UNIVERSITEIT
GENT

BIOMATH
Department of Applied Mathematics,
Biometrics and Process Control

IWA RIVER WATER QUALITY MODELLING (RWQM1) TASK GROUP

L. Somlyódy, D. Borchardt, M. Henze, L. Koncsos,
W. Rauch, P. Reichert, P. Shanahan, P. Vanrolleghem

Peter Vanrolleghem
October 26 2001

Water & Wastewater Management for Developing Countries
Kuala Lumpur, Malaysia

RUG-Biomath, Coupure 653, 9000 Gent, Belgium (e-mail Peter.Vanrolleghem@rug.ac.be)

Past Developments

- From Streeter-Phelps to QUAL2E
  (steady flow and point sources):
  A natural evolution
- IAWQ ASM Family:
  A systematic development
  COD, fractionation and matrix notation

Shortcomings in RWQM Formulations

- Lack of closed mass balances
  BOD & sediment
- Lack of sediment related processes
  attached bacteria/algae and benthic flux terms
- Inconsistency between RWQM and ASM:
  Lack of integrating WWT and river water quality

Shortcomings in RWQM Formulations

- Sewer overflow problems
- Spatial non-uniformities
  and rapid temporal changes
- Issues of calibration
- Predictive capability ?

Objectives of the RWQM Task Group

- Scientific and technical base
- "Standardized" RWQM:
  conversion model versions
- Guidelines for model selection
- Case studies
- STR: 2001

Objectives of the RWQM Task Group

- Open ended process
- Software platform
- Involvement of others
- What is not our objective?

Outputs and Events

- Vancouver (1998), Brainstorm session
  3 WS&T Papers, 1998 - Vol. 38(11)
  State-, Problems- and Future-of-the-art
- Paris (2000), Workshop
  5 WS&T Papers, 2000 - Vol. 43(5)
  Approach; Biochemical process equations;
  Submodel selection; Case study I and II
- Gent (2000), WS&T Paper, 2001 - Vol. 43(7)
  Identifiability and Uncertainty Analysis
- Scientific and Technical Report, 2001

UNIVERSITEIT GENT

BIOMATH
Department of Applied Mathematics, Biometrics and Process Control

River Water Quality Modelling : State-of-the-art

Peter Vanrolleghem
October 26 2001

Water & Wastewater Management for Developing Countries
Kuala Lumpur, Malaysia

RUG-Biomath, Coupure 653, 9000 Gent, Belgium (e-mail Peter.Vanrolleghem@rug.ac.be)

Overview

- Hydrodynamics
  - de Saint-Venant
  - Simplifications
- Transport
  - Advection-Dispersion
  - Box-model
- Conversion
  - Streeter-Phelps
  - Qual2E

Hydrodynamics

- de Saint-Venant equations
  - cross-sectionally integrated (1-dimensional -> length)
  - momentum:

$$\frac{\partial Q}{\partial t}+\frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right)+gA\frac{\partial y}{\partial x}+gA(S_f-S_0)=0$$

  - mass balance

$$\frac{\partial A}{\partial t}+\frac{\partial Q}{\partial x}=q$$

q = lateral inflow per unit length [L^2T^{-1}]; Q = streamflow [L^3T^{-1}];
x = longitudinal coordinate [L]; A = cross section [L^2];
y = channel depth [L]; S_0 = bottom slope [-];
g = gravity acceleration [LT^{-2}]. S_f = friction slope [-];

Hydrodynamics: Simplifications

- Dynamic wave -> full de Saint-Venant
- Diffusive wave -> neglects acceleration term
- Kinematic wave -> neglects pressure gradient term
  cannot handle backwater effects
- Hydrologic models -> replace momentum equation with empirical relationship:

$$\frac{\partial V}{\partial t}=Q_i-Q_e \qquad Q_e=\frac{V}{K} \qquad Q_e=\alpha\left(V/A-\beta\right)^{\gamma}$$

also termed "box models"

Transport equation

Change in concentration over time (3-dimensional)

$$\frac{\partial c}{\partial t}=-u\frac{\partial c}{\partial x}-v\frac{\partial c}{\partial y}-w\frac{\partial c}{\partial z}+\frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial c}{\partial z}\right)+\mathbf{r}(\mathbf{c},\mathbf{p})$$

Advection Dispersion Reaction

Integration over depth/width --> 1-dimensional

$$\frac{\partial(AC)}{\partial t}+\frac{\partial(QC)}{\partial x}=\frac{\partial}{\partial x}\left(AD_L\frac{\partial C}{\partial x}\right)+A\mathbf{R}(\mathbf{C},\mathbf{P})$$

Hydrologic "box" model --> 0-dimensional

$$\frac{d(VC^*)}{dt}=Q_iC_i-QC^*+V\mathbf{R}^*(\mathbf{C}^*,\mathbf{P}^*)$$

Conversion: Streeter-Phelps model

- Pioneering work (1925)
- Two state variables :
  - Dissolved Oxygen (DO)
  - Organic matter (BOD)
- Mass balances :

$$\frac{dDO}{dt} = K_2.(DO_{sat} - DO) - K_1.BOD$$

$$\frac{dBOD}{dt} = -K_1.BOD$$

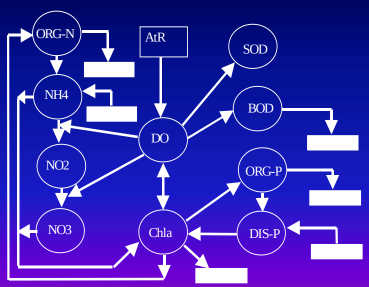
Conversion: Qual2E

- US Environmental Protection Agency (1987)
- Legislation driven
- Descendent from Streeter-Phelps (via Qual1, Qual2)
- Adds N- and P-cycling

- Steady state model
- No closed mass balances guaranteed
  sediment, BOD state variable

Conversion: Qual2E

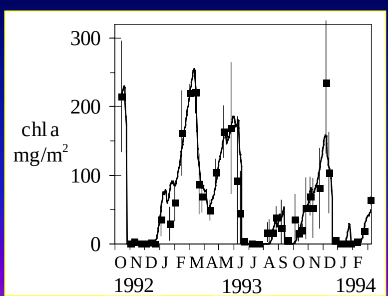
- C-, N- and P-cycles :



Software

	PROGRAM	1	2	3	4	5	6	7	8	9	10
Hydrodynamics	Extern. Input	Y	Y	N	N	Y	N	N	N	N	Y
	Simulated	N	Y	Y	Y	Y	Y	Y	Y	Y	Y
	Control structure	N	N	Y	Y	Y	Y	Y	Y	Y	Y
Transport	Advection	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
	Dispersion	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
Sediment	Quality models	N	Y	Y	N	Y	Y	N	N	open	Y
Water quality	Temperature	Y	N	Y	Y	Y	Y	Y			N
	Bacteria	N	N	Y	Y	Y	Y	Y			N
	DO-BOD	Y	Y	Y	Y	Y	Y	Y			Y
	Nitrogen	Y	Y	Y	Y	Y	Y	Y	open structure	open structure	Y
	Phosphorus	Y	Y	Y	Y	Y	Y	Y			Y
	Silicon	N	N	Y	N	Y	Y	Y			N
	Phytoplankton	Y	Y	3	Y	Y	Y	Y			Y
	Zooplankton	N	N	Y	N	Y	Y	N			N
	Benthic algae	N	N	N	N	Y	Y	Y			N
Systems analysis	Parameter estimation	N								Y	Y
	Sensitivity/uncertainty analysis	Y								Y	Y

Advanced application: Prediction of sessile algal growth
(Uehlinger et al., 1996)



UNIVERSITEIT GENT

BIOMATH
Department of Applied Mathematics, Biometrics and Process Control

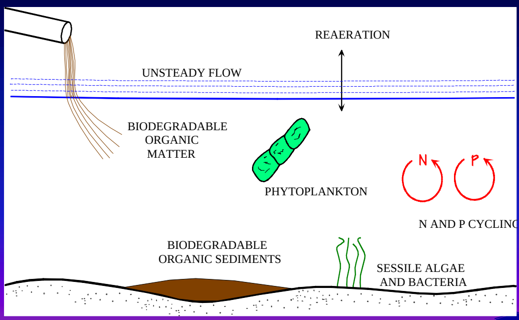
River Water Quality Model No. 1 : Modelling framework

Peter Vanrolleghem
October 26 2001

Water & Wastewater Management for Developing Countries
Kuala Lumpur, Malaysia

RUG-Biomath, Coupure 653, 9000 Gent, Belgium (e-mail Peter.Vanrolleghem@rug.ac.be)

Modelling Context
River Water Quality



Mass Balance Equation

Change in concentration over time

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z} + \frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial c}{\partial z}\right) + \mathbf{r}(\mathbf{c},\mathbf{p})$$

Advection Dispersion Reaction

Mass Balance Equation

Advective-dispersion equation

or

Defective-confusion equation

????

