Integrated water quality modeling: New perspectives using IWA RWQM1 model

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IWA RIVER WATER QUALITY MODELLING (RWQM) TASK GROUP

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INTRODUCTION AND BACKGROUND

SHORTCOMINGS IN RWQM FORMULATIONS

- LACK OF CLOSED MASS BALANCES: BOD AND SEDIMENT
- LACK OF SEDIMENT RELATED PROCESSES (attached bacteria/algae and other benthic flux terms)
- INCONSISTENCY IN RWQM AND ASM FORMULATIONS: lack of integrating wastewater treatment and river water quality

SHORTCOMINGS IN RWQM FORMULATIONS

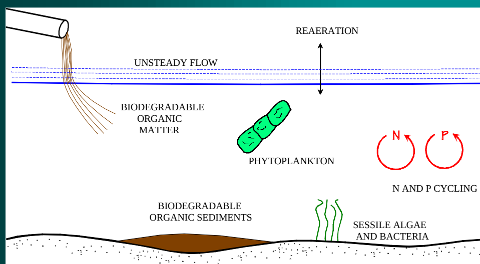
- SEWER OVERFLOW PROBLEMS
- SPATIAL NON-UNIFORMITIES AND RAPID TEMPORAL CHANGES
- ISSUES OF CALIBRATION
- PREDICTIVE CAPABILITY

OBJECTIVES OF THE RWQM TASK GROUP

- ☞ SCIENTIFIC AND TECHNICAL BASE
- ☞ "STANDARDIZED" RWQM CONVERSION MODEL VERSIONS
- ☞ GUIDELINES FOR MODEL SELECTION
- ☞ CASE STUDIES
- ☞ OPEN ENDED DEVELOPMENT PROCESS

RIVER WATER QUALITY MODEL NO. 1: I. MODELLING APPROACH

Modelling Context: River Water Quality



Mass Balance Equation

Change in concentration over time

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

Advection | Dispersion | Reaction

Model Decision Procedure

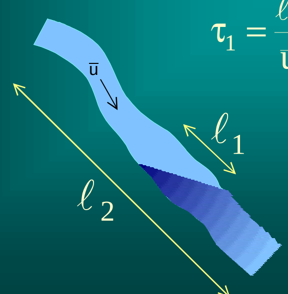
- Define temporal representation
- Determine spatial dimensions
- Determine representation of mixing
- Determine representation of advection
- Determine reaction terms
- Determine boundary conditions

Step 1. Define Temporal Representation

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

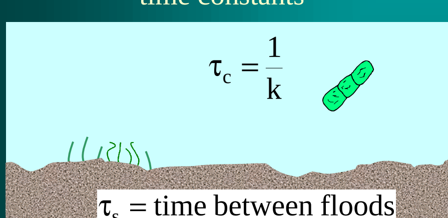
Upper- and lower-bound time constants

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



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

Water-column and sediment reaction time constants



Usually: $\tau_s > \tau_c$

Step 1. Define Temporal Representation – Water-Column Reactions

$\tau_c << \tau_1 \rightarrow$ steady-state model	$\tau_1 < \tau_c < \tau_2 \rightarrow$ dynamic model	$\tau_c >> \tau_2 \rightarrow$ reactions negligible

τ_1 τ_2

Summary: Model Decision Procedure

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

RIVER WATER QUALITY MODEL NO. 1: II. BIOCHEMICAL PROCESS EQUATIONS

Contents

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

- Features
- Simplifying Assumptions
- Components
- Processes

RWQM1 Peterson Matrix

Features

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

Simplifying Assumptions

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

Components

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

- Growth & respiration of heterotrophs (X_H) (aerobic and anoxic).
- Growth & respiration of nitrifiers (X_{N1} X_{N2}).
- Growth, respiration & death of algae (X_{ALG}).
- Growth, respiration & death of consumers (X_{CON}).
- Hydrolysis.
- Chemical equilibria.
- Adsorption and desorption of phosphate.

