thesis, the general conclusions derived from main chapters are summarized as follows:

In the last decades, the activated sludge models have been widely used in the design, operation and control of activated sludge plants for domestic and industrial wastewater treatment. It is rather simple, comprehensive and cost effective to express the overall effect of complex biological reactions on activated sludge plant response using those activated sludge models. The simulation of activated sludge system necessitates influent wastewater characteristics as a model input together with relevant model parameters. In relation to the prediction of system performance, the determination of model-based wastewater characteristics play a primary role in the

design, operation and control of activated sludge plants. For instance, the reactor configuration (i.e. plug flow, completely mixed reactor), operation strategy (i.e. non-aerated/aerated reactors, flow return cycles) and the selection of aerator capacity should be considered regarding the average and dynamic changes in wastewater characteristics for sustainable carbon and nutrient (N, P) removal efficiency.

Dedicated short-term respirometric batch tests are widely accepted tools to collect ample information on influent wastewater characteristics on the basis of a selected model. Those experiments also provide extensive information about the active fraction of the biomass, process kinetics and stoichiometry (Sperandio and Paul, 2000; Germirli Babuna *et al.*, 1998; Spanjers and Vanrolleghem, 1995). However, the utilization of these batch methods brings the difficulties of estimating model parameters from a short-term experimental data, accurately. Mostly, the over-parametrization becomes a major problem. Mostly, the requirements in estimating important model parameters often lag behind the increasing complexity of the activated sludge models. As a result, the uncertainty of the model increases and the estimates of model parameters turn out to be biased or out of confidence limits. The solutions can be generated via (i) finding a mathematical approach to optimize the number of parameters to be estimated and (ii) maximizing the information content of the experiments in order to eliminate the uncertainty over parameters to some extent using the Optimal Experimental Design (OED) techniques (Dochain and Vanrolleghem, 2001).

In domestic wastewaters, the availability of high amount of slowly biodegradable COD fraction (X_S) can be advantageous and regarded as important organic carbon source for the design and upgrade of BNR type activated sludge system (Hatziconstantinou *et al.*, 1996; Bannister and Pretorius, 1998; Moser-Engeler, 1998). Moreover, especially for activated sludge plants treating the industrial discharges, refractory characteristics of soluble hydrolyzable matter directly influence the effluent quality of activated sludge plants (Insel *et al.*, 2003a; Orhon *et al.*, 2001).

In this thesis, a theoretical identifiability approach was proposed for estimating parameters for surface saturation type hydrolysis kinetics together with slowly biodegradable COD fraction based on short term respirometric data. According to the proposed method, 7 out of 10 kinetic parameters and including the active fraction of heterotrophic biomass were found to be identifiable from batch respirograms. The

applicability of the method was tested on different types of wastewaters including industrial and domestic effluents that have high amount of slowly biodegradable COD (X_S) fraction. As a result, the selected model becomes identifiable when the initial growth and secondary hydrolysis plateaus are individually visible from batch respirometric data. The proposed method was also controlled with the method of Brun *et al.*, (2001) using the collinearity index, γ_k for parameter subsets and the eigen-value decomposition of the covariance matrix (Brouwer *et al.*, 1998) to detect identifiability problems. The collinearity indices, γ_k calculated for different experiments were found to be less than 20, which is an acceptable threshold limit for parameter identifiability according to Brun *et al.* (2002; 2001). Consequently, the parameter estimation study was conducted without detecting any convergence problem and the calculation of correlation matrix.

The parameter identifiability problems occurred while insufficient data was collected due to a fast initial transient response in oxygen uptake rate (OUR) measurements (Vanrolleghem *et al.*, 2004), which was recorded just after the addition of wastewater spike into the batch vessel containing endogenous aerated biomass. The information content of the experiment was increased with the aid of Optimal Experimental Design (OED) methodology using the scalar functions of Fisher Information Matrix, FIM (Vanrolleghem *et al.*, 1995; Dochain and Vanrolleghem, 2001). As a result, conducting the batch respirometric assays with lower initial substrate to biomass (S_0/X_0) ratio decreased the overall uncertainty on the parameters; on the other hand, it increased the degree of correlations among estimated parameters. In this respect, appropriate adjustments of initial food to microorganism ratio (S_0/X_0) can secure sufficient data in order to characterize the growth and hydrolysis kinetics, at once. In this way, the S_0/X_0 ratio should be lowered to a certain level without causing severe identifiability problems. To sum up, running the experiments with lower S_0/X_0 ratio increases the information content, however increases the correlation among the model parameters.

Accurate determination of biodegradable COD fractions together with degradation kinetics of those are key considerations in the selection and operation of activated sludge plants to be designed for nutrient removal (Hatzicostantinou *et al.*, 1996; Bannister and Pretorius, 1998). The changes in wastewater characteristics with respect to the biodegradable COD fractions, COD/N and COD/P ratios necessitate

dynamic adjustments in operation of treatment plant in order to provide stable effluent characteristics. Especially for small communities, the sequencing batch reactors, SBRs are regarded as a viable alternative achieving efficient nitrogen (nutrient) removal. And SBR systems have great operation flexibility, which allows appropriate manipulation of cyclic periods to handle the dynamic environmental conditions and wastewater characteristics.

In the literature, few methodologies have been proposed for the design of SBR providing delicate stoichiometric relationships between biomass, biodegradable substrate and nitrogen (Artan *et al.*, 2002; Teichgraber *et al.*, 2001). Although, the influent wastewater characterization (biodegradable/inert COD fractionation, TKN, TP) and model parameters are known, external inputs such as aeration intensity (characterized by process K_La) known to be the most important part may alter the expected efficiency of the plant presumed via process stoichiometry. In order to anticipate the effect of aeration, a model-based evaluation of process dynamics lead better understanding of biological processes taking place within the cycles in SBR system.

The volumetric oxygen transfer coefficient, K_La governs the airflow rate to be supplied to the system and it couples the oxygen transfer term to activated sludge models. The selection of the aerator capacity, in turn, the K_La parameter is of great importance on the process performance since the nitrification and denitrification processes are susceptible to dissolved oxygen levels in the reactor. In this study, a prior calculation approach was anticipated for the selection of process K_La to be used in the system design of a SBR. The calculation using the appropriate assumptions gave compatible results with steady state simulation of the system.

A calibration effort was carried out for visualizing the discrepancy reasons between expected and real nitrogen removal efficiency of an SBR, which was operated in pre-denitrification (MLE) mode to treat leather-tanning effluents. At the beginning of the aeration phase just after the mixed filled period transient behavior of the oxygen profile starting from low levels around 0.3 mg/l triggered extra nitrate removal through the end of the aerobic phase. The results of simulation study revealed that additional nitrate removal was due to the simultaneous nitrification and denitrification (SND) mechanism as long as the dissolved oxygen is limited (Munch *et al.*, 1996). In this respect, the necessary conditions for SND can be summarized as

follows: (1) the biodegradable COD should be available; (2) the aerobic sludge age should be sufficient to maintain nitrification and (3) lower dissolved oxygen levels are required to activate denitrification.

In SBR systems, Enhanced Biological Phosphorus Removal (EBPR) requires anaerobic mixed fill phase for phosphorus accumulating organisms, X_{PAO} to store volatile fatty acids for luxury phosphate uptake under succeeding aerobic or anoxic phases (Wentzel *et al.*, 1992). Since the mechanisms of EBPR depend upon influent wastewater concentration (i.e. VFA content), plant configuration and process conditions (i.e. competition between ordinary heterotrophs and X_{PAOs} in the availability of nitrate and VFA), a model-based evaluation is required to clarify the individual and overall effect of different processes on the plant performance. For instance, the dissolved oxygen limitation makes it difficult to solve the net effect of parallel reactions without any modeling effort. Thus, model based evaluation of process performance is required to generate operation scenarios for finding the optimum robust process conditions in terms of efficient nutrient removal.

In this thesis, a calibration methodology was developed for an SBR achieving nutrient removal under limited oxygen conditions. After model calibration using the modified ASM2d (ASM2dN), it was concluded that the contribution of simultaneous processes of autotrophs, heterotrophs and X_{PAO} governed the overall nutrient removal efficiency of the SBR system. For instance, the VFA uptake and anoxic phosphate removal were activated in the mixed/fill phase when the nitrate is still available. On the other hand, the simultaneous nitrification, denitrification and phosphate uptake namely the “simultaneous nutrient removal” takes place when the aeration is limited.

After “model calibration” step, model -based system analysis serves as a reference point to visualize possible and convenient operation scenarios of activated sludge systems (SBR in this study) in order to minimize the effluent nutrient levels. In order to increase the nutrient removal performance, manipulation of aeration intensity –in turn the activation of simultaneous nutrient removal- can be an alternative for the SBR systems. However, the selection of optimization variables (i.e. aeration intensity) should be taken into consideration since the system may become sensitive to the external disturbances. In this study, the nutrient removal performance of lab-scale SBR was increased via reduced aeration with the aid of calibrated model. On

the other hand, it was found that the stability of efficient BNR was found to be more fragile to external disturbances.

The nutrient removal mechanism in oxidation ditches is similar to the operation strategy of SBRs in a such way that the dissolved oxygen transfer is provided spatially generated via creating aerated and un-aerated zones instead of adjusting the length of the phases as in SBRs. The adjustment of oxygen transfer allows utilizing the available nitrate, N_A and denitrification potential, N_{DP} for nitrogen (or nutrient) removal. Various reactor configurations are used together with oxidation ditch plants for nutrient removal. In most cases, the reactors so called “selectors” are added to the prior to the oxidation ditch reactor not only to promote EBPR (US EPA, 1992) but also to hinder the excessive growth of filamentous microorganisms (Randall *et al.*, 1992).

Orbal type oxidation ditch activated sludge plants are operated in SND mode to achieve nitrogen removal with reduced aeration costs. However, the modeling of an Orbal using high frequency data with the aid of ASM2d revealed that the dynamics of BNR suffer from dissolved oxygen oscillations in closed loop bioreactors. So, the dissolved oxygen control should be implemented for performance stability.

In this thesis, the actual performance of full-scale oxidation ditch operated in cyclic alternating aeration mode was evaluated with the aid of dynamic model calibration methodology “BIOMATH calibration protocol” using the ASM2d. The modeling work was carried out using the measurement campaigns pertaining to different time scales. The plant performance and the importance of different processes were addressed in this regard. The system exerted high variations in nutrients in the effluent, which was well delineated with model simulations. However, after 2 years, a recalibration of the plant was required using the 2nd set of measurement campaign data. The kinetics of hydrolysis, the oxygen half saturation coefficients, endogenous parameters of X_{PAOs} were found to be important which are affecting the overall nutrient removal efficiency of oxidation ditch system. Thus, the manipulation of related parameters reflected the difference of process efficiency together with process dynamics pertaining to the periods for the first and second measurement campaign. Practically, above 10 mg/l recycled nitrate through RAS ($Q_{RAS}/Q_{in}:1$) from clarifier to the selector caused temporal loss in EBPR activity.

The design, operation and control of activated sludge plants are highly dependent upon wastewater characteristics. Especially, the biological treatment of industrial wastewaters and nutrient removal from domestic wastewaters suffer from the lack of knowledge on wastewater characteristics. The information on the availability of biodegradable COD fraction together with kinetics should be collected rapidly and properly to depict the trend of the changes in wastewater characteristics. Moreover, swift data collection is also important to take the appropriate control action in time with regard to process control. The integration of respirometric tests in comprehensive model solutions generates rapid information on biodegradable COD fractions and the degradation kinetics, efficiently. In addition, optimal experimental design (OED) allows process engineers to manipulate the experimental conditions to adjust (or maximize) the information quality of experiments. Besides, the respirometric tests enable to gather information on the oxygen requirements of the system. As already discussed above, with the inclusion of aeration term -which reflects the real situation- a model base evaluation is required to draw the real picture of the process dynamics. A model-based evaluation of lab- or full-scale treatment plants reflects the dynamics of the plant close to the reality and reveals the difference between expected quality and actual system performance. The calibrated and validated activated sludge models can then be used as full-scale optimization tools to implement the best control strategy to reach optimum operation mode. However, the effects of selected control strategies on the characteristics of activated sludge (i.e. settleability) should further be investigated. Finally, in the view of cost and time effectiveness, further investigation should also be devoted to full-scale optimal experimental design application, which facilitates the determination of relevant on-site measurement points and optimal data sampling frequency.