Model Decision Procedure

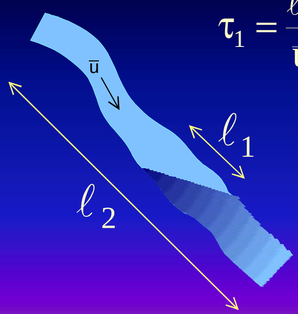
- Define temporal representation
- Determine spatial dimensions
- Determine representation of mixing
- Determine representation of advection
- Determine reaction terms
- Determine boundary conditions

Step 1. Define temporal representation

- Define upper- and lower-bound time constants
- Define water-column and sediment process time constants

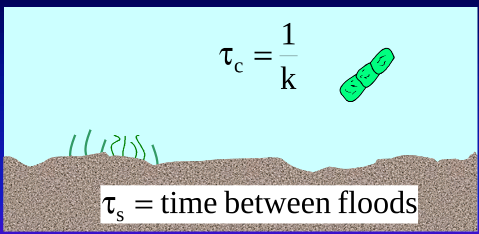
Upper- and lower-bound time constants

$$\tau_1 = \frac{\ell_1}{\bar{u}}$$



$$\tau_2 = \frac{\ell_2}{\bar{u}}$$

Water-column and sediment process time constants



Usually: $t_s > t_c$

P. Vanrolleghem - 12-01 - 25 BIOMATH

Step 1. Define Temporal Representation – Water-Column Reactions

$t_c << t_1 \rightarrow$ steady-state model	$t_1 < t_c < t_2 \rightarrow$ dynamic model	$t_c >> t_2 \rightarrow$ reactions negligible

$\longleftarrow \tau_1 \longrightarrow \tau_2 \longrightarrow$

P. Vanrolleghem - 12-01 - 26 BIOMATH

Step 1. Define Temporal Representation – Sediment Processes

- $\tau_c >> \tau_s \rightarrow$ fast sediment processes negligible
- $\tau_c > \tau_s > \tau_1 \rightarrow$ dynamic sediment model
- $\tau_s >> \tau_c \rightarrow$ time-invariant sediment process (typical case)

P. Vanrolleghem - 12-01 - 27 BIOMATH

Step 2. Determine spatial dimensions

- Define lateral and vertical length scales:
  - Lateral: $\ell_\ell = \frac{W^2}{2K_y}\bar{u}$
  - Vertical: $\ell_v = \frac{h^2}{2K_z}\bar{u}$

P. Vanrolleghem - 12-01 - 28 BIOMATH

Step 2. Determine spatial dimensions

$l_1 << l_v \rightarrow$ 3-D model	$l_v < l_1 < l_l \rightarrow$ 2-D model	$l_1 >> l_l \rightarrow$ 1-D model

$\longleftarrow \ell_v \longrightarrow \ell_\ell \longrightarrow$

P. Vanrolleghem - 12-01 - 29 BIOMATH

Step 3. Define mixing representation

- Dispersion may be neglected if:
  - Mixing is much faster than reactions

$$\tau_c >> \frac{2K_x}{\bar{u}^2}$$

  - Mixing is much faster than variations due to external sources and boundary conditions

$$\tau_e >> \sqrt{\frac{2K_x \ell^2}{\bar{u}^3}}$$

P. Vanrolleghem - 12-01 - 30 BIOMATH

Step 4. Define water column advection

t_{flow} = time constant for flow variation

$t_1 < t_{flow} < t_2$
→ hydrodynamic model

τ_1 τ_2

Step 4. Define sediment advection

t_s = time constant for sedimentation $\tau_s = \frac{h}{w_s}$

$t_s << t_1$ → suspended sediment negligible

$t_1 < t_s < t_2$ → sediment and settling model

$t_2 << t_s$ → settling negligible

τ_1 τ_2

Step 4. Define reaction terms

- See: Vanrolleghem et al. (2001)
  River Water Quality Model No. 1:
  III. Biochemical Submodel Selection

This will be presented separately

Step 6. Define Boundary Conditions

- Possible BC's:
  - O_2 flux at surface and bottom
  - COD flux at bottom
  - Water inflow or outflow due to seepage
  - Pollutant loads
- Treatment of BC's
  depends on model dimensionality

BC example: DO reaeration

- In 3-D model:
  reaeration is flux b.c. at surface

$$\varepsilon_z \left.\frac{\partial c}{\partial z}\right|_{z=z_o} = K_L (c_s - c)$$

- In 1-D model:
  reaeration is source term with rate constant

$$r_{reaeration} = K_a (c_s - c)$$

Summary: Model Decision Procedure

- Define temporal representation
- Determine spatial dimensions
- Determine representation of mixing
- Determine representation of advection
- Determine reaction terms
- Determine boundary conditions

UNIVERSITEIT GENT

BIOMATH
Department of Applied Mathematics, Biometrics and Process Control

River Water Quality Model No.1 : Conversion Process Modelling

Peter Vanrolleghem
October 26 2001

Water & Wastewater Management for Developing Countries
Kuala Lumpur, Malaysia

RUG-Biomath, Coupure 653, 9000 Gent, Belgium (e-mail Peter.Vanrolleghem@rug.ac.be)

Water Quality: Determinands

- Organic pollution
  - BOD_5, BOD_7, BOD_∞
  - COD_{tot}, COD_s
  - TOC
  - SS, TSS, Settleables
- Nitrogen pollution
  - NH_4-N, NO_2-N, NO_3-N
  - TKN, TN
- Phosphorous pollution
  - o-PO_4
  - TP
- Heavy metals:
  - Hg, Ag,
  - Cd, Zn,
  - Cu, Ni,
  - Pb, As,
  - Cr
- Pathogenic organisms
  - Coliform bacteria
- Specific pollutants
  - LAS detergent (1% !)
  - Phenols

Water Quality Determinands: BOD

BOD = Biochemical Oxygen Demand

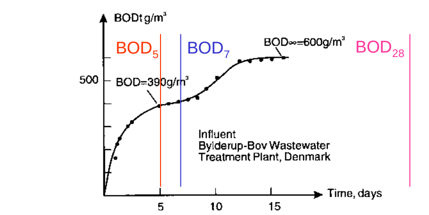


Fig 2.7 *The BODt-curve for mixed municipal and slaughterhouse wastewaters.*

Pollution + few organisms => growth + O_2 consumption

Water Quality Determinands: COD

COD = Chemical oxygen demand

- Chemical oxidation to CO_2, H_2O, NH_4, SO_4 at high temperature, very acid
- Amount of oxygen consumed = COD

e.g. 60 g Acetic acid = 64 g COD
1 $CH_3COOH + 2\ O_2 \text{-->} 2\ CO_2 + 2\ H_2O$

exercise: Ethanol = CH_3CH_2OH Methane = CH_4
Sewage = $C_{18}H_{19}O_9N$ Sulphide = H_2S
Biomass = $C_5H_7O_2N$
??? How much COD per g organic matter ???

Water Quality Determinands: TOC

TOC = Total Organic Carbon

- Oxidation to CO_2 at high temperature / catalytic
- Amount of produced CO_2 x 12/44 = TOC

e.g. 60 g Acetic acid = 24 g TOC
1 $CH_3COOH + 2\ O_2 \text{-->} 2\ CO_2 + 2\ H_2O$

Water Quality Determinands: SS

TSS = Total Suspended Solids

- Dry solids of sample after drying at 105 C = TSS

SS = Suspended Solids

- Dry solids measured after filtering of sample = SS

Settleable Solids

- Dry solids measured after 2 h settling of sample

Biological growth

- Growth = multiplication of organisms
- Requirements for growth:
  - nutrients (biomass = $C_5H_7O_2N$, + P, S, ...)
  - favorable environmental conditions (pH, temperature)
- Basic reaction :

  C-source + NH_4 + PO_4 + H^+ ==> Biomass
  + electron acceptor (O_2, NO_3) + byproducts
  + electron donor (C-source) (H_2O, CO_2, N_2, NO_3)

Biological conversion

- Because biomass grows (or at least wants to), a number of compounds are converted, e.g.
  - Organic pollutants --> CO_2 + new biomass
  - NH_4 --> NO_3
  - NO_3 --> N_2
  - Organic pollutants --> biogas (CH_4 + CO_2)
- How much is converted ?
  - Rate of the conversion reaction ==> KINETICS
  - Ratio of conversions of the different compounds ==> STOICHIOMETRY

Conversion stoichiometry

Suppose following conversion takes place:

$C_{18}H_{19}O_9N + O_2 + H^+ \rightarrow C_5H_7O_2N + CO_2 + H_2O$

for each "molecule" of pollutants degraded, a proportional amount of other products will be used (left of arrow) or produced (right of arrow)

We can therefore write:

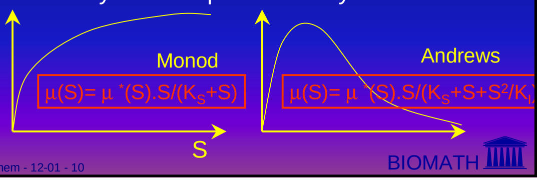
$a\ C_{18}H_{19}O_9N + b\ O_2 + c\ H^+ \rightarrow d\ C_5H_7O_2N + e\ CO_2 + f\ H_2O$

a,b,c,d,e,f are called yield or stoichiometric coefficients

note that one of the coefficients can be chosen = 1

Process kinetics

- A conversion will not occur (reaction rate = 0) when its sources (substrates) are absent
  ↳ compounds on the left of the reaction arrow
- A conversion will have a maximum rate
  - when all sources are in excess
  - inhibition by sources/products may affect max. rate



Conversion rates

Take the conversion above

$a\ C_{18}H_{19}O_9N + b\ O_2 + c\ H^+ \rightarrow 1\ C_5H_7O_2N + d\ CO_2 + e\ H_2O$

Suppose conversion kinetics: $\mu(S)=\mu^*(S).X.S/(K_S+S)$
- Monod kinetics in the substrate
- first order in the biomass concentration

The conversion of each component is then:

$C_{18}H_{19}O_9N$	: - a. $\mu(S)$	$C_5H_7O_2N$	: + 1. $\mu(S)$
O_2	: - b. $\mu(S)$	CO_2	: + d. $\mu(S)$
H^+	: - c. $\mu(S)$	H_2O	: + e. $\mu(S)$

Conversion rates (cont'd)

- Conversion rate of a compound consists of 3 parts:
  - sign (+/-) dependent on whether it is used or produced
  - stoichiometric coefficient in the conversion
  - rate of the conversion
- What if parallel conversions with same compounds ?