Biochemical Conversion Model

The Matrix

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	

RIVER WATER QUALITY MODEL NO. 1:
III. BIOCHEMICAL SUBMODEL
SELECTION

Contents

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

Contents

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

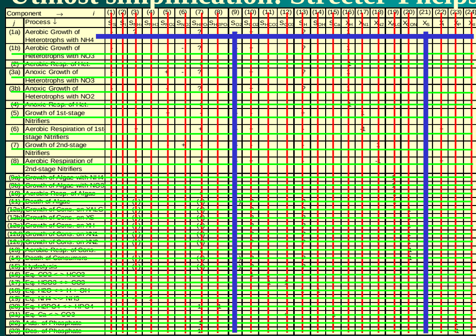
Selection criteria

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

Examples of model simplifications

- ✓ from ***23 x 24*** to ***1 x 2***

Utmost simplification: Streeter-Phelps



Utmost simplification: Streeter-Phelps

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

Items to consider

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

Relevant compartments

✓ **Is it necessary to include (Nr of variables!):**

✓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

✓**Component is eliminated from 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 !**

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**
✓ **Understanding of pH dynamics**
✓ **Possible carbon limitation of algae/nitrif.**
✓ **pH-effects on process rates**
✓ **Ammonia toxicity**

Simplified model: Example 1

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

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	

15

13

Simplified model: Ex. 2 ≅ QUAL2E

- ✓ growth is compensated by respiration: X=constant
  hydrolysis is incorporated in degradation rate

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			-	-	+	+	

5

7

Simplified model: Example 3 ≅ extended Streeter-Phelps

- ✓ ~~nitrification~~ + ~~anoxic conditions~~

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		-	-	+	+	

2

6

Note presence of growing algal biomass !

Simplified model: Example 4 ≅ Streeter-Phelps

✓ ~~algae~~

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

1

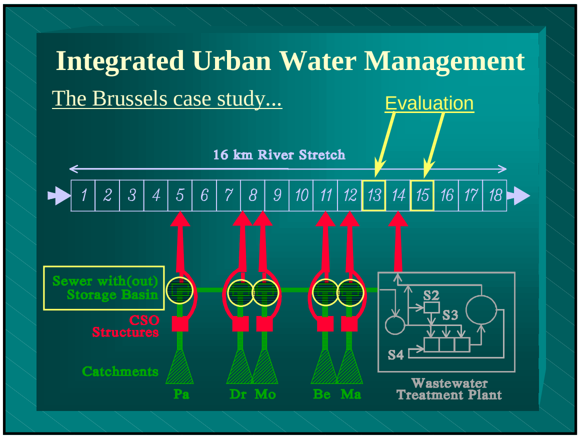
2

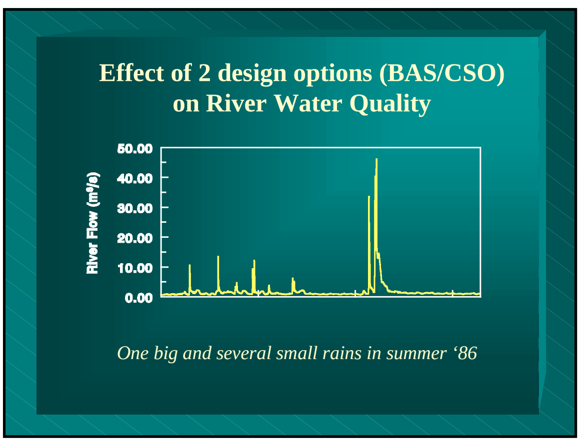
Constant heterotrophic biomass hidden
but explicitly present in degradation kinetics!

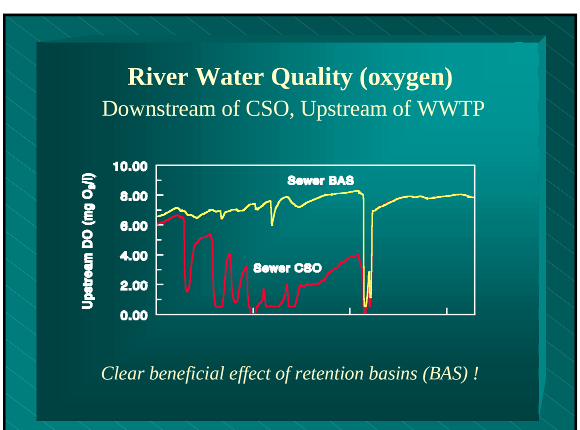
Take home

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

Ready for applications ?