REFERENCES

- Abusam, A. and Keesman, K.J.**, 1999. Effect of number of CSTRs on the modelling of oxidation ditches: steady state and dynamic analysis, *Med. Fac. Landbouww. Univ. Gent*, 64/5a.
- Alewell, C. and Manderscheid, B.**, 1998. Use of objective criteria for the assessment of biogeochemical ecosystem models, *Ecol. Modell.*, **107**, 213-224.
- Applegate, C.S., Wilder, B. and Deshaw, J.R.**, 1980. Total nitrogen removal in a multi-channel oxidation systems, *J. Wat. Pollut. Cont. Fed.*, **52(3)**, 568-577.
- APHA**, 1998. *Standard Methods for the Examination of Water and Wastewater*, 20th Eds. American Public Health Association, Washington D.C., U.S.A.
- APHA.**, 1995. *Standard Methods for the Examination of Water and Wastewater*, 19th Eds., American Public Health Association, Washington D.C., USA.
- Artan, N., Orhon, D. and Tasli, R.**, 2002a. Design of SBR systems for nutrient removal from wastewaters subject to seasonal fluctuations, *Wat. Sci. Tech.*, **46(8)**, 91-98.
- Artan, N., Wilderer, P., Orhon, D., Tasli, R. and Morgenroth, E.**, 2002b. Model evaluation and optimisation of nutrient removal potential for sequencing batch reactors, *Water SA*, **28(4)**, 423-432.
- Artan, N., Wilderer, P., Orhon, D., Morgenroth, E., and Özgür, N.**, 2001. The mechanism and design of sequencing batch reactor systems for nutrient removal – The state of the art, *Wat. Sci. Tech.*, **43(3)**, 53-61.
- ASCE Standards**, 1992. Measurement of oxygen transfer in clean water, 2nd Eds., Newyork, U.S.A.
- Avcioğlu, E., Orhon, D. and Sözen, S.**, 1998. A new method for the assessment of heterotrophic endogenous respiration rate under aerobic and anoxic conditions, *Wat. Sci. Tech.*, **38(8-9)**, 95-103.
- Ayesa, E., Oyarbide, G., Larrea, L., Garciaheras, J.L.**, 1995. Observability of reduced-order models-application to a model for control of alpha-process, *Wat.Sci. Tech.*, **31(2)**, 161-170.

- Baltes, M., Schneider, R., Sturm, C. and Reuss, M., 1994. Optimal experimental design for parameter estimation in unstructured growth models, *Biotechnol. Prog.*, **10**, 480-488.
- Bannister, S.S., and Pretorius, W.A., 1998. Optimization of primary sludge acidogenic fermentation for biological nutrient removal, *Water SA*, **24**(1), 35-41.
- Barker, P.S. and Dold, P.L., 1997. General model for biological nutrient removal activated-sludge systems: model presentation, *Water Env. Res.*, **69**(5), 969-984.
- Barker, P.S. and Dold, P.L. 1995. COD and nitrogen mass balances in activated sludge systems. *Wat. Res.*, **29**(2), 633-643.
- Barnard, J.L., 1974. Cut P and N without chemicals, *Water Wastes Eng.*, **11**, 33-36.
- Barnard, J.L., 1973. Biological denitrification. *Wat. Poll. Cont.*, **72**(6), 705-720.
- Bertanza, G., 1997. Simultaneous nitrification-denitrification process in extended aeration plants: Pilot and real scale experiences, *Wat. Sci Tech.*, **35**(6), 53-61.
- Bidstrup, S.M. and Grady, C.P.L.Jr., 1988. SSSP-Simulation of single-sludge processes, *J. Wat. Pollut. Cont. Fed.*, **60**, 351-361.
- Boeijs, G., Corstanje, R., Rottiers, A. and Schowanek, D., 1998. Adaptation of the CAS test system and synthetic sewage for biological nutrient removal. Part I: Development of a new synthetic sewage, *Chemosphere*, **38**(4), 699-709.
- Bortone, G., Saltarelli, R., Alonso, V., Sorm, R., Wanner, J. and Tilche, A., 1996. Biological anoxic phosphorus removal, *Wat. Sci. Tech.*, **34**(1-2), 119-128.
- Boyle, W.C. and Campbell, H.J.Jr., 1984. Experiences with oxygen transfer testing of diffused air systems under process conditions, *Wat. Sci. Tech.*, **16** (Vienna), 91-106.
- Brdjanovic, D., van Loosdrecht, M.C.M., Hooijmans, C.M., Mino, T., Alaerts, G.J. and Heijnen, J.J., 1999. Innovative methods for sludge characterization in biological phosphorus removal systems, *Wat. Sci. Tech.*, **39**(6), 37-43.
- Brdjanovic, D., 1998a. Modeling biological phosphorus in activated sludge. *Ph.D. thesis*, Delft University of Technology, The Netherlands.
- Brdjanovic, D., Slamet, A., van Loosdrecht, M.C.M., Hooijmans, C.M., Alaerts, G.J. and Heijnen, J.J., 1998b. Impact of excessive aeration on biological phosphorus removal from wastewaters, *Wat. Res.*, **32**(1), 200-208.

- Brouwer, H., Klapwijk, A. and Keesman, K.J., 1998.** Identification of activated sludge and wastewater characteristics using respirometric batch experiments, *Wat. Res.*, **32(4)**, 1240-1254.
- Brun, R., Kühni, M., Siegrist, H., Gujer, W. and Reichert, P., 2002.** Practical identifiability of ASM2d parameters-systematic selection and tuning of parameter subsets, *Wat. Res.*, **36**, 4113-4127.
- Brun, R., Reichert, P. and Künsch, R.K., 2001.** Practical identifiability analysis of large environmental simulation models, *Wat. Resour. Res.*, **37(4)**, 1015-1030.
- Bungaard, E., Endersen, K.L. and Petersen, G., 1989.** Biotenitro and Biotenitro systems-experiences and advanced model development: the Danish system for biological N and P removal., *Wat. Sci. Tech.*, **21(Brighton)**, 1727-1730.
- Burrows, L.J., Stokes, A.J., West, J.R., Forster, C.F. and Martin, A.D., 1999.** Evaluation of different analytical methods for tracer studies in aeration lanes of activated sludge plants, *Wat. Res.*, **33(2)**, 367-374.
- Capela, S., Gillot, S. and Héduit, A., 1999.** Oxygen transfer under process conditions: Comparison of measurement methods. In: *Proceedings 72nd Annual WEF Conference and Exposition*. New Orleans, USA, October 9-13 1999.
- Carucci, A., Kühni, M., Brun, R., Carucci, G., Koch, G., Majone, M. And Siegrist, H. 1999a.** Microbial competition for the organic substrates and its impact on EBPR systems under conditions of changing carbon, *Wat. Sci. Tech.*, **39(1)**, 75-85.
- Carucci, A., Chiavola, A., Majone, M. and Rolle, E., 1999b.** Treatment of tannery wastewater in a sequencing batch reactor, *Wat. Sci. Tech.*, **40(1)**, 253-261.
- CEC, 1991.** *Council Directive concerning urban wastewater treatment (91/271/EC)* Official Journal L135/40.
- Cech, J.S. and Hartman, P., 1993.** Competition between polyphosphate and polysaccharide accumulating bacteria in enhanced biological phosphate removal systems. *Wat. Res.*, **27(7)**, 1219-1225.
- Chambers, B., 1992.** Design methodology for optimisation of aeration efficiency in activated sludge plants. In: *Proceedings 6th Forum Applied Biotechnology. Med. Fac. Landbouww. Univ. Gent*, **57**, 1631-1642.
- Chudoba, P., Capdeville, B. and Chudoba, J., 1992.** Explanation of biological meaning of the S_0/X_0 ratio in batch cultivation, *Wat. Sci. Tech.*, **26(3-4)**, 743-751.

- Cinar, O., Daigger, G.T. and Graef, P.G., 1998.** Evaluation of IAWQ activated sludge model no2 using steady state data from four full scale wastewater treatment plants, *Water Env. Res.*, **70**, 1216-1224.
- Clayton, J.A., Ekama, G.A., Wentzel, M.C. and Marais, G.v.R., (1991)** Denitrification kinetics in biological nitrogen and phosphorus removal activated-sludge systems treating municipal wastewaters, *Wat. Sci. Tech.*, **23(4-6)**, 1025-1035.
- Coen, F., Vanderhaegen, B., Vanrolleghem, P.A. and van Meenen, P., 1997.** Improved design and control of industrial and municipal nutrient removal plants using dynamic models, *Wat. Sci. Tech.*, **35(10)**, 53-61.
- Comeau, Y., Hall, K.J. and Oldham, K., 1990.** Indirect phosphate quantification in activated sludge, *Water Pollut. Res. J. Canada*, **25(2)**, 161-174.
- Comeau, Y., Hall, K.J., Hancock, R.E.W. and Oldham, W.K., 1986.** Biochemical model for enhanced biological phosphorus removal, *Wat. Res.*, **20(12)**, 1511-1521.
- Copp, J.B., Spanjers, H. and Vanrolleghem, P.A., 2002.** Respirometry in control of the activated sludge process: Benchmarking control strategies. *IWA Scientific and Technical Report No:11*, London, UK.
- Copp, J.B. and Murphy, K.L., 1995.** Estimation of the active nitrifying biomass in activated-sludge, *Wat. Res.*, **29(8)**, 1855-1862.
- Daigger, G.T. and Littleton, H.X., 2000.** Characterization of simultaneous nutrient removal in staged, closed-loop bioreactors, *Water Env. Res.*, **72(3)**, 330-339.
- Daigger, G.T. and Nolasco, D., 1995.** Evaluation and design of full scale treatment plants using biological process model, *Wat. Sci. Tech.*, **31(2)**, 245-255.
- Daigger, G.T. and Roper, R.E., 1985.** The relationship between SVI and activated sludge settling characteristics, *J. Wat. Pollut. Cont. Fed.*, **57(8)**, 859-866.
- Demoulin, G., Rudiger, A. and Goronszy, M.C., 2001.** Cyclic activated sludge technology –recent operating experience with a 90,000 p.e. plant in Germany, *Wat. Sci. Tech.*, **43(3)**, 331-337.
- Demuynck, C., Vanrolleghem, P.A., Mingneau, C., Liessens, J and Verstraete, W., 1994.** NDBEPR process optimization in SBRs: reduction of external carbon source and oxygen supply, *Wat. Sci. Tech.*, **30(4)**, 219-227.

- De Clercq, B.**, 2003. Computational fluid dynamics of settling tanks: development of experiments and rheological, settling and scrapers submodels, *Ph.D. Thesis*, Ghent University, Faculty of Agricultural and Applied Biological Science, Belgium.
- De Clercq, B., Coen, F., Vanderhaegen, B. and Vanrolleghem, P.A.**, 1999. Calibrating simple models for mixing and flow propagation in wastewater treatment plants, *Wat. Sci. Tech.*, **39(4)**, 61-69.
- De Pauw, D.J.W., Sin, G., Insel, G., Van Hulle, S., Vandenberghe, V. and Vanrolleghem, P.A.**, 2004. Discussion of 'Assessing Parameter Identifiability of Activated Sludge Model No. 1' by Pedro Afonso and Maria da Conceicao Cunha. *J. Environ. Eng.*, 128, 748-754. *J. Environ. Eng.-ASCE*, **130(1)**, 110-112.
- De Silva, D.G. and Rittmann, E.**, 2001. Simultaneous nitrification and denitrification in one stage activated sludge process, *WEFTEC01. 74rd Annual. Conference Exposition*, Water Environ. Fed., Atlanta, Georgia, USA.
- De la Sota, A., Larrea, L., Novak, L., Grau, P. and Henze, M.**, 1994. Performance and model calibration of R-N-D processes in pilot plant, *Wat. Sci. Tech.*, **30(6)**, 355-364.
- Dochain, D. and Vanrolleghem, P.A.**, 2001. *Dynamical Modelling and Estimation In Wastewater Treatment Processes*, IWA Publishing, London.
- Dochain, D., Vanrolleghem, P.A. and Van Daele M.**, 1995. Structural identifiability of biokinetic models of activated sludge respiration, *Wat. Res.*, **29(11)**, 2571-2579.
- Dold, P.L.**, 2002. Importance of decay rate in assessing nitrification kinetics, *WEFTEC02, Water Environ. Fed. 75th Annu. Conf. Exposition*, Water Environ. Fed., Chicago, Illinois, USA.
- Dold, D.L. and Marais, G.v.R.**, 1986. Evaluation of the general activated sludge model proposed by the IAWPRC Task Group, *Wat. Sci. Tech.*, **18(6)**, 63-89.
- Dold, P.L., Ekama, G.A. and Marais, G.v.R.**, 1980. A general model for the activated sludge process, *Prog. Wat. Tech.*, **12(6)**, 47-54.
- Drews, R.J.L.C and Greeff, A.M.**, 1973. Nitrogen elimination by rapid alternation of aerobic/anoxic conditions in Orbal activated sludge plants, *Wat. Res.*, **7**, 1183-1194.
- Drews, R.J.L.C., Malan, W.M., Meiring G.J., Moffatt, B.**, 1972. The Orbal extended aeration activated sludge plant, *Wat. Res.*, **44(2)**, 221-231.
- Ekama, G.A. and Wentzel, M.C.**, 1999. Denitrification kinetics in biological N and P removal activated sludge systems treating municipal wastewaters, *Wat. Sci. Tech.*, **39(6)**, 69-77.