  $a\ C_{18}H_{19}O_9N + b\ O_2 + c\ H^+ \rightarrow 1\ C_5H_7O_2N + d\ CO_2 + e\ H_2O$
  $f\ CO_2 + g\ O_2 + h\ NH_4^+ \rightarrow 1\ C_5H_7O_2N + i\ NO_3 + j\ H_2O + k H^+$
- ==> $C_5H_7O_2N$, O_2, CO_2, H^+, H_2O occur more than once

$C_5H_7O_2N$	: + 1. μ_1 + 1. μ_2	O_2	: - b. μ_1 - g. μ_2
CO_2	: + d. μ_1 - f. μ_2	H^+	: - c. μ_1 + k. μ_2

General conversion model

- For the i-th compound, S_i:

$$r(S_i) = \Sigma_j \text{ sign}(ji)\ v_{ji}.\rho_j$$

where

ρ_j = the rate of the j-th reaction in which S_i participates
v_{ji} = the stoichiometric coefficient for S_i in the j-th reaction
sign(ji) = sign (+/-) indicating whether S_i is substrate or product in the j-th reaction

Temperature effect on conversion rate

$\mu(T)= \mu(20).e^{k(T-20)}$

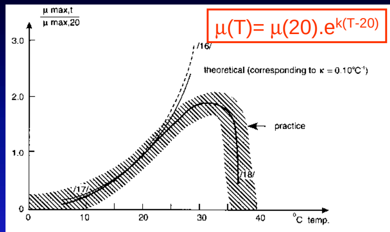
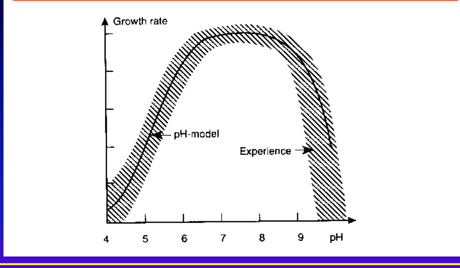


Fig 3.7 *Nitrification as a function of temperature. As opposed to the other biological processes in wastewater treatment, thermophilic nitrifying bacteria are unknown.*

Rule of thumb: Doubling of reaction rate for temperature increase with 10ºC

pH effect on conversion rates

$\mu(pH)= \mu(pH_{opt}).K_{pH}/(K_{pH} -1+10^{| pH-pHopt |})$



Process is changing the system pH by production of H^+ (e.g. nitrification, digestion) or OH^- (denitrification)

Conversion Processes (1)

- Aerobic organic substrate removal
  - in the presence of O_2 (aerobic)
  - heterotrophic organisms (i.e. C-source is organic)
  - $C_{18}H_{19}O_9N + O_2$ (+ H^+) + NH_4 --> $C_5H_7O_2N + CO_2 + H_2O$
  - high yield (1 g substrate-COD --> 0.4 g biomass-COD)

Conversion Processes (2)

- Nitrification
  - in the presence of O_2 (aerobic)
  - autotrophic organisms (i.e. C-source is inorganic: CO_2)
  - $NH_4 + CO_2 + O_2$ + --> $C_5H_7O_2N + NO_3 + H_2O + H^+$
  - low yield (0.24 g COD/g N oxidised)
  - slow growth rate
  - highly sensitive to lots of disturbances (pH, T, inhibitors)
  - in fact: two-step process (NH_4 -> NO_2 -> NO_3)

Conversion Processes (3)

- Denitrification
  - in the absence of O_2 (anoxic)
  - in the presence of NO_3 and COD
  - heterotrophic organisms
  - $C_{18}H_{19}O_9N + NO_3 + H^+ + NH_4$ --> $C_5H_7O_2N + CO_2 + H_2O + N_2$
  - relatively high yield (0.3 g biomass-COD/g COD)
  - performs both nitrogen and COD removal !
  - recuperates O_2 invested in nitrification !

Peterson (1965) matrix notation

Components, Processes, Stoichiometry & Kinetics:

Continuity →
Mass Balance ↓

Component → / i j Process ↓	1 X_B	2 S_S	3 S_O	Process Rate, ρ_j $[ML^{-3}T^{-1}]$
1 Growth	1	$-\frac{1}{Y}$	$-\frac{1-Y}{Y}$	$\frac{\hat{\mu} S_S}{K_S + S_S} X_B$
2 Decay	−1		−1	bX_B
Observed Conversion Rates $ML^{-3}T^{-1}$	$r_i = \sum_j r_{ij} = \sum_j \nu_{ij}\rho_j$			Kinetic Parameters: Maximum specific growth rate: $\hat{\mu}$ Half-velocity constant: K_S Specific decay rate: b
Stoichiometric Parameters: True growth yield: Y	Biomass [M(COD) L^{-3}]	Substrate [M(COD) L^{-3}]	Oxygen (negative COD) [M(−COD) L^{-3}]	

Mass balancing

- Vertical summation of

  Stoichiometry term * Kinetics

  terms gives total conversion

$$r(S_i) = \Sigma_j \; \text{sign}(ji) \; v_{ji}.\rho_j$$

Add the transport terms ==> the mass balance !

Continuity check

- Horizontal summation of the product of stoichiometric coefficients and composition (I_{ci}) should equal 0 !

$$\Sigma_i \; v_{ji}.i_{ci} = 0$$

Provided:
- consistent units have been used
- all substrates/products are included

This can be done for COD, N, P, Charge, Mass

--> Example: ASM3 !

j ∨	Process (Component i > / expressed as >)	1 S_O O_2	2 S_I COD	3 S_S COD	4 S_{NH} N	5 S_{N2} N	6 S_{NO} N	7 S_{HCO} Mole	8 X_I COD	9 X_S COD	10 X_H COD	11 X_{STO} COD	12 X_A COD	13 X_{TS} TSS
1	Hydrolysis		f_{SI}	$1-f_{SI}$	y_1			z_1		-1				$-i_{XS}$
Heterotrophic organisms, denitrification														
2	Aerobic storage of COD	x_2		-1	y_2			z_2				Y_{STO}		t_2
3	Anoxic storage of COD			-1	y_3	$-x_3$	x_3	z_3				Y_{STO}		t_3
4	Aerobic growth	x_4			y_4			z_4			1	$-1/Y_H$		t_4
5	Anoxic growth (denitrification)				$-i_{NBM}$	$-x_5$	x_5	z_5			1	$-1/Y_H$		t_5
6	Aerobic endog. respiration	$-(1-f_I)$			y_6			z_6	f_I		-1			t_6
7	Anoxic endog. respiration				y_6	$-x_7$	x_7	z_7	f_I		-1			t_7
8	Aerobic respiration of PHA	-1										-1		-0.60
9	Anoxic respiration of PHA					$-x_9$	x_9	z_9				-1		-0.60
Autotrophic organisms, nitrification														
10	Nitrification	x_8			y_{10}		$1/Y_A$	z_{10}					1	i_{TSBM}
11	Aerobic endog. respiration	$-(1-f_I)$			y_{11}			z_{11}	f_I				-1	t_{11}
12	Anoxic endog. respiration				y_{12}	$-y_{12}$	y_{12}	z_{12}	f_I				-1	t_{12}
Composition matrix $\iota_{k,I}$														
k	Conservatives													
1	COD g COD	-1	1	1		-1.71	-4.57		1	1	1	1	1	
2	Nitrogen g N		i_{NSI}	i_{NSS}	1	1	1		i_{NXI}	i_{NXS}	i_{NBM}		i_{NBM}	
3	Ionic charge Mole +				1/14		-1/14	-1						
	Observables													
4	TSS g TSS								i_{TSXI}	i_{TSXS}	i_{TSBM}	0.60	i_{TSBM}	

ASM3 Composition matrix Solubles

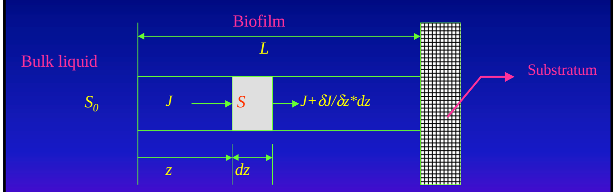
	Component / expressed as >	S_O O_2	S_I COD	S_S COD	S_{NH} N	S_{N2} N	S_{NO} N	S_{HCO} Mole
Composition matrix $\iota_{k,i}$								
k	Conservatives							
1	COD g COD	-1	1	1		-1.71	-4.57	
2	Nitrogen g N		i_{NSI}	i_{NSS}	1	1	1	
3	Ionic charge Mole +				1/14		-1/14	-1
	Observables							
4	TSS g TSS							

ASM3 Composition matrix Particulates

	Component / expressed as	X_I COD	X_S COD	X_H COD	X_{STO} COD	X_A COD	X_{TS} TSS
Composition matrix $\iota_{k,i}$							
k	Conservatives: Conservation equation						
1	COD g COD	1	1	1	1	1	
2	Nitrogen g N	i_{NXI}	i_{NXS}	i_{NBM}		i_{NBM}	
3	Ionic charge Mole +						
	Observables: Composition equation						
4	TSS g TSS	i_{TSXI}	i_{TSXS}	i_{TSBM}	0.60	i_{TSBM}	

Biofilm processes

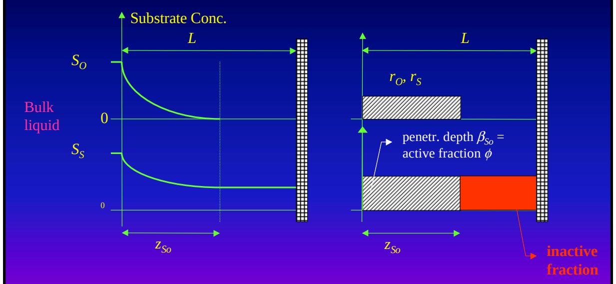
- Conversion + DIFFUSION
  Principle:



