UNIVERSITEIT GENT

BIOMATH
Department Applied Mathematics, Biometrics and Process Control

The Usefulness of Models in Environmental Engineering

Peter Vanrolleghem

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

Models in Control...

Overview

- Models
  - What are they?
  - How do I build them ?
- Application of Models
  - Understanding / Education / Training
  - Experimental Design
  - Intelligent Sensors
  - Model-based Control
  - Decision support (Risk Assessment - System Design)

Definitions

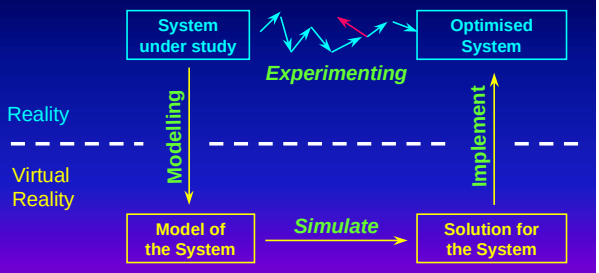
- System
  Part of reality that is separated from its environment on the basis of a purpose defined by the researcher
- Model
  An approximate description of a part of reality considering only those aspects of interest
- Simulation
  = Virtual Experimentation: Manipulation of a model to gain insight in the "behaviour" of the real system

Types of Models

- Mental models (ideas, concepts, ...)
- Verbal models ("description in words")
- Scale models ("house in cardbord")
- Computer models ("house in AutoCad")
- Mathematical models ("equations")

Why Modelling ?

Solving Problems for complex systems

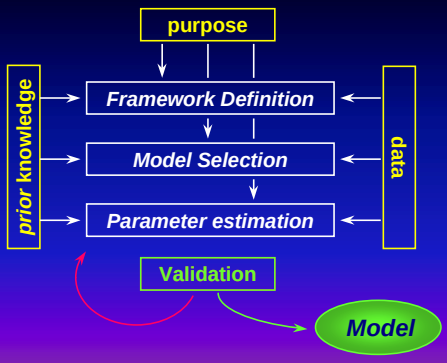


Model building: Starting points

- Purpose of the model
  - Increasing understanding of a system *(Think tank)*
  - Summary of knowledge/data *(Communication)*
  - Prediction of future behaviour *(Control)*
- *Prior* knowledge
  - Experience
  - Existing models
  - Literature (facts, phenomena, theories, ...)
- Data
  - Existing data
  - New data collected in view of model building

BIOMATH

Model building: Subtasks



BIOMATH

Overview

- Models
  - What are they?
  - How do I build them ?
- Application of Models
  - Understanding / Education / Training
  - Experimental Design
  - Intelligent Sensors
  - Model-based Control
  - Decision support (Risk Assessment - System Design)

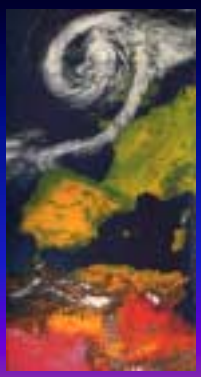
BIOMATH

Models to the General Public

$$E = mc^2$$

BIOMATH

Models to the General Public



Weather Forecasting

(Reading, UK)

BIOMATH

Models in Environmental Engineering

Only two types of application:

- Describing the past (*$E=mc^2$*)
  - Understanding (research - education - training)
  - Summary of knowledge
- Prediction of the future (*Weather*)
  - Forecasting the future state of an existing system
  - Forecasting the future behaviour of a changed system

BIOMATH

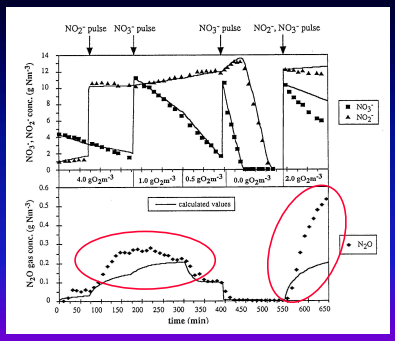
Models for understanding

- Hypothesis is generated on the basis of
  - data as such (apple falls off a tree -> model)
  - discrepancy of data with an existing model
- New insight is acquired when the new model is accepted by the scientific community

  ... until the next (better) data set comes along...