- Ekama, G.A., and Marais, G.v.R., 1986a.** Sludge settleability and secondary settling tank design procedures, *Wat. Pollut. Control*, **85(1)**, 101-113.
- Ekama, G.A., Dold, P.L. and Marais G.v.R., 1986b.** Procedures for determining influent COD fractions and the maximum specific growth rate of heterotrophs in activated sludge systems. *Wat. Sci. Tech.*, **18**, 91-114.
- Ekama, G.A. and Marais, G.v.R., 1979.** Dynamic behaviour of the activated sludge process, *J. Water. Pollut. Cont. Fed.*, **51(3)**, 534-556.
- Filipe, C.D.M., Daigger, G.T. and Grady, C.P.L.Jr., 2001.** Stoichiometry and kinetics of acetate uptake under anaerobic conditions by an enriched culture of phosphorus accumulating organisms at different pHs, *Biotechnol. Bioeng.*, **76**, 32-43.
- Filipe, C.D.M and Daigger, G.T., 1999.** Evaluation of the capacity of phosphorus accumulating organisms to use nitrate and oxygen as final electron acceptors: A theoretical study on population dynamics, *Water Env. Res.*, **71(6)**, 1140-1150.
- Filipe, C.D.M., and Daigger, G.T. 1998.** Development of a revised metabolic model for the growth of phosphorus-accumulating organisms, *Wat. Env. Res.*, **70(1)**, 67-79.
- Furumai, H., Kazmi, A.A., Fujita, M., Furuya, Y. and Sasaki, K., 2001.** Modelling long-term nutrient removal in a sequencing batch reactor, *Wat.Res.*, **33**, 2708-2714.
- Germirli Babuna, F., Orhon, D., Ubay Çokgor, E., Insel, G. and Yapraklı, B., 1998.** Modelling of activated sludge for textile wastewaters, *Wat. Sci. Tech.*, **38(4-5)**, 9-17.
- Germirli, F., Orhon, D. and Artan, N., 1991.** Assessment of the initial inert soluble COD in industrial wastewaters, *Wat. Sci. Tech.*, **23(4-6)**, 1077-1086.
- Gernaey, K., Petersen, B., Dochain, D. and Vanrolleghem, P.A., 2002.** Modelling aerobic carbon source degradation processes using titrimetric and combined respirometric-titrimetric data: structural and practical identifiability, *Biotechnol. Bioeng.*, **79(7)**, 754-767.
- Gernaey, K., Vanrolleghem, P. and Lessard, P., 2001.** Modelling of a reactive primary clarifier, *Wat. Sci. Tech.*, **43(7)**, 73-81.
- Godfrey, K.R., and Distefano, J.J., 1985.** Identifiability of model parameters, in *Identification and System parameter estimation*, pp. 89-144. Pergamon Press, Oxford.

- Goel, R., Mino, T., Satoh, H. and Matsuo, T., 1998. Comparison of hydrolytic enzyme systems in pure culture and activated sludge under different electron acceptor conditions, *Wat. Sci. Tech.*, **37(4-5)**, 91-114.
- Goel, R., Mino, T., Satoh, H. and Matsuo, T., 1997. Effect of electron acceptor conditions on hydrolytic enzyme synthesis in bacterial cultures. *Wat. Res.*, **31(10)**, 2597-2603.
- Görgün, E., Çokgör, E.U., Orhon, D., Germirli, F. and Artan, N., 1995. Modelling biological treatability for meat processing effluent, *Wat. Sci. Tech.*, **32(12)**, 43-52.
- Grady, C.P.L.Jr., Daigger, G.T. and Lim, H.C., 1999. *Biological Wastewater Treatment*, Marcel Dekker Inc., Newyork, U.S.A.
- Grady, C.P.L.Jr., Smets, B.F. and Barbeau, S., 1996. Variability in kinetic parameter estimates: a review of possible causes and a proposed terminology, *Wat. Res.*, **30(3)**, 742-748.
- Gujer, W., Henze, M., Mino, T. and van Loosdrecht, M.C.M., 2000. Activated Sludge Model No.3., in: Activated Sludge Models ASM1, ASM2, ASM2d and ASM3, Henze, M., Gujer, W., Mino, T., van Loosdrecht, M.C.M. Eds. IWA Scientific and Technical Report No.9. IWA London.
- Gujer, W., Henze, M., Mino, T. and van Loosdrecht, M.C.M., 1999. Activated sludge model No 3., *Wat. Sci. Tech.*, **39(1)**, 183-193.
- Gujer, W. and Larsen, T.A., 1995. The implementation of biokinetics and conservation principles in ASIM, *Wat. Sci. Tech.*, **31(2)**, 257-266.
- Hanaki, K., Wantawin, C. and Ohgaki, S., 1990. Nitrification at low levels of dissolved oxygen with and without organic loading in a suspended-growth reactor, *Wat. Res.*, **24(3)**, 297-302.
- Hanhan, O., Artan, N. and Orhon, D., 2003. Retrofitting activated sludge systems to intermittent aeration for nitrogen removal, *Wat. Sci. Tech.*, **46(8)**, 75-82.
- Hatziconstantinou, G.J., Yannakopoulos, P. and Andreakis, A., 1996. Primary sludge hydrolysis for biological nutrient removal, *Wat. Sci. Tech.*, **34(1-2)**, 417-423.
- Hellinga, C., Schellen, A.A.J.C., Mulder, J.W., Van Loosdrecht, M.C.M and Heijnen, J.J., 1998. The SHARON process: an innovative method for nitrogen removal for ammonium-rich wastewater. *Wat. Sci. Tech.*, **37**, 135-42.
- Henze, M., Aspegren, H., Jansen, J.L., Nielsen, P.H. and Lee, N., 2002. Effect of solids retention time and wastewater characteristics on biological phosphorus removal, *Wat. Sci. Tech.*, **45(6)**, 137-144.

- Henze, M., Gujer, W., Mino, T., and van Loosdrecht, M.C.M., 2000. Activated Sludge Models: ASM1, ASM2, ASM2d and ASM3, *Scientific and Technical Report No:9*, IWA Publishing, London.
- Henze, M., Gujer, W., Mino, T., Matsuo, T., Wentzel, M. C., Marais, G. v. R. and van Loosdrecht, M. C. M., 1999. Activated sludge model No.2d, ASM2d, *Wat. Sci. Tech.*, **39**(1), 165-182.
- Henze, M., Gujer, W., Mino, T., Matsuo, T., Wentzel, M.C. and Marais, G.v.R., 1995a. *Activated sludge model No.2.*, IAWPRC Task Group on Mathematical Modelling for Design and Operation of Biological Treatment, IAWQ, London.
- Henze, M., Harremoës, P., Jansen, J.C. and Arvin, E. 1995b. Biological and Chemical Processes, in *Wastewater Treatment*, Springer-Verlag, Berlin.
- Henze, M., Gujer, W., Mino, T., Matsuo, T., Wentzel, M.C. and Marais, G.v.R., 1995c. Wastewater and biomass characterization for the activated sludge model no.2: Biological phosphorus removal. *Wat. Sci. Tech.*, **31**(2), 13-23.
- Henze, M., Dupont, R., Grau, P and De la Sota, A., 1993. Rising sludge in secondary settlers due to denitrification, *Wat. Res.*, **27**(2), 231-236.
- Henze, M., 1992. Characterization of wastewater for modelling of activated sludge processes, *Wat. Sci. Tech.*, **25**(6), 1-15.
- Henze, M. and Mladenovski, C., 1991. Hydrolysis of particulate substrate by activated sludge under aerobic, anoxic and anaerobic conditions, *Wat. Res.*, **25**(1), 61-64.
- Henze, M., Grady C.P.L.Jr., Gujer, W., Marais, G.v.R. and Matsuo, T., 1987. *Activated sludge model No.1*, IAWPRC Science and Technical Report No. 1, IAWPRC, London.
- Henze, M., 1986. Nitrate versus oxygen utilization rates in wastewater and activated sludge systems. *Wat. Sci. Tech.*, **18**(6), 115-122.
- Hidalgo, M.E. and Ayesa, E., 2001. Numerical and graphical description of the information matrix in calibration experiments for state-space models, *Wat. Res.*, **35**(13), 3206-3214.
- Holmberg, A., 1982. On the practical identifiability of microbial growth models incorporating Michaelis-Menten type nonlinearities, *Math. Biosci.*, **62**, 23-43.
- Hvala, N., Zec, M., Ros, M. and Strmenik, S., 2001. Design of a sequencing batch reactor sequence with an input load partition in a simulation-based experimental environment, *Water Environ. Res.*, **73**, 146 –153.

- Hu, Z.R., Sotemann, S., Moodley, R., Wentzel, M.C. and Ekama, G.A., 2003a.** Experimental investigation of the external nitrification biological nutrient removal activated sludge (ENBNRAS) system, *Biotechnol. Bioeng.*, **83(3)**, 260-273.
- Hu, Z.R., Wentzel, M.C. and Ekama, G.A., 2003b.** Modelling biological nutrient removal activated sludge systems - a review, *Wat. Res.*, **37(14)**, 3430-3444.
- Hu Z.R., Wentzel, M.C. and Ekama, G.A., 2001.** External nitrification in biological nutrient removal activated sludge systems. *Wat. Sci. Tech.*, **43(1)**, 251-260.
- Hulsbeek, J.J.W., Kruit, J., Roeleveld, P.J., van Loosdrecht, M.C.M., 2002.** A practical protocol for dynamic modelling of activated sludge systems, **45(6)**, 127-136.
- Insel, G., Sin, G., Lee, D.S. and Vanrolleghem, P.A., 2004.** A calibration methodology and model-based system analysis for nutrient removing SBRs, *3rd IWA International conference on SBR*, February 22-26th, Noosa, Queensland, Australia.
- Insel, G., Orhon, D. and Vanrolleghem, P.A., 2003a.** Identification and modelling of aerobic hydrolysis mechanism-application of optimal experimental design, *J. Chem. Tech. Biotech.*, **78(4)**, 437-445.
- Insel, G., De Pauw, D., Lee, D.S. and Vanrolleghem, P.A., 2003b.** Dynamic calibration of an intermittently aerated carousel plant-Report No1, Technical Report, Gent University, Applied Mathematics, Biometrics and Process Control.
- Insel, G., Sin, G., Lee, D.S. and Vanrolleghem, P.A., 2003b.** A calibration methodology and model-based system analysis for nutrient removing SBRs, *3rd IWA International conference on SBR*, Queensland, Australia.
- Insel, G., Karahan Gül, Ö., Orhon, D., Vanrolleghem, P.A. and Henze, M., 2002.** Important limitations in the modeling of activated sludge-biased calibration of the hydrolysis process, *Wat. Sci. Tech.*, **45(12)**, 23-36.
- Irvine, R.L., Wilderer, P.A. and Flemming, H.C., 1997.** Controlled unsteady state processes and technologies-an overview, *Wat. Sci. Tech.*, **35(1)**, 11-18.
- Isaacs, S., Hansen J.A., Schmidt, K. and Henze, M., 1995.** Examination of the activated sludge model no.2 with an alternating process, *Wat. Sci. Tech.*, **31(2)**, 55-66.