BIOMATH

Biofilm processes

Active fraction concept

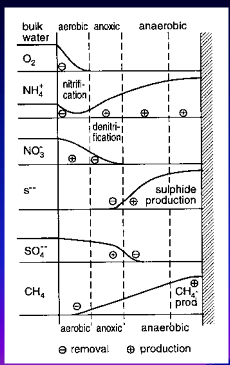


BIOMATH

Biofilm Processes

The active fraction concept: leads to the interpretation of biofilms as systems in which layers exist with different conversion processes taking place

The layers change in size as the process conditions change



BIOMATH

UNIVERSITEIT GENT

BIOMATH
Department of Applied Mathematics, Biometrics and Process Control

River Water Quality Model No. 1 : Biochemical Process Equations

Peter Vanrolleghem

October 26 2001

Water & Wastewater Management for Developing Countries
Kuala Lumpur, Malaysia

RUG-Biomath, Coupure 653, 9000 Gent, Belgium (e-mail Peter.Vanrolleghem@rug.ac.be)

Contents

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z} + \frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial c}{\partial z}\right) + \mathbf{r(c,p)}$$

Contents

- Model Description
  - Simplifying Assumptions
  - Composition of Organic Compounds
  - Components and Processes
  - Summary
- Identifiability and Uncertainty Analysis
  - Kinetic parameters
  - Stoichiometric parameters

Simplifying Assumptions

- Constant elemental composition of compounds
- Constant process stoichiometry
- No adaptation of biomasss
- No anaerobic conditions (nitrate available)
- Influence of macrophytes as varying surface for growth of sessile organisms neglected
- No silicate limitation

Composition of Organic Compounds

Characterization by mass fractions of C, H, O, N, P:

$$\alpha_C + \alpha_H + \alpha_O + \alpha_N + \alpha_P = 1$$

COD, i_N and i_P can then be calculated:

$$COD = 32\ (\ \alpha_C/12 + \alpha_H/4 + \alpha_O/32 + 3\alpha_N/56 + 5\alpha_P/124\ )\ OM$$

Why Elemental Mass Fractions ?

- Increasing realization of the importance
- Elemental analyses are increasingly available
- Other measurement units than COD are in use in limnology (e.g. organism counts, org. C, dry weight)
- Rigorous theoretical base
- Possibility for sensitivity analysis

Components and Processes

Complex, "complete" model
Recommendations for model simplifications (see later)
Decisions / Problems:

- Inclusion of nitrite
  (even if process modelling is still uncertain)
- Only one type of X_S/X_I
  (although composition of X_H, X_{N1}, X_{N2}, X_{ALG}, X_{CON} different)
- Death and respiration of X_{ALG} and X_{CON}
  (although difficult to separate)
- Phosphorus adsorption and desorption

Components (24)

S -> soluble
X -> particulate

Organisms: X_H, X_{N1}, X_{N2}, X_{ALG}, X_{CON}
Org. material: X_S, X_I, S_S, S_I
Nutrients: S_{NH4}, S_{NH3}, S_{NO2}, S_{NO3}, S_{HPO4}, S_{H2PO4}
Oxygen: S_{O2}
Inorg. material: X_P, X_{II}, S_{CO2}, S_{HCO3}, S_{CO3}, S_H, S_{OH} , S_{Ca}

Processes (30)

Growth and respiration of heterotrophs
(aerobic and anoxic)
Growth and respiration of nitrifiers (2 types)
Growth, respiration and death of algae
Growth, respiration and death of consumers
Hydrolysis
Chemical equilibria
Adsorption and desorption of phosphate

Process Stoichiometry / Concepts

Based on
- elemental composition of organic compounds
- stoichiometric parameters (yields and inert fractions)

the stoichiometric coefficients can be calculated using charge and mass balances

Equations are given in the STR
MS Excel spreadsheet can be downloaded from http://www.eawag.ch/~reichert.

Process Stoichiometry / Summary

Component →	i	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)
j	Process ↓	S_S	S_I	S_{NH4}	S_{NH3}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{H2PO4}	S_{O2}	S_{CO2}	S_{HCO3}	S_{CO3}	S_H	S_{OH}	S_{Ca}	X_H	X_{N1}	X_{N2}	X_{ALG}	X_{CON}	X_S	X_I	X_P	X_{II}
(1a)	Aerobic Growth of Heterotrophs with NH4	-		?				?		-	+			?			1								
(1b)	Aerobic Growth of Heterotrophs with NO3	-					-	?		-	+			?			1								
(2)	Aerobic Resp. of Het.			+				+		-	+			-			-1						+		
(3a)	Anoxic Growth of Heterotrophs with NO3	-				+	-	?			+			?			1								
(3b)	Anoxic Growth of Heterotrophs with NO2	-				-		?			+			?			1								
(4)	Anoxic Resp. of Het.			+			-	+			+			-			-1						+		
(5)	Growth of 1st-stage Nitrifiers			-		+		-		-	-			+				1							
(6)	Aerobic Respiration of 1st-stage Nitrifiers			+				+		-	+			-				-1					+		
(7)	Growth of 2nd-stage Nitrifiers					-	+	-		-	-			-					1						
(8)	Aerobic Respiration of 2nd-stage Nitrifiers			+				+		-	+			-					-1				+		
(9a)	Growth of Algae with NH4			-				-		+	-			-						1					
(9b)	Growth of Algae with NO3						-	-		+	-			-						1					
(10)	Aerobic Resp. of Algae			+				+		-	+			-						-1			+		
(11)	Death of Algae			(+)				(+)		(+)	?			?						-1		+	+		
(12a)	Growth of Cons. on XALG			(+)				(+)		-															
(12b)	Growth of Cons. on XS			(+)				(+)		-															
(12c)	Growth of Cons. on XH			(+)				(+)		-															
(12d)	Growth of Cons. on XN1			(+)				(+)		-															
(12e)	Growth of Cons. on XN2			(+)				(+)		-															
(13)	Aerobic Resp. of Cons.			+				+		-															
(14)	Death of Consumers			(+)				(+)		(+)															
(15)	Hydrolysis	+		(+)				(+)		(+)															
(16)	Eq. CO2 <-> HCO3																								
(17)	Eq. HCO3 <-> CO3																								
(18)	Eq. H2O <-> H + OH																								
(19)	Eq. NH4 <-> NH3			-1	1																				
(20)	Eq. H2PO4 <-> HPO4							1	-1																
(21)	Eq. Ca <-> CO3																								
(22)	Ads. of Phosphate							-1																	
(23)	Des. of Phosphate							1																-1	

+ always positive
- always negative
? Not predictable
(+) elemental composition chosen such that +

Process Kinetics

- Monod-type limitation factors
  for consumed oxygen and nutrients
- Monod and inhibition factors as switching functions
- Exponential temperature dependence
- Steele-type light dependence of algae growth
- Dynamic formulation of chemical equilibria
  i.e. a forward and backward reaction
  (rather than set of non-linear algebraic equations)

Summary

Compilation of formulations used in the literature
with special emphasis on
- compatibility with activated sludge models
- closing of mass balances
- calculation of pH

Use of elemental mass balances
makes connection to ASM more difficult

Contents

- Model Description
  - Simplifying Assumptions
  - Composition of Organic Compounds
  - Components and Processes
  - Summary
- Identifiability and Uncertainty Analysis
  - Kinetics parameters
  - Stoichiometric parameters

Identifiability and Uncertainty Analysis of Process Kinetics

Reichert and Vanrolleghem, Watermatex 2000; WST 43(7)

Problem: It is not possible to identify all model parameters using typically available data

Goals: Identify subsets of practically identifiable kinetic model parameters as a function of the measurement layout

Estimate model prediction uncertainty.

Technique

Use a simplified model with constant biomass
Ignore uncertainty in process stoichiometry

Identify practically identifiable parameter subsets
using sensitivity analysis
analysis of near linear dependence of sensitivity functions

Use Monte Carlo simulation
to calculate prediction uncertainty
based on estimated prior uncertainty of model parameters

Assessment of Prior Uncertainties and Scale Parameters

Relative uncertainties:

50%: kinetic parameters
with exception of growth rates
20%: growth rates, temperature coefficients
5%: physical parameters, inflows,
external parameters.
0%: stoichiometric parameters

Scale parameters:
upstream inflow concentrations used

Experimental Layouts

Layout	Measured variables
1	S_{O2}
2	+ $S_{NH4}+S_{NH3}$
3	+ S_{NO2}
4	+ S_{NO3}
5	+ $S_{HPO4}+S_{H2PO4}$
6	+ pH
7	+ S_{Cond}

Conclusions of Kinetic Parameter Identifiability and Uncertainty Analysis

- Measurements of O_2, NH_3 and NO_2 allow to identify 5-7 (of the 51) parameters of this model
- Adding measurements of NO_3, PO_4, pH, ions and conductivity does not significantly increase the identifiability of kinetic model parameters (but are useful to test the model and identify stoichiometric parameters)
- Without site-specific calibration, model prediction uncertainty is very large
- All these conclusions hold only for the specific case study

Sensitivity Analysis of Process Stoichiometry

(Reichert and Estermann, to be published)

Problem: Uncertainty induced by sensitivity of stoichiometric coefficients to the uncertainty of elemental mass fractions

Goal: Estimate the range of variability of stoichiometric coefficients induced by changes in elemental mass fractions within their natural variability ranges

Preliminary Results

- Small changes in elemental mass composition can lead to changes of about 20% in stoichiometric coefficients
- Reasonable variations of elemental composition can give changes in stoichiometric coefficients up to a factor of 2
- Significant changes can occur in all stoichiometric coefficients (oxygen, nutrients, CO_2 and H)