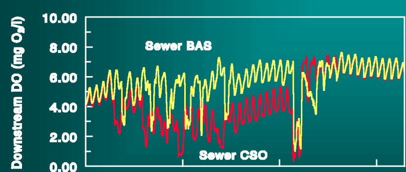

Integrated Urban Water Management
The Brussels case study...
Evaluation
16 km River Stretch
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
Sewer with(out) Storage Basin
CSO Structures
Catchments
Pa
Dr Mo
Be Ma
S2
S3
S4
Wastewater Treatment Plant


Effect of 2 design options (BAS/CSO) on River Water Quality
River Flow (m³/s)
50.00
40.00
30.00
20.00
10.00
0.00
One big and several small rains in summer '86


River Water Quality (oxygen)
Downstream of CSO, Upstream of WWTP
Upstream DO (mg O2/l)
10.00
8.00
6.00
4.00
2.00
0.00
Sewer BAS
Sewer CSO
Clear beneficial effect of retention basins (BAS) !

River Water Quality (oxygen)

Downstream of CSO, Downstream of WWTP



Beneficial effect of basins is reduced due to lower efficiency of WWTP by increased loading from basins

GREAT-ER project

Geography-referenced **R**egional **E**xposure **A**ssessment **T**ool for **E**uropean **R**ivers

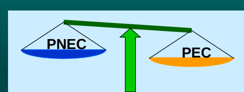
- prediction of the fate of specific **"down-the-drain" chemicals** in **surface water**
- using **Geographical Information Systems** (GIS)
- for use within **Environmental Risk Assessment**

Environmental Risk Assessment

- Aim = **assess** the probability and severeness of negative **effects** on ecosystems after exposure to **chemicals**
- steps:
  - **exposure**: Predicted Environmental Concentration (PEC)
    → how much ends up in the environment ? where ?
  - **effects**: Predicted No Effects Concentration (PNEC)
    → how toxic / dangerous is the chemical for the environment ?

Environmental Risk Assessment

- Aim = **assess** the probability and severeness of negative **effects** on ecosystems after exposure to **chemicals**
- steps:
  - **exposure**: **P**redicted **E**nvironmental **C**oncentration **(PEC)**
  - **effects**: **P**redicted **N**o **E**ffects **C**oncentration **(PNEC)**
  - risk ratio: $\frac{\text{PEC}}{\text{PNEC}} < 1$?



Environmental exposure assessment

Current methods (advised in EU legislation):
multimedia fate models:

Environmental exposure assessment

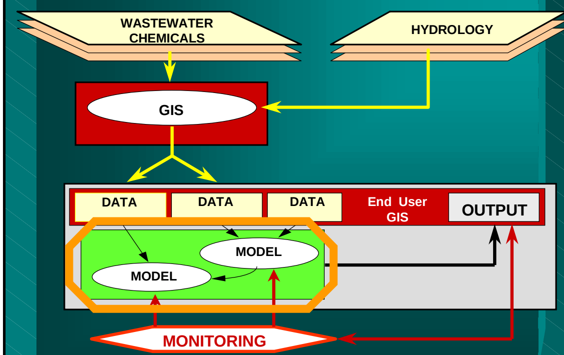
- **Current methods**:
  - **multimedia fate models**
  - **no spatial nor temporal variability considered** → **limited accuracy**

FACTOR > 100-1000 !