- Jetten, M.S.M., Strous, M., de Pas-Schoonen, K.T., Schalk, J., van Dongen, G.J.M. van de Graaf, A.A., Logemann, S., Muyzer, G., van Loosdrecht, M.C.M., Kuenen, J.G., 1999.** The anaerobic oxidation of ammonium, *FEMS Microbial. Rev.*, **22**, 421-437
- Kappeler, J. and Gujer, W., 1992.** Estimation of kinetic parameters of heterotrophic biomass under aerobic conditions and characterization of wastewater for activated sludge modelling. *Wat. Sci. Tech.*, **25(6)**, 125-139.
- Kayser R., 1999.** Activated Sludge Process, 13th Section IN: Rehm J and Reed G, *Biotechnology*, 2nd Edition, Wiley-VCH, Vol. 11a, Weinheim, Germany.
- Kazmi, A.A., Fujita, M. and Furumai, H., 2001.** Modeling effect of remaining nitrate on phosphorus removal in SBR, *Wat. Sci. Tech.*, **43(3)**, 175-182.
- Keller, J., Watts, S., Battye-Smith, W. and Chong, R., 2001.** Full-scale demonstration of biological nutrient removal in a single tank process,. *Wat. Sci. Tech.*, **43(3)**, 355-362.
- Keesman, K.J., Spanjers, H. and van Straten, G., 1998.** Analysis of endogenous process behavior in activated sludge, *Biotechnol. Bioeng.*, **57(2)**, 155-163.
- Kern-Jespersen, J.P. and Henze, M., 1993.** Biological phosphorus uptake under anoxic and aerobic conditions, *Wat. Res.*, **27(4)**, 617-624.
- Ketchum, L.H.Jr., 1997.** Design and physical features of sequencing batch reactors, *Wat. Sci. Tech.*, **35(1)**, 1-10.
- Koch, G., Pianta, R., Krebs, P. and Siegrist, H., 1999.** Potential of denitrification and solids removal in the rectangular clarifier, *Wat. Res.*, **33(2)**, 309-318.
- Krebs, P., Armbruster, M., and Rodi, W., 2000.** Numerische Nachklärbecken-Modelle. KA, *Wasserwirtschaft Abwasser Abfall*, **47(7)**, 985-999.
- Kuba, T., van Loosdrecht, M.C.M. and Heijnen, J.J., 1996.** Effect of cyclic oxygen exposure on the activity of denitrifying phosphorus removing bacteria, *Wat. Sci. Tech.*, **34(1-2)**, 33-40.
- Kuba, T., Wachtmeiser, A., van Loosdrecht, M.C.M. and Heijnen, J.J., 1994.** Effect of nitrate on phosphorus release in biological phosphorus removal systems, *Wat. Sci. Tech.*, **30(6)**, 263-269.
- Kuba, T., Smolders, G.J.F., van Loosdrecht, M.C.M. and Heijnen, J.J., 1993.** Biological phosphorus removal from wastewater by anaerobic-anoxic sequencing batch reactor. *Wat. Sci. Tech.*, **27(5-6)**, 241-252.

- Langergraber, G., Rieger, L., Winkler, S., Alex, J., Wiese, J., Owerdieck, C., Ahnert, M., Simon, J. and Maurer, M.,** 2003. A guideline for simulation studies of wastewater treatment plants, In proceedings: *9th IWA conference on Design Operation and Economics of LWWTP*, pp. 201-208, 1st -4th September 2003, Praha, Czech Republic.
- Lau, A.D., Strom, P.F. and Jenkins, D.,** 1984. Growth kinetics of *Spharetilus natans* and a floc former in pure and dual continuous culture, *J. Wat. Pollut. Cont. Fed.*, **56(1)**, 41-51.
- Levine, A.D., Tchobanoglous, G., Asano, T.,** 1991. Size distributions of particulate contaminants in wastewater and their impact on treatability, *Wat. Res.*, **25**, 911-922.
- Lin, Y.F. and Jing, S.R.,** 2001. Characterization of denitrification and nitrification in a step-feed alternating anoxic-oxic sequencing batch reactors, *Water Environ. Res.*, **73**, 526-533.
- Lin, K.C. and Tsang, K.W.R.,** 1989. Nitrogen removal in an intermittently aerated completely mixed reactor, *Env. Tech. Lett.*, **10(1)**, 1-8.
- Lishman, L.A. and Murphy, K.L.,** 1994. The significance of hydrolysis in microbial death and decay, *Wat. Res.*, **28(11)**, 2417-2419.
- Liu, R.,** 2000. Monitoring, modeling and control of nutrient removal in the activated sludge process, *PhD Thesis*, University of Georgia, Georgia, U.S.A.
- Littleton, H.X., Daigger, G.T., Strom, P.F. and Jin, R.,** 2002. Simulation of Bio-P removal in CFD environment-Analysis of macro environment variations in simultaneous biological nutrient removal systems, *WEFTEC02, Water Environ. Fed. 75th Annual Conference Exposition*, Chicago, Illinois, U.S.A.
- Makinia, J., Swinarski, M. and Dobiegala, E.,** 2002. Experiences with computer simulation at two large wastewater treatment plants in northern Poland, *Wat. Sci. Tech.*, **45(6)**, 209-218.
- Mamais, D., Jenkins, D. and Pitt, P.,** 1993. A rapid physical chemical method for the determination of readily biodegradable soluble COD in municipal wastewaters, *Wat. Res.*, **27**, 195-197.
- Manga, J., Ferrer, J., Garcia-Usach, F. and Seco, A.,** 2001. A modification to the Activated Sludge Model No. 2 based on the competition between phosphorus-accumulating organisms and glycogen-accumulating organisms. *Wat. Sci. Tech.*, **43(11)**, 161-171.
- Manning, J.F. and Irvin, R.L.,** 1985. The biological removal of phosphorous in a sequencing batch reactor, *J. Water Pollut. Control. Fed.*, **57**, 87-94.

- Maurer, M. and Gujer, W.,** 1994. Prediction of the performance of enhanced biological phosphorus removal plants, *Wat. Sci. Tech.*, **30(6)**, 333-343.
- Meijer, S.C.F., van Loosdrecht, M.C.M. and Heijnen J.J.,** 2001. Metabolic modeling of full-scale biological nitrogen and phosphorus removing WWTPs, *Wat. Res.*, **35(11)**, 2711-2723.
- Meinhold, J., Filipe, C.D.M., Daigger, G.T. and Isaacs, S.,** 1999. Characterization of the denitrifying fraction of phosphate accumulating organisms in biological phosphate removal, *Wat. Sci. Tech.*, **39(1)**, 31-42.
- Metcalf and Eddy,** 2003. *Wastewater Engineering, Treatment and Reuse*, McGraw Hill, New York.
- McCarty, P.L.,** 1972. Stoichiometry of biological reactions, *Prog. Wat. Technol.*, **7**, 157-173.
- Mino, T., Liu, W.T., Kurisu, F. and Matsuo, T.,** 1995a. Modeling glycogen storage and denitrification capability of microorganisms in enhanced biological phosphorus removal processes, *Wat. Sci. Tech.*, **31(2)**, 25-34.
- Mino, T., San Pedro, D.C. and Matsuo, T.,** 1995b. Estimation of the rate of slowly biodegradable COD (SBCOD) hydrolysis under anaerobic, anoxic and aerobic conditions by experiments using starch as model substrate, *Wat. Sci. Tech.*, **31(2)**, 95-103.
- Miyake, H. and Morgenroth, E.,** 2002. Optimization of enhanced biological phosphorus removal after periods of low loading. *WEFTEC02, Water Environ. Fed. 75th Annual Conf. Exposition*, Chicago, Illinois, U.S.A.
- Moser-Engeler, R., Udert K.M., Wild D. and Siegrist, H.,** 1998. Products from primary sludge fermentation and their suitability for nutrient removal, *Wat. Sci. Tech.*, **38(1)**, 265-273.
- Muller, J.S. and Stensel, H.D.,** 1990. Biologically enhanced oxygen transfer in the activated sludge process, *Research Journal WPCF*, **62(2)**, 193-203.
- Mueller, J.S. and Boyle, W.,** 1988. Oxygen transfer under process conditions, *J. Wat. Pollut. Control Fed.*, **60**, 332-341.
- Muller, A., Wentzel, M.C., Loewenthal, R.E. and Ekama, G.A.,** 2003. Heterotrophic anoxic yield in anoxic aerobic activated sludge systems treating municipal wastewater, *Wat. Res.*, **37(10)**, 2435-2441.

- Munch, E.V., Lant, P. and Keller, J., 1996.** Simultaneous nitrification and denitrification in bench-scale sequencing batch reactors, *Wat. Res.*, **30(2)**, 277-284.
- Munack, A., 1989.** Optimal feeding strategy for identification of Monod type models by fed-batch experiments, in *Computer Applications in Fermentation Technology: Modelling and Control of Biotechnological Processes*, pp. 195-204, Eds. Fish, N., Fox, R., Thornhill, N., Elsevier, Amsterdam, the Netherlands.
- Mura, G., 2003.** Model-based optimisation of SBRs: Effect of oxygen set-point and SRT, *MSc. Thesis*, Ghent University, Gent, Belgium.
- Murat, S., Ateş Genceli, E., Tasli, R., Artan, N. and Orhon, D., 2002..** Sequencing batch reactor treatment of tannery wastewater for carbon and nitrogen removal, *Wat. Sci. Tech.*, **46(9)**, 219–227.
- Murnleitner, E., Kuba, T., van Loosdrecht, M.C.M. and Heijnen, J.J. 1997.** An integrated metabolic model for the aerobic and denitrifying biological phosphorus removal, *Biotechnol Bioeng.*, **54(5)**, 434-450.
- Naidoo, K., Ndlovu, V., Mjadu, L., Goatley, K. and Kerdachi, D.A., 2002.** The exceptional simultaneous removal of carbon, nitrogen and phosphorus in a simple activated sludge treatment system at Kingsburgh Wastewater Treatment Works, *Water SA, WISA Proceedings*, 67-72.
- Nowak, O., Franz, A., Svardal, K., Müller, V. and Kühn, V., 1999.** Parameter estimation for activated sludge models, *Wat. Sci. Tech.*, **39(4)**, 113-120.
- Novak, L., Larrea, L. and Wanner, J., 1995.** Mathematical model for soluble carbonaceous substrate biosorption, *Wat. Sci. Tech.*, **31(2)**, 67-77.
- Novak, L., Larrea, L. and Wanner, J., 1994.** Estimation of maximum specific growth-rate of heterotrophic and autotrophic biomass-a combined technique of mathematical-modeling and batch cultivations, *Wat. Sci. Tech.*, **30(11)**, 171-180.
- Oh, J. and Silverstein, J., 1999.** Oxygen inhibition of activated sludge denitrification, *Wat. Res.*, **33(8)**, 1925-1937.
- Olsson, G. and Jeppson, U., 1994.** Establishing cause-effect relationships in activated sludge plants-what can be controlled? *Proceedings of Fac. Landbouww.*, Gent University, 59/4a.
- Omlin, M., Brun R., and Reichert P., 2001.** Biogeochemical model of lake Zurich: sensitivity, identifiability and uncertainty analysis, *Ecol. Modell.* **141**, 105-123.
- Omlin, M. and Reichert, P., 1999.** A comparison of techniques for the estimation of model prediction uncertainty, *Ecol. modell.*, **115**, 45-59.

- Orhon, D., Okutman, D. and Insel, G., 2002.** Characterization and biodegradation of settleable organic matter for domestic wastewater, *Water SA*, **28(3)** 299-305.
- Orhon, D., Babuna, F.G. and Insel, G., 2001.** Characterization and modelling of denim-processing wastewaters for activated sludge, *J. Chem. Tech. Biotech.*, **76(9)**, 919-931.
- Orhon, D., Ates Genceli, E. and Sözen, S., 2000.** Experimental evaluation of the nitrification kinetics for tannery wastewaters, *Water SA*, **26(1)**, 43–50.
- Orhon, D., Taşlı, R. and Sözen, S., 1999a.** Experimental basis of activated sludge treatment for industrial wastewaters – the state of the art, *Wat. Sci. Tech.*, **40(1)**, 1-11.
- Orhon, D., Karahan, Ö. and Sözen, S., 1999b.** The effect of residual microbial products on the assessment of the particulate inert COD in wastewaters, *Wat. Res.*, **33(14)**, 3191-3203.
- Orhon, D., Ubay Çokgör, E. and Sözen, S., 1999c.** Experimental basis for the hydrolysis of slowly biodegradable substrate in different wastewaters, *Wat. Sci. Tech.*, **39(1)**, 87-95.
- Orhon, D., Ates, Genceli, E. and Ubay Çokgör, E., 1999d.** Characterization and modeling of activated sludge for tannery wastewater, *Water Environ. Res.*, **71(1)**, 50–63.
- Orhon, D., Sözen, S. and Artan, N., 1996.** The effect of heterotrophic yield on the assessment of the correction factor for anoxic growth, *Wat. Sci. Tech.*, **34(5-6)**, 67-74.
- Orhon, D. and Artan, N., 1994.** Modelling of Activated Sludge Systems, Technomic Press, Lancaster PA.
- Orhon, D., Artan, N., Buyukmurat, S. and Görgün, E., 1992.** The effect of residual COD on the biological treatability of textile wastewaters, *Wat. Sci. Tech.*, **26(3-4)**, 815-825.
- Park, H.D. and Noguera, D.R., 2002.** Effect of dissolved oxygen on ammonia oxidizing bacterial communities, *WEFTEC02, Water Environ. Fed. 75th Annual Conf. Exposition*, Chicago, Illinois, U.S.A.
- Petersen, B., Gernaey, K., Henze, M. and Vanrolleghem, P.A., 2003.** Calibration of activated sludge models: A critical review of experimental designs. In: *Biotechnology for the Environment: Wastewater Treatment and Modeling, Waste Gas Handling*. Eds. Agathos S.N. and Reineke W., Kluwer Academic Publishers, Dordrecht, The Netherlands. 101-186.