Overall Conclusions

The presented model formulations summarize past efforts in water quality modelling

The use of elemental mass fractions is a rigorous basis for analyzing the uncertainty in process stoichiometry

The model parameters are hardly identifiable and the predictive power may be poor

UNIVERSITEIT GENT

BIOMATH
Department of Applied Mathematics, Biometrics and Process Control

River Water Quality Model No. 1 : Biochemical submodel selection

Peter Vanrolleghem
October 26 2001

Water & Wastewater Management for Developing Countries
Kuala Lumpur, Malaysia

RUG-Biomath, Coupure 653, 9000 Gent, Belgium (e-mail Peter.Vanrolleghem@rug.ac.be)

The horror Matrix ...
Biochemical Conversion Model

Component →	i	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)
j	Process ↓	S_S	S_I	S_{NH4}	S_{NH3}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{H2PO4}	S_{O2}	S_{CO2}	S_{HCO3}	S_{CO3}	S_H	S_{OH}	S_{Ca}	X_H	X_{N1}	X_{N2}	X_{ALG}	X_{CON}	X_S	X_I	X_P	X_{II}
(1a)	Aerobic Growth of Heterotrophs with NH4	-		?				?		-	+			?			1								
(1b)	Aerobic Growth of Heterotrophs with NO3	-					-	?		-	+			?			1								
(2)	Aerobic Resp. of Het.			+				+		-	+			-			-1						+		
(3a)	Anoxic Growth of Heterotrophs with NO3	-				+	-	?			+			?			1								
(3b)	Anoxic Growth of Heterotrophs with NO2	-				-		?			+			?			1								
(4)	Anoxic Resp. of Het.			+			-	+			+			-			-1						+		
(5)	Growth of 1st-stage Nitrifiers			-		+		-		-	-			+				1							
(6)	Aerobic Respiration of 1st-stage Nitrifiers			+				+		-	+			-				-1					+		
(7)	Growth of 2nd-stage Nitrifiers					-	+	-		-	-			-					1						
(8)	Aerobic Respiration of 2nd-stage Nitrifiers			+				+		-	+			-					-1				+		
(9a)	Growth of Algae with NH4			-				-		+	-			-						1					
(9b)	Growth of Algae with NO3						-	-		+	-			-						1					
(10)	Aerobic Resp. of Algae			+				+		-	+			-						-1			+		
(11)	Death of Algae			(+)				(+)		(+)	?			?						-1		+	+		
(12a)	Growth of Cons. on XALG			(+)				(+)		-	?			?						-	1	+			
(12b)	Growth of Cons. on XS			(+)				(+)		-	?			?							1	-			
(12c)	Growth of Cons. on XH			(+)				(+)		-	?			?			-				1				
(12d)	Growth of Cons. on XN1			(+)				(+)		-	?			?				-			1				
(12e)	Growth of Cons. on XN2			(+)				(+)		-	?			?					-		1				
(13)	Aerobic Resp. of Cons.			+				+		-	+			-							-1		+		
(14)	Death of Consumers			(+)				(+)		(+)	?			?							-1	+	+		
(15)	Hydrolysis	+		(+)				(+)		(+)	?			?								-1			
(16)	Eq. CO2 <-> HCO3										-1	1		+											
(17)	Eq. HCO3 <-> CO3											-1	1	+											
(18)	Eq. H2O <-> H + OH													1	1										
(19)	Eq. NH4 <-> NH3			-1	1									+											
(20)	Eq. H2PO4 <-> HPO4							1	-1					+											
(21)	Eq. Ca <-> CO3												+			1									
(22)	Ads. of Phosphate							-1																1	
(23)	Des. of Phosphate							1																-1	

r(c,p)

 BIOMATH

Contents

$$\frac{\partial \mathbf{c}}{\partial t} = -u\frac{\partial \mathbf{c}}{\partial x} - v\frac{\partial \mathbf{c}}{\partial y} - w\frac{\partial \mathbf{c}}{\partial z} + \frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial \mathbf{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial \mathbf{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial \mathbf{c}}{\partial z}\right) + \mathbf{r}(\mathbf{c},\mathbf{p})$$

Selection criteria
- ✓ Components
- ✓ Processes
- ✓ General rules for model selection

Examples of model simplifications
- ✓ from *23 x 24* to *1 x 2*

 BIOMATH

Utmost simplification: Streeter-Phelps

Component →	i	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)	(18)	(19)	(20)	(21)	(22)	(23)	(24)
j	Process ↓	S_S	S_I	S_{NH4}	S_{NH3}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{H2PO4}	S_{O2}	S_{CO2}	S_{HCO3}	S_{CO3}	S_H	S_{OH}	S_{Ca}	X_H	X_{N1}	X_{N2}	X_{ALG}	X_{CON}	X_S	X_I	X_P	X_{II}
(1a)	Aerobic Growth of Heterotrophs with NH4	-		?				?		-	+			?			1								
(1b)	Aerobic Growth of Heterotrophs with NO3	-					-	?		-	+			?			1								
(2)	Aerobic Resp. of Het.			+				+		-	+			-			-1						+		
(3a)	Anoxic Growth of Heterotrophs with NO3	-				+	-	?			+			?			1								
(3b)	Anoxic Growth of Heterotrophs with NO2	-				-		?			+			?			1								
(4)	Anoxic Resp. of Het.			+			-	+			+			-			-1						+		
(5)	Growth of 1st-stage Nitrifiers			-		+		-		-	-			+				1							
(6)	Aerobic Respiration of 1st-stage Nitrifiers			+				+		-	+			-				-1					+		
(7)	Growth of 2nd-stage Nitrifiers					-	+	-		-	-			-					1						
(8)	Aerobic Respiration of 2nd-stage Nitrifiers			+				+		-	+			-					-1				+		
(9a)	Growth of Algae with NH4			-				-		+	-			-						1					
(9b)	Growth of Algae with NO3						-	-		+	-			-						1					
(10)	Aerobic Resp. of Algae			+				+		-	+			-						-1			+		
(11)	Death of Algae			(+)				(+)		(+)	?			?						-1		+	+		
(12a)	Growth of Cons. on XALG			(+)				(+)		-	?			?						-	1	+			
(12b)	Growth of Cons. on XS			(+)				(+)		-	?			?							1	-			
(12c)	Growth of Cons. on XH			(+)				(+)		-	?			?			-				1				
(12d)	Growth of Cons. on XN1			(+)				(+)		-	?			?				-			1				
(12e)	Growth of Cons. on XN2			(+)				(+)		-	?			?					-		1				
(13)	Aerobic Resp. of Cons.			+				+		-	+			-							-1		+		
(14)	Death of Consumers			(+)				(+)		(+)	?			?							-1	+	+		
(15)	Hydrolysis	+		(+)				(+)		(+)	?			?								-1			
(16)	Eq. CO2 <-> HCO3										-1	1		+											
(17)	Eq. HCO3 <-> CO3											-1	1	+											
(18)	Eq. H2O <-> H + OH													1	1										
(19)	Eq. NH4 <-> NH3			-1	1									+											
(20)	Eq. H2PO4 <-> HPO4							1	-1					+											
(21)	Eq. Ca <-> CO3												+			1									
(22)	Ads. of Phosphate							-1																1	
(23)	Des. of Phosphate							1																-1	

 BIOMATH

Utmost simplification: Streeter-Phelps

Component →	i	(7)	(16)
j	Process ↓	S_{O2}	X_S
(1+2)	Aerobic Degradation of organic material	-	-

 BIOMATH

Items to consider when simplifying

- ✓ Relevant compartments ?
- ✓ Variable or constant component conc. ?
- ✓ Nitrite
- ✓ Anoxic conditions
- ✓ Nitrifiers
- ✓ Algae
- ✓ Chemical equilibria
- ✓ General rules

 BIOMATH

Relevant compartments

- ✓ Is it necessary to include (Nr of states !):
  - ✓ Water column
  - ✓ Sediment (pore water and particles)
  - ✓ Biofilm (attached surface)

Large river: ~~sediment~~, only water column

Small river: large surface - bulk liquid ratio
==> sediment compartment necessary (Case I)
==> biofilm compartment necessary (Case II)

State variables or constants ?

Biomass concentrations
=> algae, consumers, heterotrophs, nitrifiers
=> especially useful for short term dynamics

When component is eliminated from the matrix
=> Kinetics are simplified (states ==> constants)
=> Processes are combined (e.g. growth+decay)

Note: This does not mean that component concentrations are eliminated from the model !

Nitrite

- ✓ Only necessary when significant build-up
  - ✓ when there is a large NH_4 input
  - ✓ during start-up of nitrification
- ✓ If not necessary
  - ✓ consolidate columns 5 & 6 ==> S_{NO}
  - ✓ consolidate columns 17 & 18 ==> X_N
  - ✓ combine growth and respiration processes
  - ✓ combine consumer growth processes

==> similar to ASM1 !

Anoxic conditions

- ✓ If always aerobic (high aeration-low loading)
- ✓ Eliminate: anoxic growth & respiration

Nitrifiers

- ✓ If hydraulic retention time is insufficient
- ✓ If oxygen supply is insufficient
- ✓ Biofilm formation overgrown with heterotrophs
- ✓ Eliminate: nitrifier growth, respiration, consumption

Algal activity

- ✓ Conditions:
  - ✓When hydraulic retention time < 4 - 6 d
  - ✓When Chl-a < 10 Og/l
- ✓ Eliminate:
  - algal growth
  - algal death
  - algal respiration
  - consumers of algae
- ✓ Note: not applicable for sessile algae/macrophytes

Chemical equilibria

- ✓ S_{OH} / S_H only 2 extra parameters to be estimated !
  S_{NH3}/S_{NH4}
  S_{H2CO3} / S_{HCO3} / S_{CO3} / S_{Ca}
  S_{H2PO4} / S_{HPO4}
- ✓ Normally eliminated
- ✓ Except for:
  - ✓ Understanding of pH dynamics
  - ✓ Possible carbon limitation of algae/nitrifiers
  - ✓ pH-effects on process rates
  - ✓ Ammonia toxicity

General submodel selection rules

- ✓ S_S, S_{O2}, S_{NH4}, X_S are generally selected
- ✓ Eliminating one component can lead to the elimination of other components/processes
- ✓ For any component with a negative relation in a row (uptake), the reaction cannot occur if that component is absent in the water
- ✓ If a column empty ==> Eliminate the component for r(c,p) , but not for its transport !