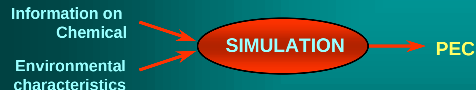
- **GREAT-ER: refine PEC calculations**
  - 'real' **geo-referenced** data
  - **variability**
  - geo-referenced → **validation** is possible

AIM = FACTOR < 3-5

GREAT-ER: Overview

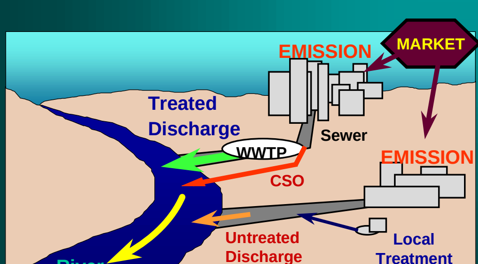


Overall simulation approach



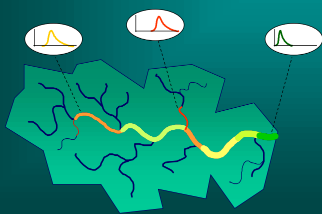
- Steady state models (no dynamics)
- Stochastic / deterministic
- Input / Output - Statistical distributions
  - Geo-referenced

The underlying model



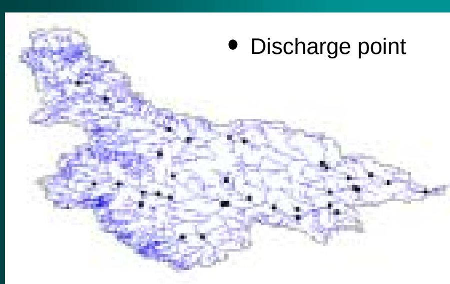
Simulation Data Analysis

- direct GREAT-ER simulation results: geo-referenced predicted concentrations



GREAT-ER Validation

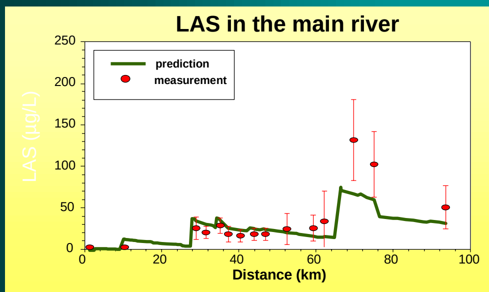
Catchment in Yorkshire (UK)



GREAT-ER Validation

LAS concentrations in the river stretches

Validation of GREAT-ER



Case study Integrated Model: Lambro

Treatment plant of Merone (north of Milano, Italy)

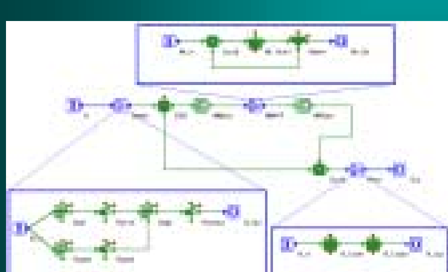
- overloaded during day time under dry conditions
- expansion of plant with increased hydraulic capacity

Effect of upgrade on river water quality is assessed using an integrated model:

- WWTP (anoxic/aerobic activated sludge)
- River (modified RWQM1, 47 tanks)

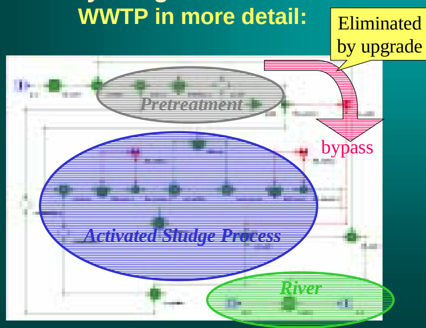
with WEST modelling & simulation platform

Case study Integrated Model: Lambro
Implementation in WEST (hierarchical !)



Case study Integrated Model: Lambro

WWTP in more detail:

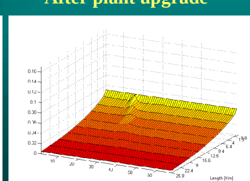


Case study Integrated Model: Lambro

The LAS concentration is followed along the river as function of time and distance

Before plant upgrade

After plant upgrade



Conclusions

INTEGRATED WATER QUALITY MODELLING HAS BEEN MUCH FACILITATED THANKS TO:

- ☞ New RWQM1 conversion model that is ASM-compatible
- ☞ Suggested guidelines for (simple) submodel selection
- ☞ Increased interest in integrated analysis by authorities leads to an increasing number of illustrative case studies
- ☞ Open modelling & simulation platform (WEST)