- Petersen, B., Gernaey, K., Henze, M. and Vanrolleghem, P.A., 2002.** Evaluation of an ASM1 model calibration procedure on a municipal-industrial wastewater treatment plant, *J. Hydroinformatics*, **4(1)**, 15-38.
- Petersen, B., Gernaey, K. and Vanrolleghem, P.A., 2001a.** Practical identifiability of model parameters by combined respirometric-titrimetric measurements, *Wat. Sci. Tech.*, **43(7)**, 347-355.
- Petersen B., Gernaey K., Henze M. and Vanrolleghem P.A., 2001b.** Calibration of activated sludge models: A critical review of experimental designs, in: *Biotechnology for the Environment*, pp.80., Eds. Agathos S. and Reineke W., Focus on Biotechnology, Vol. 3. Kluwer Academic Publishers, Dordrecht, the Netherlands.
- Petersen, B., 2000.** Calibration identifiability and optimal experimental design of activated sludge models, *PhD Thesis*, Applied Mathematics Biometrics and Process Control (BIOMATH) Department, Belgium.
- Pochana, K. and Keller, J., 1999.** Study of factors affecting simultaneous nitrification and denitrification –SND, *Wat.Sci. Tech.*, **39(6)**, 61-68.
- Pohjanpalo, H., 1978.** System identifiability based on the power series expansion of the solution, *Math. Biosci.*, **41**, 21-33.
- Randall, C.W., Barnard, L.B. and Stensel, H.D., 1992.** Design and Retrofit of Wastewater Treatment Plants for Biological Nutrient Removal, Technomic Publishing Inc., Lancaster, PA.
- Reichert, P., 2003.** UNCSIM Course, Swiss Federal Institute for Environmental Science and Technology (EAWAG), CH-8600, Dübendorf, Switzerland, 25-26 September.
- Reichert, P. and Vanrolleghem, P., 2001.** Identifiability and uncertainty analysis of the River Water Quality Model No:1 (RWQM1), *Wat. Sci. Tech.*, **43(7)**, 329-338.
- Reichert, P., Ruchti, J. and Simon, W., 1998.** *AQUASIM 2.0*, Swiss Federal Institute for Environmental Science and Technology (EAWAG), CH-8600 Duebendorf, Switzerland.
- Reichert, P., von Scultness, R. and Wild, D., 1995.** The use of AQUASIM for estimating parameters of activated sludge models, *Wat. Sci. Tech.*, **31(2)**, 135-147.
- Reichert, P., 1994.** AQUASIM-A Tool for simulation and data analysis of aquatic systems, *Wat. Sci. Tech.*, **30(2)**, 21–30.
- Reiger, L., Koch, G., Kühni, M., Gujer, W. and Siegrist, H., 2001.** The EAWAG Bio-P module for activated sludge Model No.3., *Wat. Res.*, **35(16)**, 3887-3903.

- Rittmann, B.E. and Langeland, W.E., 1985.** Simultaneous denitrification with nitrification in single-channel oxidation ditches, *J. Wat. Poll. Cont. Fed*, **57(4)**, 300-308.
- Rodrigo, M.A., Seco, A., Penya Roja, J.M., Ferrer, J., 1996.** Influence of sludge age on enhanced phosphorus removal in biological systems, *Wat. Sci. Tech.*, **34(1-2)**, 41-48.
- Roeleveld, P.J. and van Loosdrecht, M.C.M., 2002.** Experiences with guidelines for wastewater characterization in the Netherlands, *Wat. Sci. Tech.*, **45(6)**, 77-87.
- Romansky, J., Heider, M. and Weismann, U., 1997.** Kinetics of anaerobic orthophosphate release and substrate uptake in enhanced biological phosphorus removal from synthetic wastewaters, *Wat. Res.*, **31(12)**, 3137-3145.
- Rozzi, A., Ficara, E., Cellemare, C.M. and Bortone, G., 1999.** Characterization of textile wastewater and other industrial wastewaters by respirometric and titration biosensors, *Wat. Sci. Tech.*, **40(1)**, 161-168.
- Satoh, H., Okuda, E., Mino, T. and Matsuo, T., 2000.** Calibration of kinetic parameters in the IAWQ Activated Sludge Model: a pilot scale experience, *Wat. Sci. Tech.*, **42(3-4)**, 29-34.
- Satoh, H., Mino, T. and Matsuo, T., 1994.** Deterioration of enhanced biological phosphorus by the domination of microorganisms without polyphosphate accumulation. *Wat. Sci. Tech.*, **30(6)**, 203-211.
- Scheer, H. and Seyfried, C.F., 1996.** Enhanced biological phosphate removal: modelling and design in theory and practice, *Wat. Sci. Tech.*, **38(8-9)**, 95-103.
- Servais, P., Seidl, M. and Mouchel, J.M., 1999.** Comparison of parameters characterizing organic matter in a combined sewer during rainfall events and dry weather, *Water. Env. Res.*, **71(4)**, 408-417.
- Siegrist, H., Reiger, L., Koch, G., Kühni, M. and Gujer, W., 2002.** The EAWAG Bio-P module for activated sludge No3., *Wat. Sci. Tech.*, **45(6)**, 61-76.
- Siegrist, H., Brunner I., Koch, G., Linh Con Phan and Van Chieu Le., 1999.** Reduction of biomass decay rate under anoxic and anaerobic conditions, *Wat. Sci. Tech.*, **39(1)**, 129-137.
- Siegrist, H. and Tschui, M., 1992.** Interpretation of experimental data with regard to the activated sludge model no. 1 and calibration of the model for municipal wastewater treatment plants, *Wat. Sci. Tech.*, **25(6)**, 167-183.

- Smith, G.**, 1996. Increasing oxygen delivery in anoxic tanks to improve denitrification, *WEFTEC96, Water Environ. Fed. 69th Annual Conf. Exposition*, Dallas, Texas, 5, 345.
- Smolders, G.J.F.**, 1995. A metabolic model of the biological phosphorus removal-stoichiometry, kinetics and dynamic behavior, *PhD thesis*, Delft University of Technology, Department of biochemical engineering, the Netherlands.
- Smolders, G.J.F., van der Meij, J., van Loosdrecht, M.C.M. and Heijnen, J.J.**, 1994a. Model of the anaerobic metabolism of the biological phosphorus removal process: stoichiometry and pH influence. *Biotech. Bioeng.*, **43**(6), 461-470
- Smolders, G.J.F., van der Meij, J., van Loosdrecht, M.C.M. and Heijnen, J.J.**, 1994b. Stoichiometric model of the aerobic metabolism of the biological phosphorus removal process, *Biotech. Bioeng.*, **44**, 837-848.
- Sollfrank, U. and Gujer, W.**, 1991. Characterization of domestic wastewater for mathematical modelling of the activated sludge process, *Wat. Sci. Tech.*, **23**(4-6), 1057-1066.
- Sözen, S., Ubay Çokgör, E., Orhon, D. and Henze, M.**, 1998. Respirometric analysis of activated sludge behaviour-II. Heterotrophic growth under aerobic and anoxic conditions, *Wat. Res.*, **32**(2), 476-488.
- Sözen, S., Orhon, D. and San, H.A.**, 1996. A new approach for the evaluation of the maximum specific growth rate in nitrification. *Wat. Res.*, **30**(1), 43-50.
- Spagni, A., Buday, J., Ratini, P. and Bortone, G.**, 2001. Experimental considerations on monitoring ORP, pH, conductivity and dissolved oxygen in nitrogen and phosphorus biological removal processes., *Wat. Sci. Tech.*, **43**(11), 197-204.
- Spanjers, H., Vanrolleghem, P.A., Olsson, G. and Dold, P.L.**, 1998. Respirometry in Control of the Activated Sludge Process Principles, *IAWQ Scientific and Technical Report No. 7*, London, UK.
- Spanjers, H. and Vanrolleghem, P.A.**, 1995. Respirometry as a tool for rapid characterization wastewater and activated sludge. *Wat. Sci. Tech.*, **31**(2), 105-114.
- Spanjers, H.**, 1993. Respirometry in activated sludge, *PhD Thesis*, Wageningen Agricultural University, Wageningen, the Netherlands.
- Sperandio, M. and Paul, E.**, 2000. Estimation of wastewater biodegradable COD fractions by combining respirometric experiments in various S0/X0 ratios, *Wat. Res.*, **34**(4), 1233-1244.

- Stenström, M.K. and Poduska, R.A., 1980.** The effect of dissolved oxygen concentration on nitrification, *Wat. Res.*, **14(6)**, 643-649.
- Stamou, A.I., 1997.** Modelling of oxidation ditches using an open channel flow 1-D advection dispersion equation and ASM1 process description, *Wat. Sci. Tech.*, **36(5)**, 269-276.
- STOWA, 2001.** The combined Sharon-Anammox process, *STOWA report*. IWA Publishing.
- Strous, M., 2000.** Anammox and Nitrification. In: *Microbiology of Anaerobic Ammonium Oxidation*, Ph.D. thesis, 63-81, the Netherlands.
- Taşlı, R., Artan, N. and Orhon, D., 2001.** Retrofitting SBR systems to nutrient removal in sensitive tourist areas, *Wat. Sci. Tech.*, **44(1)**, 121-129.
- Taşlı, R., Orhon, N. and Artan, N., 1999.** The effect of substrate composition on the nutrient removal potential of sequencing batch reactors, *Water SA*, **25(3)**, 337-344.
- Takács, I., Patry, G. and Nolasco, D., 1991.** A dynamic model of the clarification-thickening process, *Wat. Res.*, **25(10)**, 1263-1271.
- Teichgräber, B., Schreff, D., Ekkerlein, C. and Wilderer, P.A., 2001.** SBR technology in Germany - an overview, *Wat. Sci. Tech.*, **43(3)**, 323-330.
- Tijhuis, L. and van Loosdrecht, M.C.M., 1993.** A thermodynamically based correlation for maintenance Gibbs energy requirements in aerobic and anaerobic chemotrophic growth, *Biotechnol Bioeng.*, **42(4)**, 509-519.
- Temmink, H., Petersen, B., Isaacs, S. and Henze, M., 1996.** Recovery of biological phosphorus removal after periods of low organic loading, *Wat Sci. Tech.*, **34(1-2)**, 1-8.
- Tilche, A., Bortone, G., Malaspina, F., Piccinini, S. and Stante, L., 2001.** Biological nutrient removal in a full-scale SBR treating piggy wastewater: results and modelling, *Wat. Sci. Tech.*, **43(3)**, 363-371.
- Ubay Çokgör, E., Sözen, S., Orhon, D. and Henze, M., 1998.** Respirometric analysis of activated sludge behaviour-I. Assessment of readily biodegradable substrate, *Wat. Res.*, **32(2)**, 461-475.
- Ubisi, M.F., Joodi, T.W., Wentzel, M.C. and Ekama, G.A., 1997.** Activated sludge mixed liquor heterotrophic active biomass, *Water SA*, **23(3)**, 239-248.
- U.S. EPA., 1992.** Evaluation of oxidation ditches for nutrient removal. *Technical Report*. No:832; R-92-003, Washington D.C., USA.