Simplified model: Example 1

- ✓ ~~Consumers, pH, P-adsorption/desorption~~

15

Component → *i*		(1)	(2)	(3)	(5)	(6)	(7)	(9)	(16)	(17)	(18)	(19)	(21)	(22)
j	Process ↓	S_S	S_I	S_{NH4}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{O2}	X_H	X_{N1}	X_{N2}	X_{ALG}	X_S	X_I
(1a)	Aerobic Growth of Heterotrophs with NH4	-		?			?	-	1					
(1b)	Aerobic Growth of Heterotrophs with NO3	-				-	?	-	1					
(2)	Aerobic Respiration of Heterotrophs			+			+	-	-1					+
(3a)	Anoxic Growth of Heterotrophs with NO3	-			+	-	?		1					
(3b)	Anoxic Growth of Heterotrophs with NO2	-			-		?		1					
(4)	Anoxic Respiration of Heterotrophs			+		-	+		-1					+
(5)	Growth of 1st-stage			-	+		-	-		1				
(6)	Aerobic Respiration of 1st-stage Nitrifiers			+			+	-		-1				+
(7)	Growth of 2nd-stage				-	+	-	-			1			
(8)	Aerobic Respiration of 2nd-stage Nitrifiers			+			+	-			-1			+
(9a)	Growth of Algae with NH4			-			-	+				1		
(9b)	Growth of Algae with NO3					-	-	+				1		
(10)	Aerobic Respiration of			+			+	-				-1		+
(11)	Death of Algae			(+)			(+)	(+)				-1	+	+
(15)	Hydrolysis	+		(+)			(+)	(+)					-1	

13

Simplified model: Ex. 2 ≅ QUAL2E

- ✓ Growth is compensated by respiration: X=const. hydrolysis is incorporated in degradation rate

5

Component → *i*		(3)	(5)	(6)	(7)	(9)	(19)	(21)
j	Process ↓	S_{NH4}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{O2}	X_{ALG}	X_S
(1+2)	Aerobic Degradation of organic material	+			+	-	-	-
(3+4)	Anoxic Degradation of organic material	+		-	+		-	-
(5+6)	Growth and respiration of 1st-stage Nitrifiers	-	+			-		
(7+8)	Growth and respiration of 2nd-stage Nitrifiers		-	+		-		
(9b)	Growth of Algae with NO3			-	-	+	+	

7

Simplified model: Example 3 ≅ extended Streeter-Phelps

- ✓ ~~Nitrification~~ + ~~anoxic conditions~~

2

Component → *i*		(3)	(6)	(7)	(9)	(19)	(21)
j	Process ↓	S_{NH4}	S_{NO3}	S_{HPO4}	S_{O2}	X_{ALG}	X_S
(1+2)	Aerobic Degradation of organic material	+		+	-	-	-
(9b)	Growth of Algae with NO3		-	-	+	+	

6

Note presence of growing algal biomass !

Simplified model: Example 4 ≅ Streeter-Phelps

- ✓ ~~Algae~~

1

Component → *i*		(7)	(16)
j	Process ↓	S_{O2}	X_S
(1+2)	Aerobic Degradation of organic material	-	-

2

Constant heterotrophic biomass hidden but explicitly present in degradation kinetics!

Take home

- ✓ Wake up from your horror dream :
  - ✓Simplification is nearly always possible
  - ✓No clear cut decision criteria
  - ✓Guidelines were given
  - ✓Some general rules were deduced
  - ✓Examples were provided (Qual2E, S-P)
- ✓ To be combined with 5 other steps

UNIVERSITEIT GENT

BIOMATH
Department of Applied Mathematics, Biometrics and Process Control

River Water Quality Model no. 1 (RWQM1)

Oxygen and nitrogen conversion in the river Glatt (Switzerland)

Peter A. Vanrolleghem & Peter Reichert

October 26 2001

Water & Wastewater Management for Developing Countries
Kuala Lumpur, Malaysia

RUG-Biomath, Coupure 653, 9000 Gent, Belgium (e-mail Peter.Vanrolleghem@rug.ac.be)

Study Site

River Glatt: 35 km length; from Greifensee to river Rhine. High percentage of treated waste water.

Study site: last 10 km

Steep, highly aerated, with small drops every 50 m and some cascades.

Upstream and downstream measurement stations with no significant tributaries in between

On-line analysis at both stations: T, pH, NH_4, NO_2, O_2

Downstream cumulative samples: many ions

Previous results

Reichert, Berg, Holzer, Kändler, Wanner:
- Evaluation of 6 complete data series:
  - Good fit possible (6 parameters) for each data series
  - No significant correlation between environmental conditions and conversion rate parameters

Uehlinger, König, Reichert:
- Evaluation of 123 oxygen data series:
  - Variation of production and respiration rates correlate primarily with temperature, seasonal temperature gradient, time and radiation
  - Effect of discharge and time since last flood was not significant (in contrast to other rivers).

Goals of this study

Test the applicability and appropriateness of the proposed modeling approach by applying several submodels of the RWQM1 to the Glatt data set.

Perform speculative model applications that try to increase the predictive capability of river water quality models.

Submodel 1: Constant Biomass

Variables:

S_S, S_{NH4}, S_{NO2}, S_{NO3}, S_{HPO4}, S_{O2}

Parameters:

X_H, X_{N1}, X_{N2}, X_{ALG}, X_S

Processes:

Growth and respiration of heterotrophs and nitrifiers

Growth, respiration and death of algae

Hydrolysis

Submodel 1: Constant Biomass

Component →	*i*	(1)	(3+4)	(5)	(6)	(7+8)	(9)
j	Process ↓	S_S	S_{NH4}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{O2}
(1a)	Aerobic Growth of Heterotrophs with NH4	-	?			?	-
(1b)	Aerobic Growth of Heterotrophs with NO3	-			-	?	-
(2)	Aerobic Respiration of Heterotrophs		+			+	-
(5)	Growth of 1st-stage Nitrifiers		-	+		-	-
(6)	Aerobic Respiration of 1st-stage Nitrifiers		+			+	-
(7)	Growth of 2nd-stage Nitrifiers			-	+	-	-
(8)	Aerobic Respiration of 2nd-stage Nitrifiers		+			+	-
(9a)	Growth of Algae with NH4		-			-	+
(9b)	Growth of Algae with NO3				-	-	+
(10)	Aerobic Respiration of Algae		+			+	-
(11)	Death of Algae		(+)			(+)	(+)
(15)	Hydrolysis	+	(+)			(+)	(+)

Submodel 1: Constant Biomass

Initial conditions:

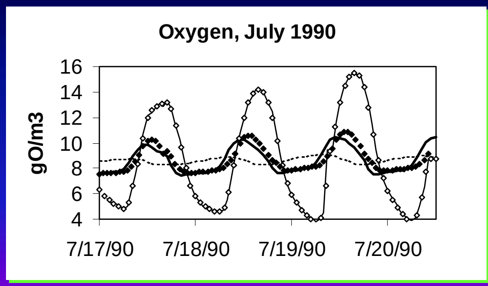
Simulation results only used after one transport time. Results are then independent of initial conditions

Input:

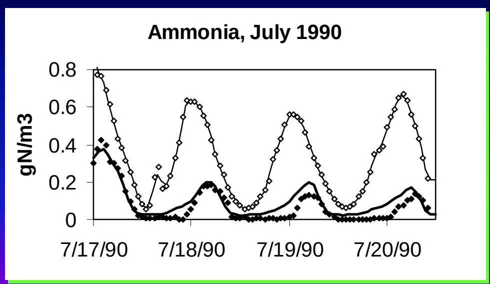
Known inputs for S_{NH4}, S_{NO2}, S_{O2}

Constant inputs assumed for S_S, S_{NO3}, S_{HPO4} (based on cumulative samples)

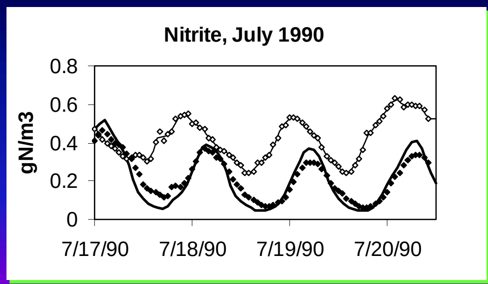
Submodel 1: Constant Biomass



Submodel 1: Constant Biomass



Submodel 1: Constant Biomass



Submodel 2: Extension to pH

Variables:

S_S, S_{NH4}, S_{NH3}, S_{NO2}, S_{NO3}, S_{HPO4}, S_{H2PO4}, S_{O2}, S_{CO2}, S_{HCO3}, S_H, S_{OH}, S_{Ca}

Parameters:

X_H, X_{N1}, X_{N2}, X_{ALG}, X_S

Processes:

Growth and respiration of heterotrophs and nitrifiers
Growth, respiration and death of algae
Hydrolysis
Chemical equilibria