BIOMATH

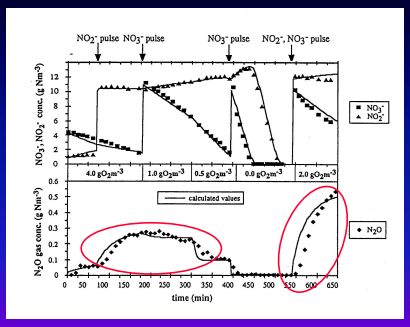
Understanding N_2O emissions



Model is insufficiently "flexible"

BIOMATH

Understanding N_2O emissions

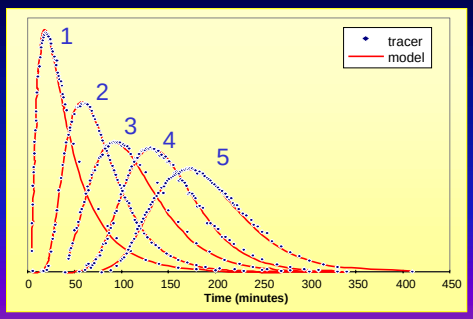


Model is much better !

BIOMATH

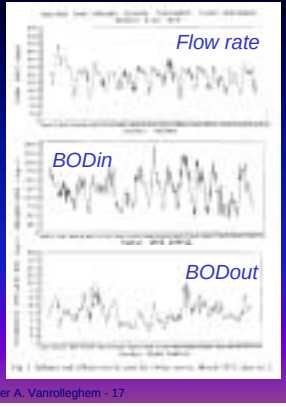
Models for description/summary

Mixing behaviour in a river (only 5 numbers !)



BIOMATH

Time series of data



Summary of data:

Time series models:

Bout(t) =

0.55 Bout(t-1) + 0.3 Bout(t-7)
+0.49 Bin(t) - 0.12 Bin(t-1)
-25 dt(t) + 32.5 dt(t-1) - 6.7dt(t-7)
-0.3 SSin(t-1) +0.22 SS(t-2)
+N(t)

The whole data series is condensed into a few numbers (only 9)!

BIOMATH

Use of models for Optimal Experimental Design (OED)

- Purpose of experimental design:
  create experimental conditions such that data allow
  - model selection
  - accurate parameter estimation
  - validation of a model

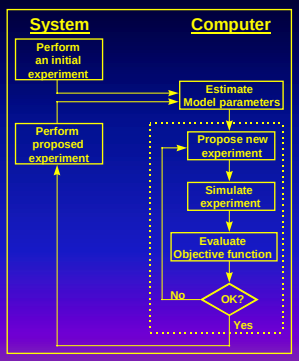
BIOMATH

Questions to be answered by Experimental Design

- What variables should we measure ?
- What is the required accuracy ?
- Over what period should be measured ?
- At what frequency are the data to be collected ?
- At what location should the measurements be done ?

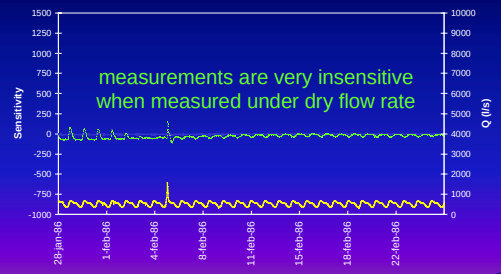
Quantified in an Objective Function
to be optimised by the OED algorithm