- U.S. EPA., 1975.** Process design manual for nitrogen control, Office of Technology Transfer, U.S. Environmental Protection Agency, Washington, DC, USA.
- U.S. Filter/Envirex, 2002.** The Orbal System for biological treatment. <http://www.usfilter.com/water>
- Wilderer, P., Irvine, R. and Goronszy, M., 2001.** Sequencing Batch Reactor Technology, *IWA Scientific and Technical Report No. 10.*, London.
- Walter, E. and Pronzato, L., 1995.** On the identifiability distinguishability testing for linear and non-linear parametric models., *Symposium applications of modelling and control in agriculture and bioindustries (IMACS)*, p. V.A.3-1-V.A.3-8, Brussels, Belgium.
- Walter, E. and Pronzato, L., 1990.** Qualitative and quantitative experiment design for phenomenological models-a survey, *Automatica*, **26(2)**, 195-213.
- Walter, E., 1982.** Identifiability of State Space Models, Springer, Berlin.
- Wanner, O., Kappeler, J. and Gujer, W., 1992.** Calibration of an activated-sludge model based on human expertise and on a mathematical optimization technique - a comparison, *Wat. Sci. Tech.*, **25(6)**, 141-148.
- Wentzel, M.C., Ekama, G.A. and Marais, G.v.R., 1992.** Processes and modeling of nitrification denitrification biological excess phosphorus removal systems - a review, *Wat. Sci. Tech.*, **25(6)**, 59-82.
- Wentzel, M.C., Ekama, G.A., Dold, P.L. and Marais, G.v.R., 1990.** Biological excess phosphorus removal-steady state process design, *Water SA*, **16**, 29-48.
- Wentzel, M.C., Dold, P.L., Ekama, G.A. and Marais, G.v.R., 1989a** Enhanced polyphosphate organism cultures in activated sludge systems, Part III, Kinetic model, *Water SA*, **15(2)**, 89-102.
- Wentzel, M.C., Ekama G.A., Loewenthal, R., Dold P. and Marais, G.v.R., 1989.** Enhanced polyphosphate organism cultures in activated sludge systems, Part II: Experimental behavior, *Water SA*, **15(2)**, 71-88.
- Wentzel, M.C., Loewenthal, R.E., Ekama, G.A. and Marais, G.v.R., 1988.** Enhanced poly phosphate organism cultures in activated sludge systems Part I: Enhanced cultures development. *Water SA.*, **14(2)**, 81-92.
- Weijers, S.R., 1999.** Online BOD tests for the determination of biodegradable COD for calibrating activated sludge model no.1, *Wat. Sci. Tech.*, **39(4)**, 177-184.

- Weijers, S.R. and Vanrolleghem, P.A., 1997.** A procedure for selecting the most important parameters in calibrating the activated sludge model no.1 with full-scale plant data, *Wat. Sci. Tech.*, **36(5)**, 69-79.
- W.E.R.F., 1999.** *Methods for wastewater characterization in activated sludge modeling*, Report No: 99 WWF 3, Alexandria, USA.
- W.E.R.F., 1996.** Aeration-a wastewater treatment process, Report No: 68, Water Environment Research Federation, Newyork, USA.
- Wilderer, P., Irvine, RL., Goronszy, M.C., 2001.** *Sequencing Batch Reactor Technology*, IWA Scientific and Technical Report No:10, London.
- Wouters-Wasiak, K., Heduit, A. and Audic, J.M., 1996.** Consequences of an occasional secondary phosphorus release on enhanced biological phosphorus removal, *Water SA*, **22(2)**, 91-96.
- van Dongen, U., Jetten, M.S.M. and van Loosdrecht, M.C.M., 2001.** The SHARON-Anammox process for treatment of ammonium rich wastewater., **44(1)**, 153-160.
- van Haandel, A.P.C, Ekama, G.A. and Marais, G.v.R., 1981.** The activated sludge process 3-single sludge denitrification, *Wat. Res.*, **15**, 1135-1152.
- Vanhooren, H., Meirlaen, J., Amerlinck, Y., Claeys, F., Vangheluwe, H. and Vanrolleghem, P.A., 2003.** WEST: Modeling biological wastewater treatment, *J. Hydroinformatics*, **5**, 27-50.
- van Loosdrecht, M.C.M. and Heijnen, J.J., 2002.** Modelling of activated sludge processes with structured biomass, *Wat.Sci. Tech.*, **45(6)**, 13-23.
- van Loosdrecht, M.C.M. and Henze, M., 1999.** Maintenance, endogenous respiration, lysis, decay and predation, *Wat. Sci. Tech.*, **39(1)**, 107-117.
- van Loosdrecht, M.C.M., Brandse, F.A. and de Vries, A.C., 1998.** Upgrading of wastewater treatment processes for integrated nutrient removal-the BCFS[®] process, *Wat. Sci. Tech.*, **37(9)**, 209-217.
- Vanrolleghem, P.A., Sin, G. and Gernaey, K.V., 2004.** Transient response of aerobic and anoxic activated sludge activities to sudden substrate concentration changes, *Biotech. Bioeng.*, (in press)
- Vanrolleghem, P.A., Insel, G., Petersen, B, Sin, G., De Pauw, D., Nopens, I., Dovermann, H., Weijers, S. and Gernaey, K., 2003.** A comprehensive model calibration procedure for activated sludge models, *WEFTEC 2003, 76th Annual Technical Exhibition and Conference*, October 11-15, 2003, Los Angeles, California U.S.A.

- Vanrolleghem, P.A. and Gillot, S., 2002.** Robustness and economic measures as control benchmark performance criteria, *Wat. Sci. Tech.*, **45(4-5)**, 117-126.
- Vanrolleghem, P.A., Spanjers, H., Petersen, B., Ginestet, P. and Takacs, I., 1999.** Estimating (combinations of) Activated Sludge Model No.1 parameters and components by respirometry, *Wat. Sci. Tech.*, **39(1)**, 195-214.
- Vanrolleghem, P.A., Coen, F., Gernaey, K., Petersen, B., De Clercq, B. and Ottoy, J.P., 1998.** Limitations of short term experiments designed for identification of activated sludge biodegradation models by fast dynamic phenomena, *7th IFAC Conference on Computer Application in Biotechnology*, Osaka, Japan, May 31-June 4.
- Vanrolleghem, P.A., Van Daele, M. and Dochain, D., 1995.** Practical identifiability of a biokinetic model of activated sludge respiration, *Wat. Res.*, **29(11)**, 2561-2570.
- Vanrolleghem, P.A. and Verstraete, W., 1993.** Simultaneous biokinetic characterization of heterotrophic and nitrifying populations of activated sludge with an on-line respirographic biosensor, *Wat. Sci. Tech.*, **28(11-12)**, 377-387.
- Versyck, K.J.E. and Van Impe, J.F.M., 2000.** Review on operation modes in bioreactor experiments aimed at parameter estimation of the Monod growth kinetics, *IWA-Watermatex 2000 Conference*, 7/28-7/35.
- Vialas, C., Cheruy, A. and Gentil, S., 1986.** An experimental approach to improve the Monod model identification in *Modelling and Control of Biotechnological Processes*, pp 155-160, Pergamon Press, Oxford.
- Yagci, N., Insel, G., Artan, N. and Orhon, D., 2004.** Modeling and calibration of phosphate and glycogen accumulating organism competition for acetate uptake in sequencing batch Reactor, *Wat. Sci. Tech.*, **50(6)**, 241-250.

ANNEX A: Table A.1. Matrix representation of ASM2dN-Soluble Components

ASM2dN	1	2	3	4	5	6	7	8	9	10
No Processes/Components	S_{O_2}	S_F	S_A	S_{NH}	S_{ND}	S_{NO_3}	S_{PO_4}	S_I	S_{ALK}	S_{N_2}
1 Hydrolysis		$1-f_{SI}$					$i_{PXS}-(1-f_{SI}) i_{PSF}-i_{PSI} f_{SI}$	f_{SI}	$-i_{PXS}-(1-f_{SI}) i_{PSF}-i_{PSI} f_{SI}$	$(1.5/31)$
2 Hydrolysis of entrapped-N					$+1$					
3 Fermentation		-1	$+1$				i_{PSF}		$-1/64-i_{PSF} (1.5/31)$	
4 Ammonification				1	-1				$1/14$	
5 Aerobic growth of Heterotrophs, X_H on S_A	$1 - \frac{Y_H}{Y_H}$		$-\frac{1}{Y_H}$	$-i_{NBM}$			$-i_{PBM}$		$(1.5/31) i_{PBM}-i_{NBM}/14+1/(64 Y_H)$	
6 Aerobic growth of Heterotrophs, X_H on S_F	$1 - \frac{Y_H}{Y_H}$	$-\frac{1}{Y_H}$		$-i_{NBM}$			$-i_{PBM}+i_{PSF}/Y_H$		$-(1.5/31) (-i_{PBM}+i_{PSF}/Y_H)-i_{NBM}/14$	
7 Anoxic growth of Heterotrophs, X_H on S_A			$-\frac{1}{Y_{HNO_3}}$	$-i_{NBM}$		$-\frac{1-Y_{HNO_3}}{2.86 Y_{HNO_3}}$	$-i_{PBM}$		$-(1.5/31)(-i_{PBM}+i_{PSF}/Y_H)-i_{NBM}/14+1/(64 Y_{HNO_3})+(1/14)(1-Y_{HNO_3})/(2.86 Y_{HNO_3})$	$(1-Y_{HNO_3})/(2.86 Y_{HNO_3})$
8 Anoxic growth of Heterotrophs on S_F		$-\frac{1}{Y_{HNO_3}}$		$-i_{NBM}$		$-\frac{1-Y_{HNO_3}}{2.86 Y_{HNO_3}}$	$-i_{PBM}+i_{PSF}/Y_H$		$-(1.5/31)(-i_{PBM}+i_{PSF}/Y_H)-i_{NBM}/14+1/(14)(1-Y_{HNO_3})/(2.86 Y_{HNO_3})$	$(1-Y_{HNO_3})/(2.86 Y_{HNO_3})$
9 Growth of Autotrophs, X_{AUT}	$4.57 - \frac{Y_{NH}}{Y_{NH}}$			$-(i_{NBM}+1/Y_{NH})$		$\frac{1}{Y_{NH}}$	$-i_{PBM}$		$(1.5/31) i_{PBM}+i_{NBM}/14-2/(14 Y_{NH})$	
10 Lysis of Autotrophs, X_{AUT}							i_{PBM}		$-(1.5/31) i_{PBM}$	
11 Lysis of Heterotrophs, X_H							i_{PBM}		$-(1.5/31) i_{PBM}$	
12 Storage of X_{PHA}			-1				Y_{PO_4}		$1/64-(1.5/31) Y_{PO_4}$	
13 Aerobic Storage of X_{PP}	$-Y_{PHA}$						-1		$1.5/31-1/31$	
14 Anoxic Storage of X_{PP}						$-Y_{PHA}/2.86$	-1		$1.5/31-1/31+(1/14) Y_{PHA}/2.86$	$Y_{PHA}/2.86$
15 Aerobic growth of X_{PAOS}	$1 - \frac{Y_H}{Y_H}$			$-i_{NBM}$			$-i_{PBM}$		$1.5/31 i_{PBM}-i_{NBM}/14$	
16 Anoxic growth of X_{PAOS}				$-i_{NBM}$		$-\frac{1-Y_H}{2.86 Y_H}$	$-i_{PBM}$		$i_{PBM} 1.5/31-i_{NBM}/14+(1-Y_H)/(2.86 Y_H)$	$(1-Y_H)/(2.86 Y_H)$
17 Lysis of X_{PAO}							i_{PBM}		$-1.5/31 i_{PBM}$	
18 Lysis of X_{PHA}			$+1$						$-1/64$	
19 Lysis of X_{PP}							1		$-1.5/31 + 1/31$	

Table A.1. Matrix representation of ASM2dN-Particulate Components (Cont.)