Submodel 2: Extension to pH

Component → *i*		(1)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)
j	Process ↓	S_S	S_{NH4}	S_{NH3}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{H2PO4}	S_{O2}	S_{CO2}	S_{HCO3}	S_{CO3}	S_H	S_{OH}	S_{Ca}
(1a)	Aerobic Growth of Heterotrophs with NH4	-	?				?		-	+			?		
(1b)	Aerobic Growth of Heterotrophs with NO3	-				-	?		-	+			?		
(2)	Aerobic Respiration of Heterotrophs		+				+		-	+			-		
(5)	Growth of 1st-stage Nitrifiers		-		+		-		-	-			+		
(6)	Aerobic Respiration of 1st-stage Nitrifiers		+				+		-	+			-		
(7)	Growth of 2nd-stage Nitrifiers				-	+	-		-	-			-		
(8)	Aerobic Respiration of 2nd-stage Nitrifiers		+				+		-	+			-		
(9a)	Growth of Algae with NH4		-				-		+	-			-		
(9b)	Growth of Algae with NO3					-	-		+	-			-		
(10)	Aerobic Respiration of Algae		+				+		-	+			-		
(11)	Death of Algae		(+)				(+)		(+)	?			?		
(15)	Hydrolysis	+	(+)				(+)		(+)	?			?		
(16)	Equilibrium CO2 <-> HCO3									-1	1		+		
(17)	Equilibrium HCO3 <-> CO3										-1	1	+		
(18)	Equilibrium H2O <-> H + OH												1	1	
(19)	Equilibrium NH4 <-> NH3		-1	1									+		
(20)	Equilibrium H2PO4 <-> HPO4						1	-1					+		
(21)	Equilibrium Ca <-> CO3											+			1

Submodel 2: Extension to pH

Initial conditions:

Simulation results only used after one transport time.
Results are then independent of initial conditions

Input:

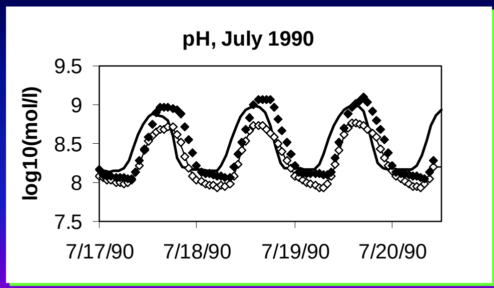
Known inputs for S_{NH4}, S_{NH3}, S_{NO2} , S_{O2} , S_H , S_{OH}

Constant inputs assumed for S_S, S_{NO3} , S_{HPO4} , S_{H2PO4} , S_{ca} (based on cumulative samples)

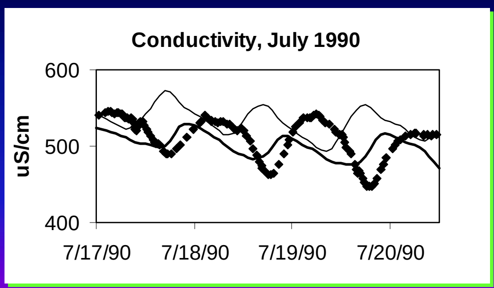
Constant concentrations used for: S_K, S_{Mg}, S_{Na}, S_{Cl}, S_{SO4}

Calculated inputs (charge, chem. eq.): S_{HCO3}, S_{CO2}, S_{CO3}

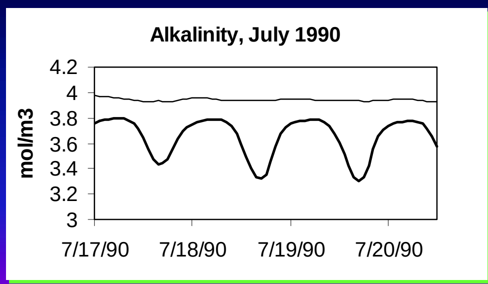
Submodel 2: Extension to pH



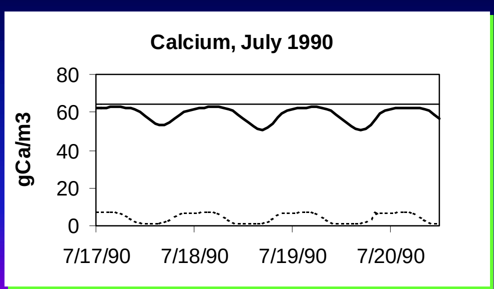
Submodel 2: Extension to pH



Submodel 2: Extension to pH



Submodel 2: Extension to pH



Submodel 3: Benthic Biomass Dynamics

Variables:

S_S, S_{NH4}, S_{NO2}, S_{NO3}, S_{HPO4} , S_{O2},
$X_{H,s}$, $X_{N1,s}$, $X_{N2,s}$, $X_{ALG,s}$, $X_{CON,s}$, $X_{S,s}$, $X_{I,s}$, X_S, X_I

Processes:

Growth and respiration of heterotrophs and nitrifiers

Growth, respiration and death of algae

Growth, respiration and death of consumers

Hydrolysis

Submodel 3: Benthic Biomass Dynamics

Component → i		(1)	(3+4)	(5)	(6)	(7+8)	(9)	(16s)	(17s)	(18s)	(19s)	(20s)	(21s)	(22s)	(21)	(22)
j	Process ↓	S_S	S_{NH4}	S_{NO2}	S_{NO3}	S_{HPO4}	S_{O2}	$X_{H,s}$	$X_{N1,s}$	$X_{N2,s}$	$X_{ALG,s}$	$X_{CON,s}$	$X_{S,s}$	$X_{I,s}$	X_S	X_I
(1a)	Aerobic Growth of Heterotrophs with NH4	-	?			?	-	A								
(1b)	Aerobic Growth of Heterotrophs with NO3	-			-	?	-	A								
(2)	Aerobic Respiration of Heterotrophs		+			+	-	-A						+		
(5)	Growth of 1st-stage Nitrifiers		-	+		-	-		A							
(6)	Aerobic Respiration of 1st-stage Nitrifiers		+			+	-		-A					+		
(7)	Growth of 2nd-stage Nitrifiers			-	+	-	-			A						
(8)	Aerobic Respiration of 2nd-stage Nitrifiers		+			+	-			-A				+		
(9a)	Growth of Algae with NH4		-			-	+				A					
(9b)	Growth of Algae with NO3				-	-	+				A					
(10)	Aerobic Respiration of Algae		+			+	-				-A			+		
(11)	Death of Algae		(+)			(+)	(+)				-A		+	+		
(12a)	Growth of Consumers on XALG		(+)			(+)	-				-	A	+			
(12b)	Growth of Consumers on XS		(+)			(+)	-					A	-			
(12c)	Growth of Consumers on XH		(+)			(+)	-	-				A				
(12d)	Growth of Consumers on XN1		(+)			(+)	-		-			A				
(12e)	Growth of Consumers on XN2		(+)			(+)	-			-		A				
(13)	Aerobic Respiration of Consumers		+			+	-					-A		+		
(14)	Death of Consumers		(+)			(+)	(+)					-A	+	+		
(15)	Hydrolysis	+	(+)			(+)	(+)						-A			

BIOMATH

Submodel 3: Benthic Biomass Dynamics

Additional considerations:

Rate limitation in benthic biofilms: $\frac{1}{1+\frac{k_{gro}}{r_{max}}X}$

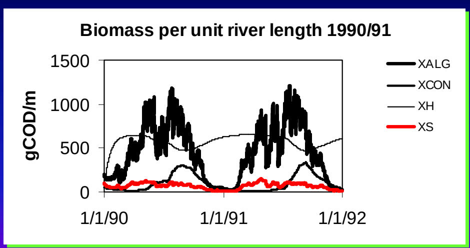
Detachment and sedimentation

Food accessibility

These additional processes
with their non-identifiable parameters
make the model application speculative.

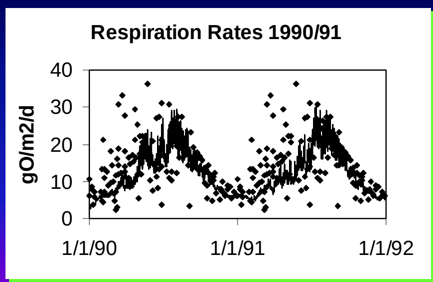
BIOMATH

Submodel 3: Benthic Biomass Dynamics



BIOMATH

Submodel 3: Benthic Biomass Dynamics



BIOMATH

Conclusions

The simplified model with constant benthic biomass leads to a good description of the data.

Extension to pH modeling appears promising

Speculative modeling of benthic biomass dynamics (intended to increase the predictive capabilities of river water quality models)

Lack of knowledge on relevant processes does not give such models high predictive power yet

BIOMATH

UNIVERSITEIT GENT

BIOMATH
Department of Applied Mathematics, Biometrics and Process Control

River Water Quality Model No. 1 : Integrated Urban Wastewater System

Jurgen Meirlaen, Tolessa Deksissa and Peter Vanrolleghem
October 26 2001

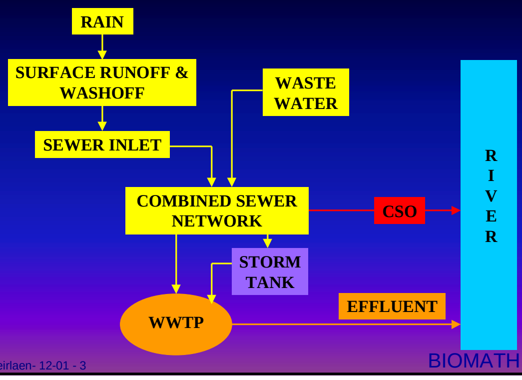
Water & Wastewater Management for Developing Countries
Kuala Lumpur, Malaysia

RUG-Biomath, Coupure 653, 9000 Gent, Belgium (e-mail Jurgen.Meirlaen@rug.ac.be)

Overview

- Introduction
- Problems in integrated modelling
- Proposed solutions
- Conclusions

Introduction: IUWS



Introduction

- Integrated modelling
  - includes sewer system, WWTP and receiving water
  - judge effect of CSO's and WWTP effluent on RWQ
  - apply emission based Real Time Control (RTC)
- Simultaneous integrated modelling
  - incorporate two-way interaction between sewer system, WWTP and receiving water
  - apply 'immission' based RTC

Problems in integrated modelling

- Problem 1: Different state variables
  - integrated simulations
- Problem 2: Complex hydraulic equations
  - fast simulations
- Problem 3: Different software packages
  - simultaneous simulation

Problem 1: Different state variables

- Organic pollution:
  - BOD (sewer and river models)
  - COD (activated sludge models)
  - TOC (measurement at low concentrations)
  - …
- Complex and varying relationships
- Different conditions in different parts of the system
  - what happens with biomass ?
- Closed mass balances ?