Model based Experimental Design



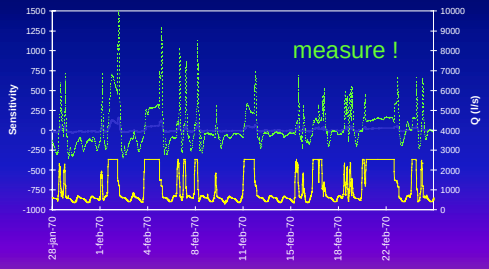
Application of OED

Calculated sensitivity to a settling parameter
during dry weather conditions



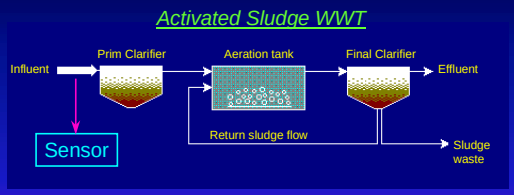
Application of OED

Calculated sensitivity to a settling parameter
during wet weather conditions



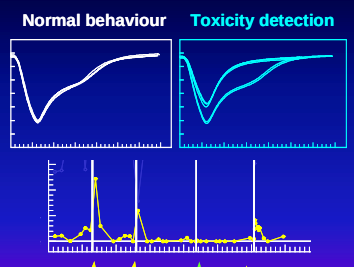
Intelligent sensors

- Raw data + Model



Intelligent sensors

2 series of
5 respirograms in 2h



No action leads to pollution

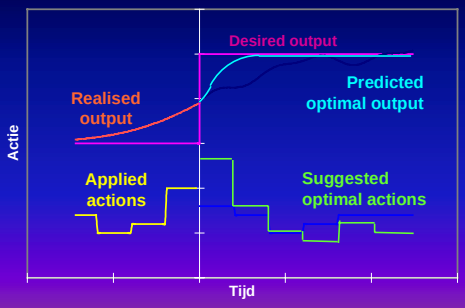
Control prevents pollution

Use of Models in Process Control

- Controllers with built-in model
  eg. Model based predictive control
- Support during the design of the control structure
  Choice of actuators, sensors, control laws
- Support during the tuning of controllers
  eg. Tuning the parameters of a PID-controller
- Prediction of disturbances
  eg. Rain - runoff / diurnal waste flow pattern

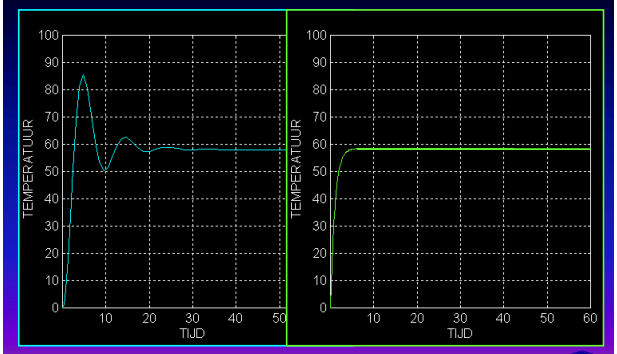
BIOMATH

Model-based Control: MBPC (Model Based Predictive Control)



BIOMATH

Controller tuning



BIOMATH

Use of Models in Decision Support

- Wastewater treatment plant design
  using Economic Cost calculations ==> MoSS-CC
- Integrated urban water management
  using sewer/WWT/river models ==> Brussels
- Environmental Risk Assessment of
  "down-the-drain" chemicals ==> GREAT-ER

BIOMATH

MoSS-CC project

Model based Simulation System
for Cost Calculation

- Calculation of the investment cost
  of a new or upgrade WWTP design
- Calculation of the (fixed & variable) operating costs
  of a new or upgrade WWTP design

=> Better design

BIOMATH

Investment Cost Relationships

- Power laws are applied:

$$COST = \Theta(Process\ Size)^n$$

- *Process size:* an easy to measure plant characteristic:
  - volume
  - area
  - length
  - design flow rate
  - pumping capacity
  - installed mechanical power

BIOMATH

Operating Cost Relationships

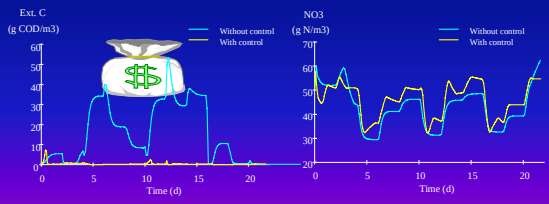
- Maintenance costs ==> proportional to investment
- Sludge treatment/disposal costs
- Pumping energy
- Aeration energy
- Mixing energy
- Effluent taxes

→ SIMULATION

Example of Cost Reduction

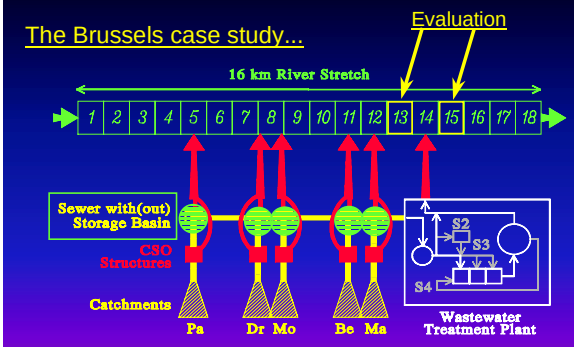
- Industrial plant with nitrogen problem:
  Question: Include automatic control or not ?

External Carbon for Denitrif. | Effluent nitrate conc.

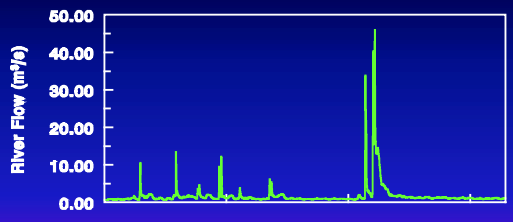


Integrated Urban Water Management

The Brussels case study...