ASM2dN	11	12	13	14	15	16	17	18	19	20	21
No Processes/Components	X_I	X_S	X_{ND}	X_H	X_{PAO}	X_{PP}	X_{PHA}	X_{NH}	X_{MEOH}	X_{MEP}	TSS
1 Hydrolysis		-1									$-i_{TSS,XS}$
2 Hydrolysis of entrapped-N			-1								
3 Fermentation											
4 Ammonification											
5 Aerobic growth of Heterotrophs, X_H on S_A				1							$i_{TSS,BM}$
6 Aerobic growth of Heterotrophs, X_H on S_F				1							$i_{TSS,BM}$
7 Anoxic growth of Heterotrophs, X_H on S_A				1							$i_{TSS,BM}$
8 Anoxic growth of Heterotrophs on S_F				1							$i_{TSS,BM}$
9 Growth of Autotrophs, X_{AUT}								1			$i_{TSS,BM}$
10 Lysis of Autotrophs, X_{AUT}	f_{XI}	$1 - f_{XI}$	$i_{N,BM} f_{XI} i_{N,XI}$					-1			$(1 - f_{XP}) i_{TSS,XS} + f_{XP} i_{TSS,XI} - i_{TSS,BM}$
11 Lysis of Heterotrophs, X_H	f_{XI}	$1 - f_{XI}$	$i_{N,BM} f_{XI} i_{N,XI}$	-1							$(1 - f_{XP}) i_{TSS,XS} + f_{XP} i_{TSS,XI} - i_{TSS,BM}$
12 Storage of X_{PHA}					$-Y_{PO4}$	1	1				$-Y_{PO4} i_{TSS,XI} + i_{TSS,XPHA}$
13 Aerobic Storage of X_{PP}						1	$-Y_{PHA}$				$i_{TSS,XPP} - Y_{PHA} i_{TSS,XPHA}$
14 Anoxic Storage of X_{PP}						1	$-Y_{PHA}$				$i_{TSS,XPP} - Y_{PHA} i_{TSS,XPHA}$
15 Aerobic growth of X_{PAOs}					1		$\frac{-1}{Y_H}$				$i_{TSS,BM} (1/Y_H) i_{TSS,XPHA}$
16 Anoxic growth of X_{PAOs}					1		$\frac{-1}{Y_H}$				$i_{TSS,BM} (1/Y_H) i_{TSS,XPHA}$
17 Lysis of X_{PAO}	f_{XI}	$1 - f_{XI}$	$i_{N,BM} f_{XI} i_{N,XI}$	-1							$(1 - f_{XP}) i_{TSS,XS} + f_{XP} i_{TSS,XI} - i_{TSS,BM}$
18 Lysis of X_{PHA}							-1				$-i_{TSS,XPHA}$
19 Lysis of X_{PP}						-1					$-i_{TSS,XPP}$

Table A.1. Processes of ASM2dN (Cont.)

	Processes	Rate Equation
1	Hydrolysis	$k_h \frac{X_S/X_H}{K_X + X_S/X_H} \left(\frac{S_O}{K_O + S_O} + \eta_{HNO_3} \frac{K_O}{K_O + S_O} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} + \eta_{fe} \frac{K_O}{K_O + S_O} \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \right) X_H$
2	Hydrolysis of entrapped-N	$\rho_I \frac{X_{ND}}{X_S}$
3	Fermentation	$Q_{fe} \frac{S_F}{K_F + S_F} \frac{K_O}{K_O + S_O} \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{K_{NO_2}}{K_{NO_2} + S_{NO_2}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_H$
4	Ammonification	$k_a S_{ND} X_H$
5	Aerobic growth of Heterotrophs, X_H on S_A	$\mu_H \frac{S_O}{K_O + S_O} \frac{S_A}{K_A + S_A} \frac{S_F}{S_F + S_A} \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_{PO}}{K_{PO} + S_{PO}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_H$
6	Aerobic growth of Heterotrophs, X_H on S_F	$\mu_H \frac{S_O}{K_O + S_O} \frac{S_F}{K_F + S_F} \frac{S_A}{S_A + S_F} \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_{PO}}{K_{PO} + S_{PO}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_H$
7	Anoxic growth of Heterotrophs, X_H on S_A	$\eta_{NO_3het} \mu_H \frac{K_O}{K_O + S_O} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_A}{K_A + S_A} \frac{S_F}{S_F + S_A} \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_{PO}}{K_{PO} + S_{PO}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_H$
8	Anoxic growth of Heterotrophs on S_F	$\eta_{NO_3het} \mu_H \frac{K_O}{K_O + S_O} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_F}{K_F + S_F} \frac{S_A}{S_A + S_F} \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_{PO}}{K_{PO} + S_{PO}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_H$
9	Growth of Autotrophs, X_{AUT}	$\mu_{NH} \frac{S_O}{K_{ONH} + S_O} \frac{S_{NH}}{K_{NHNH} + S_{NH}} \frac{S_{PO}}{K_{PO} + S_{PO}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_{AUT}$
10	Lysis of Autotrophs, X_{AUT}	$b_{NH} X_{AUT}$
11	Lysis of Heterotrophs, X_H	$b_H X_H$
12	Storage of X_{PHA}	$q_{PHA} \frac{S_A}{K_A + S_A} \frac{X_{PP}/X_{PAO}}{K_{PP} + X_{PP}/X_{PAO}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_{PAO}$
13	Aerobic Storage of X_{PP}	$q_{PP} \frac{S_{PO}}{K_{PS} + S_{PO}} \frac{S_O}{K_O + S_O} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \frac{K_{max} - X_{PP}/X_{PAO}}{K_{IPP} + K_{max} - X_{PP}/X_{PAO}} X_{PAO}$
14	Anoxic Storage of X_{PP}	$\eta_{NO_3PAO} q_{PP} \frac{S_{PO}}{K_{PS} + S_{PO}} \frac{K_O}{K_O + S_O} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} \frac{K_{max} - X_{PP}/X_{PAO}}{K_{IPP} + K_{max} - X_{PP}/X_{PAO}} X_{PAO}$
15	Aerobic growth of X_{PAOs}	$\mu_{PAO} \frac{S_O}{K_O + S_O} \frac{S_{PO}}{K_P + S_{PO}} \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} X_{PAO}$
16	Anoxic growth of X_{PAOs}	$\eta_{NO_3} \mu_{PAO} \frac{K_O}{K_O + S_O} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_{PO}}{K_P + S_{PO}} \frac{S_{NH}}{K_{NH} + S_{NH}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{X_{PHA}/X_{PAO}}{K_{PHA} + X_{PHA}/X_{PAO}} X_{PAO}$
17	Lysis of X_{PAO}	$b_{PAO} X_{PAO} \frac{S_{ALK}}{K_{ALK} + S_{ALK}}$
18	Lysis of X_{PHA}	$b_{PHA} X_{PHA} \frac{S_{ALK}}{K_{ALK} + S_{ALK}}$
19	Lysis of X_{PP}	$b_{PP} X_{PP} \frac{S_{ALK}}{K_{ALK} + S_{ALK}}$

ANNEX B

Annex B1:

Table B.1. Plant performance and average influent wastewater characteristics

Influent wastewater Characteristics	Unit	Measurement
COD _{total}	mgCOD/l	590
COD _{filter}	mgCOD/l	234
TKN	mgN/l	66
TKN _{sol}	mgN/l	6
NH ₄ -N	mgN/l	48
PO ₄ -P	mgP/l	7.3
TP	mgP/l	12
TSS	mgSS/l	395
Flowrates		
Average Flowrate, Q _{av} (Dry weather)	m ³ /day	6310
Q _{peak} /Q _{av}	-	1.6
Q _{peak} /Q _{min}	-	5.0
Plant Load		
COD _{total}	kgCOD/day	3723
TKN load	kgN/day	417
TP load	kgP/day	76
COD/TKN	-	8.9
COD/TP	-	49
Effluent wastewater characteristics (yearly average basis)		
COD _{total}	mgCOD/l	33 (30 [*])
NO ₃ -N	mgN/l	5.5 (5.4 [*])
NH ₄ -N	mgN/l	0.6 (0.6 [*])
TP	mgP/l	1.3 (1.4 [*])
TKN	mgN/l	2.6
TSS	mgSS/l	5
Plant operation		
SRT	day	~22
HRT	day	1.8
Q _{internal} /Q	-	219
V _{sel} /V _{total} (reac)	-	0.12
MLSS(carrousel)	mgSS/l	4700-5000
Sludge Blanket Height (Settler)	m	No blanket

* Flux based steady state simulation

Annex B2

Mass balance to check/verify the SRT of the Haaren WWTP

The mass balance of total-P over the system was calculated in order to determine the exact sludge age of the system. First the average wastage flow-rate, Q_{was} , is calculated using the TP balance as follows:

$$Q_{in,ave} \cdot TP_{in,ave} = Q_{out,ave} \cdot TP_{out,ave} + Q_{was,ave} \cdot TP_{was}$$

$$Q_{was,ave} = (6310 \cdot 12 - 6030 \cdot 1.3) / 230 = 295 \text{ m}^3/\text{d}$$

The estimated $Q_{was,ave}$ (295 m³/d) using the TP balance was higher than the reported $Q_{was,ave}$ (280 m³/d). Therefore, the SRT of the system is calculated using the corrected sludge wastage rate:

$$SRT = \frac{MLSS_{ave} \cdot V_{total}}{Q_{was,ave} \cdot MLSS_{was,ave} + Q_{eff,ave} \cdot TSS_{eff,ave}}$$

$$SRT = \frac{4.6 \cdot 14,000}{295 \cdot 8.1 + 6030 \cdot 0.005} = 21.67 \text{ days}$$

The calculated SRT of the Haaren WWTP based on the corrected wastage flowrate is found to be 21.67 days which is quite close to the reported SRT of the Haaren WWTP which is 22 days. The 1.5% error in the calculated SRT is acceptable for a good quality of calibration studies (Meijer *et al.*, 2001).

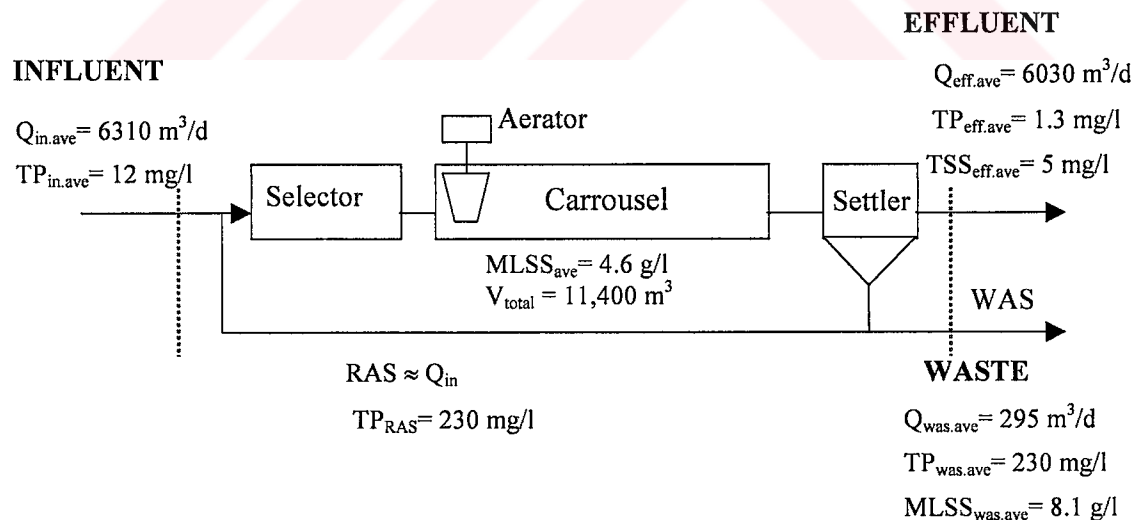


Figure B1. TP mass balance over the system

Evaluation of data quality: Flow balance

The raw flow data obtained from the SCADA system of the Haaren WWTP were analysed prior to use in the dynamic simulations. The raw data from the on-line flow sensors are stored at high frequency, which is 1 data per minute. The flow data set presented in Figure B2 is for the 8 days window that starts on 16/06/2003 as day zero and continues until 23/06/2003. The raw flow data is clearly observed to contain high frequency noise, which is usually the case with on-line sensors in WWTPs (a similar observation is made for the raw effluent flowrate data too, results not shown). This high frequency noise was filtered prior to use in dynamic simulations.

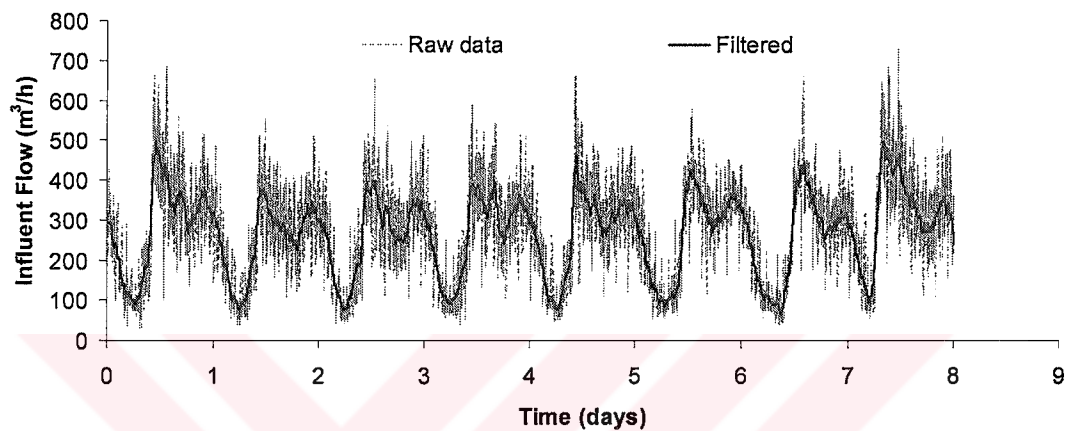


Figure B.2. The influent flowrate data; the dashed line represents raw data and the bold line represents the filtered data (Savitzky-Golay with polynomial order 1 and window size 51).