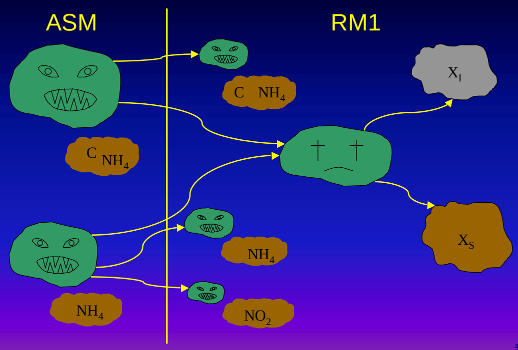
Solution: River Water Quality Model No. 1

- Biochemical conversion processes for cycles of C, O, N and P
- COD-based
- Consistency in mass and elemental balances
- Compatible with IWA Activated Sludge Models
- Suited for integration in IUWS modelling

Solution: Connector ASM-RM1

- List of conversion equations
- Closed elemental balances (C, H, O, N and P)
  - powerful model check
  - elemental compositions of all state variables
- Problems
  - compositions for components not present in ASM1
  - fate of biomass

Solution: Fate of biomass



Problems in integrated modelling

- Problem 1: Different state variables
  - integrated simulations
- Problem 2: Complex hydraulic equations
  - fast simulations
- Problem 3: Different software packages
  - simultaneous simulation

Problem 2: Complex hydraulics

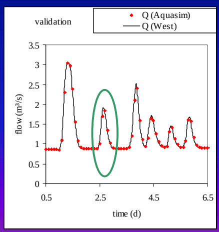
- ‘de Saint-Venant’ equations
  - flow propagation in channels and pipes
  - used in state-of-the-art models
    - sewer (Mouse, Hydroworks)
    - rivers (Duflow, Isis, Mike11)
  - non-linear partial differential equations
  - long calculation times
  - important data requirements
    - sewer pipes (slopes, diameters, roughness, …)
    - rivers (slopes, roughness,cross-sectional shape, …)

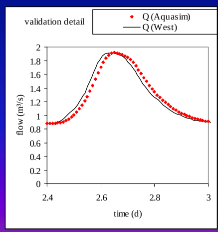
Solution: Kosim-like approach

- Run-off and flow propagation
  - Nash-Cascade
  - transportation time
  - reasonable prediction of overflow volumes and peak discharges
- Used in integrated modelling by Schütze (1998)
- Calculation times much shorter
- Needs to be calibrated against hydraulic model

Solution: Tanks-in-series model

- Capable of predicting flood-wave propagation
- Number of tanks determines dispersion
- Conversion models can be implemented in tanks





Problems in integrated modelling

- Problem 1: Different state variables
  - integrated simulations
- Problem 2: Complex hydraulic equations
  - fast simulations
- Problem 3: Different software packages
  - simultaneous simulation

Problem 3: different software packages

- Manual sequential integration
  - file transfer
  - file format
  - different state variables
  - no interaction
- SYNOPSIS
  - interface routines
  - interaction sewer/WWTP
- Integrated Catchment Simulator (ICS)
  - links MOUSE, STOAT and MIKE11
  - controls communication between models

Solution: WEST-IUWS

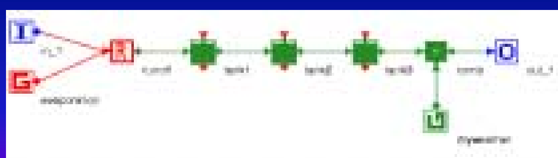
- Integrated Urban Wastewater System in WEST®
- WEST®
  - state-of-the-art simulator comparable to STOAT
  - more flexibility
  - parameter estimation
  - open model structure
  - state-of-the-art models for WWTP

Solution: WEST-IUWS

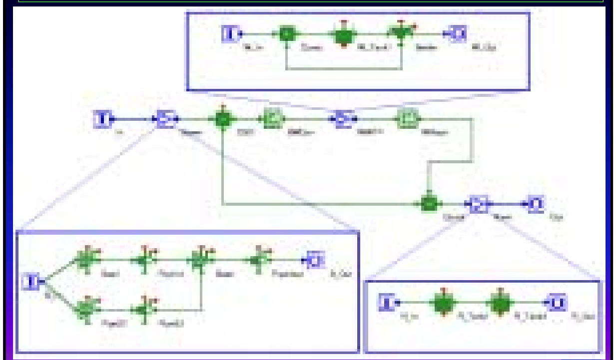
- Integrated Urban Wastewater System in WEST®
  - All models in WEST®
    - Kosim
    - ASM
    - RWQM1
    - Connectors
  - No file transfer
  - No data exchange
  - Simultaneous simulation
  - Hierarchical modelling
    - develop models separately
    - link afterwards

Solution: Kosim-like approach

- Implementation in WEST®
  - transformation of difference to differential equations
  - modelling of Nash-Cascade
  - translation time implementation



Solution: WEST-IUWS



Conclusions: WEST-IUWS

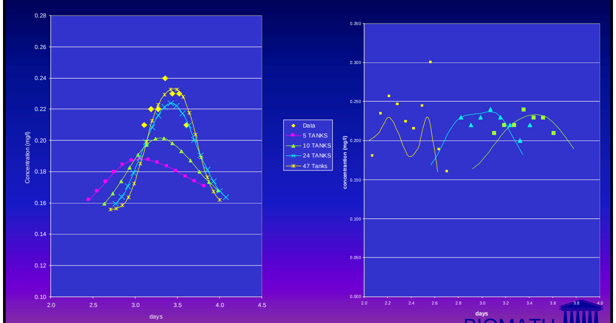
- WEST-IUWS implements
  - COD based models
    - ASM, RM1 + connector with closed mass balances
  - simplified models
    - Kosim approach for run-off and sewer system modelling
    - standard WWTP modelling
    - Tanks-in-series model for river hydraulics
  - integrated in one software package
    - no file transfer
    - no inter-software communication
    - simultaneous simulations

Case-study: Lambro

- Tributary of Po in Italy
- Studied stretch of 26 km North of Milano
- Main pollution at Merone WWTP
  - 120,000 IE
  - hydraulically limited
  - daily bypass even under dry weather !
  - studied within GREAT-ER project => large data set
- Aim of the study:
  - predict LAS concentration

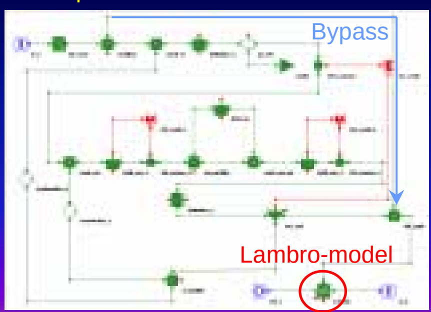
Case-study : Lambro

Decision on number of tanks in series (tracer test)



Case-study: Lambro

Implementation in WEST-IUWS

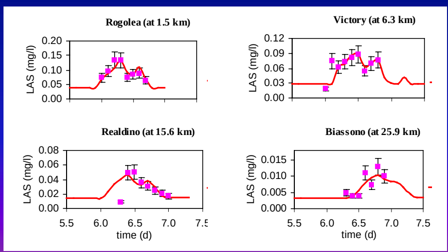


Case-study: Lambro

- Extension of RWQM1 to model specific chemical
- LAS = household detergent, 1% of COD in WW
- LAS degradation:
  - according to first order kinetics
  - only aerobically
  - no volatilisation
  - attaches to particles
- One additional column/row in RWQM1
- No algae, no consumers

Case-study: Lambro

- Model calibration on large LAS-data set
- Interesting data due to bypass
  which leads to "waves" of LAS going downstream

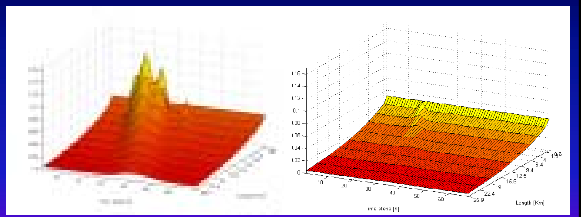


J. Meirlaen- 12-01 - 25

BIOMATH

Case-study: Lambro

Model prediction of LAS under a WWT upgrade

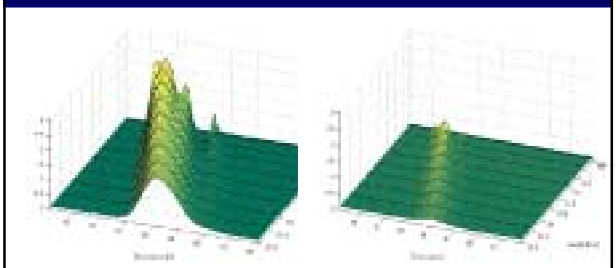


J. Meirlaen- 12-01 - 26

BIOMATH

Case-study: Lambro

Model prediction of NH_4 under a WWT upgrade



J. Meirlaen- 12-01 - 27

BIOMATH