To check the quality of the flow data, a flow balance was performed around the system boundaries shown in Figure B1, both using raw measurements and filtered measurements as follows:

$$\text{Balance} = Q_{\text{in}} - (Q_{\text{eff}} + Q_{\text{was}})$$

Table B.1.bis. Evaluation of flow data quality

Raw data balance (percentage error)		Filtered data balance (percentage error)	
Average	Standard deviation	Average	Standard deviation
-5.667	38.128	1.4257	8.092

The results of the flow balance are plotted in Figure B2. The percentage error of the flow balance is calculated as follows:

$$\text{Flow balance error} = (\text{Balance}/Q_{\text{in}}) * 100$$

The average and standard deviations for the flow balance errors were calculated for raw and filtered flow measurements and given in Table B1bis. The results show that the flow balance had an average error of 5.7% with 38% of standard deviation.

Filtering the raw flow data aided to bring the error on the flow balance down to 1.5% with 8% of standard deviation (see Table B1bis). In Figure B3, the flow balance errors are also plotted for both raw and filtered data which clearly indicates the improvement to the quality of the flow data. Figure B3 indicates that the error on the flow balance was mainly caused by the high frequency noise contained in the raw flow data. This could be considerably decreased after filtering. The filtered and quality-improved flow data are shown in Figure B4.

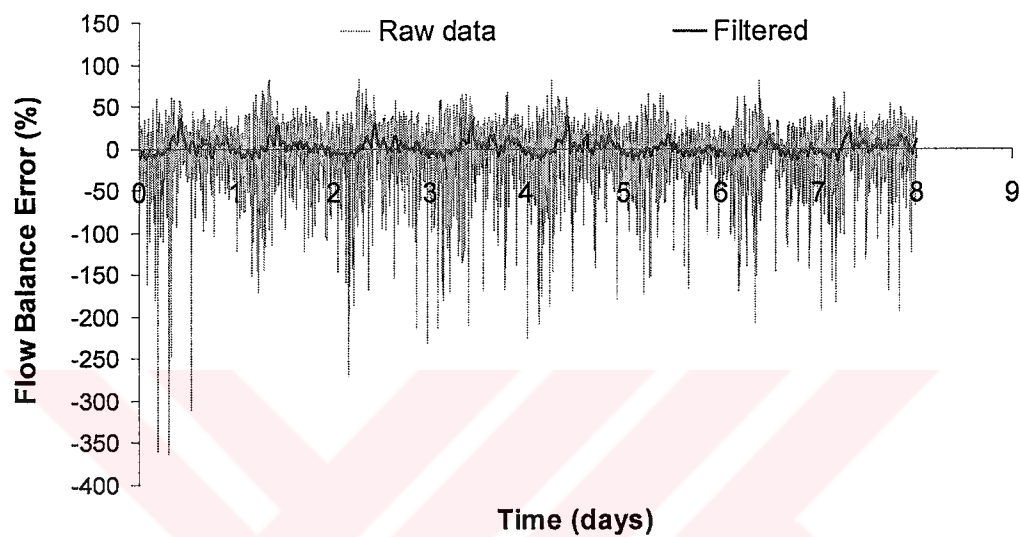


Figure B.3. Flow balance errors calculated for raw flow and filtered data

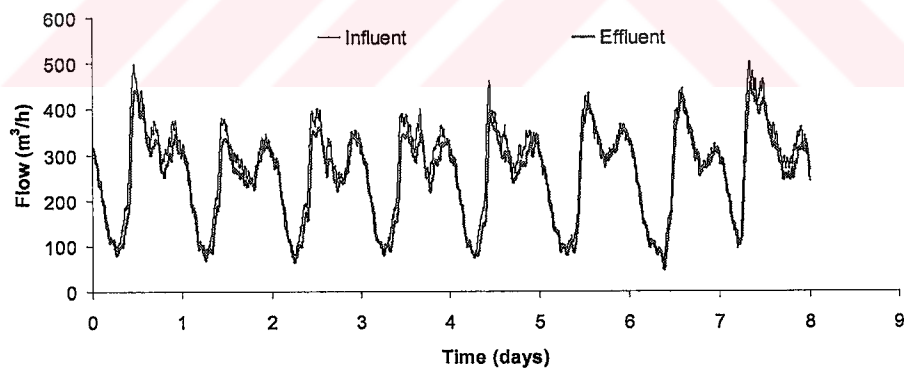


Figure B.4. Filtered (balanced) influent and effluent flow rates. Note that the corrected sludge wastage rate is 12.2 m³/h (or similarly 295 m³/day)

Annex B3.

Table B.2. The experimental results of the b_H experiment

Date	Time	OUR	OUR	ln(OUR)
(day)	(day)	(mgO ₂ /l-h)	(mgO ₂ /l-d)	
8-May-03	0.0			
13-May-03	5.5	7.5	180	5.19
14-May-03	6.6	5.7	136.8	4.92
15-May-03	7.6	4.6	110.4	4.70
16-May-03	8.4	3.7	88.8	4.49
17-May-03	9.4	3.1	74.4	4.31
18-May-03	10.5	2.5	60	4.09
19-May-03	11.6	2.1	50.4	3.92
20-May-03	12.6	1.7	40.8	3.71
21-May-03	13.6	1.4	33.6	3.51
22-May-03	14.6	1.3	31.2	3.44

Note: pH is 7.1, Temperature is around 19 °C and ATU is added to the batch reactor at around 30 mg/l.

CURRICULUM VITAE



H. Güçlü Insel was born in İstanbul, Turkey on July 12th, 1974. He completed primary and secondary school at Şişli Terakki Lisesi, Nişantaşı. In 1995, he graduated as an Environmental Engineer from Environmental Engineering Department of İstanbul Technical University (İ.T.Ü). He received his Master of Science degree from the same department in 1997. He started his Ph.D. study in 1998. He was involved in many projects about modeling and optimization of activated sludge process, industrial wastewater treatment and reuse. From 2001 until 2003, he worked as a researcher at Applied Mathematics, Biometric and Process Control Department, Gent University. He has been working as a research assistant since 1998 at İ.T.Ü. Environmental Engineering Department. His research fields are biological nutrient removal, modeling and optimization of activated sludge plants, biological treatment of industrial wastewaters and optimal experimental design.

PUBLICATION LIST

- Insel, G., Artan N. and Orhon, D., 2005. Effect of aeration on nutrient removal performance of oxidation ditch systems, *Env. Eng. Sci.* (accepted).
- Özgür Yagci, N., Insel G., Tasli, R., Artan, N., Randall, C.W. and Orhon D., 2005. A new interpretation of ASM2d for modeling of SBR performance for enhanced biological phosphorus removal, *Biotech. Bioeng.* (accepted).
- Insel, G., Artan, N. and Orhon, D., 2004. Effect of Aeration on the performance of small sequencing batch reactors for organic carbon and nitrogen removal. *6th Specialist Conference on Small Water and Wastewater Systems*, 11-14 February, Perth, Australia.
- Insel, G., Sin, G., Lee, D.S. and Vanrolleghem, P.A., 2004. A calibration methodology and model-based system analysis for nutrient removing SBRs, *3rd IWA International conference on SBR*, Queensland, Australia.
- Özgür Yagci, N., Insel, G., Artan, N., and Orhon, D., 2004. Modeling and Calibration of Phosphate and Glycogen Accumulating Organism Competition for Acetate Uptake in Sequencing Batch Reactor, *Wat. Sci. Tech.*, **50(6)**, 241-250.
- Orhon, D., Kabdasli, I., Babuna, F.G., Sözen, S., Dulkadiroğlu, H., Doğruel, S., Gül, Ö.K. and Insel, G., 2003. Wastewater reuse for the minimization of fresh water demand in coastal areas - Selected cases from the textile finishing industry, *J Env. Sci. and Health Part A-Toxic/Hazardous Substances & Environmental Engineering*, **38(8)**, 1641-1657.
- Murat, S., Insel, G., Artan, N. and Orhon, D., 2004. Effect of temperature on the nitrogen removal performance of a sequencing batch reactor treating tannery wastewater, *Wat. Sci. Tech.*, **48(11-12)**, 319-326.

- De Pauw, D.J.W., Sin, G., Insel, G., Van Hulle, S., Vandenberghe, V. and Vanrolleghem, P.A., 2004. Discussion of 'Assessing Parameter Identifiability of Activated Sludge Model No. 1' by Pedro Afonso and Maria da Conceicao Cunha. *J. Environ. Eng.*, 128, 748-754. *J. Environ. Eng.-ASCE* 130(1), 110-112.
- Insel, G., Russell, D., Beck, B. and Vanrolleghem, P.A., 2003. Evaluation of Nutrient Removal Performance for an Orbal® Plant Using The ASM2d Model, *WEFTEC 2003: 76th Annual Technical Exhibition and Conference*, October 11-15, 2003, Los Angeles, California U.S.A.
- Vanrolleghem, P.A., Insel, G., Petersen, B., Sin, G., De Pauw, D., Nopens, I., Dovermann, H., Weijers, S. and Gernaey, K., 2003. A comprehensive model calibration procedure for activated sludge models. *WEFTEC 2003: 76th Annual Technical Exhibition and Conference*, October 11-15, 2003, Los Angeles, California U.S.A.
- Insel, G., Orhon, D., and Vanrolleghem, P.A., 2003. Identification and modelling of aerobic hydrolysis mechanism-application of optimal experimental design, *J. Chem.Tech. Biotech.*, 78(4), 437-445.
- Dogrue, S., Germirli-Babuna, F., Kabdasli, I., Insel, G. and Orhon, D. 2003. Effect of stream segregation on ozonation for the removal of significant COD fractions from textile wastewater, *J. Chem.Tech. Biotech.*, 78(1), 6-14
- Insel, G., Gül, Ö.K., Orhon, D., Vanrolleghem, P.A. and Henze, M., 2002. Important limitations in the modeling of activated sludge: biased calibration of the hydrolysis process, *Wat. Sci. Tech.*, 45(12), 23-36.
- Orhon, D., Okutman, D. and Insel, G., 2002. Characterization and biodegradation of settleable organic matter for domestic wastewater, *Water SA*, 28(3), 299-305.
- Koch, M., Yediler, A., Lienert, D., Insel, G. and Kettrup, A., 2002. Ozonation of hydrolyzed azo dye reactive yellow 84 (CI), *Chemosphere*, 46(1), 109-113.
- Orhon, D., Okutman, D. and Insel, G., 2001. Characterization and biodegradation of settleable Organic matter for domestic wastewater, *Water SA*, 28(3), 299-306.
- Orhon, D., Germirli Babuna, F. and Insel, G., 2001. Characterization and modelling of denim processing wastewaters for activated sludge, *J.Chem Tech. Biotech.*, (9), 919-931.
- Insel, G., Sözen, S., Görgün, E., Orhon, D. and Hanhan, O., 2001. Evaluation of nitrogen removal efficiencies for pre-denitrification and alternating system, *Fresen. Env. Bull.*, 10 (3) 257-261.
- Orhon, D., Sözen, S., Kabdaşlı, I., Germirli Babuna, F., Karahan-Gül, Ö., Insel, G., Dulkadiroğlu, H., Doğrue, S., Baban, A. and Kemerdere Kaya, N. 2000. Recovery and reuse in Textile Industry- A case study in wool and blends finishing mill, Chemical Water and Wastewater Treatment VI, İstanbul Gothenburg Conference, 02-04 October 2000, 305-314.
- Orhon, D., Germirli Babuna, F., Kabdaşlı, I., Insel, G., Karahan, Ö., Dulkadiroğlu, H., Doğrue, S., Sevimli F. and Yediler, A., 1999. A scientific approach to wastewater recovery and reuse in the textile industry, *Wat. Sci. Tech.*, 43(11), 223-232.
- Karahan Ö., Insel G., Dulkadiroglu D., Kabdasli I., Yediler A. Orhon D. and Kettrup A., 2000. Industrial wastewater management for recycle and reuse-A case study for the textile Industry, *Fresen. Env. Bull.*, 9(5-6), 314-321.
- Germirli Babuna, F., Orhon, D., Ubay Çokgör, E., Insel, G. and Yapraklı, B., 1998. Modelling of activated sludge for textile wastewaters, *Wat. Sci. Tech.*, 38(4-5), 9-17.