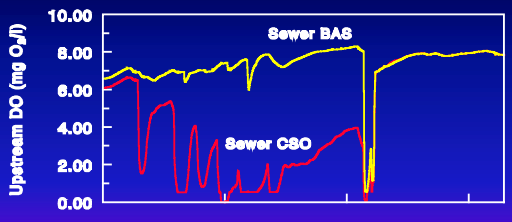
Effect of 2 design options (BAS/CSO) on River Water Quality



One big and several small rain events in summer '86

River Water Quality (oxygen)

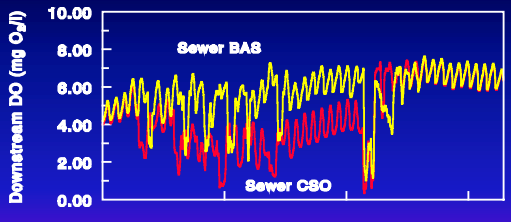
Downstream of CSO, Upstream of WWTP



Clear beneficial effect of retention basins (BAS) in sewer !

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 Regional Exposure Assessment Tool for European Rivers

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

BIOMATH

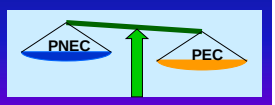
Environmental Risk Assessment

- 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 ?

BIOMATH

Environmental Risk Assessment

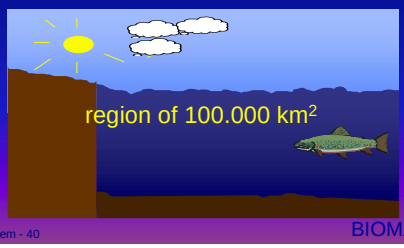
- Aim = **assess** the probability and severeness of negative **effects** on ecosystems after exposure to **chemicals**
- steps:
  - **exposure**: Predicted Environmental Concentration **(PEC)**
  - **effects**: Predicted No Effects Concentration **(PNEC)**
  - **risk ratio**: $\frac{PEC}{PNEC} < 1$?



BIOMATH

Environmental exposure assessment

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



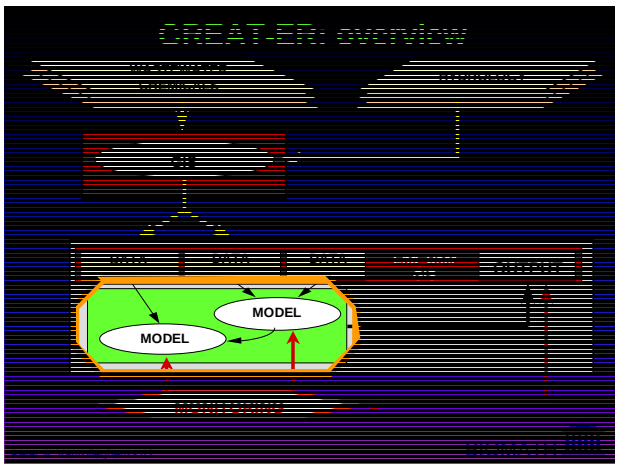
BIOMATH

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

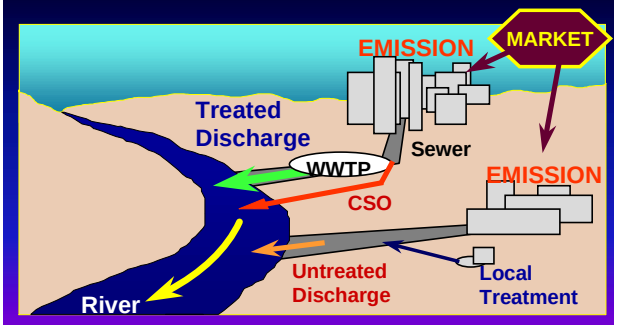
BIOMATH



Overall simulation approach

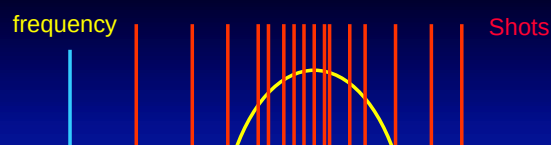
– 'Steady state' models (no dynamics)
– Stochastic / deterministic
– Input / Output - Statistical distributions
- Geo-referenced

Deterministic Model

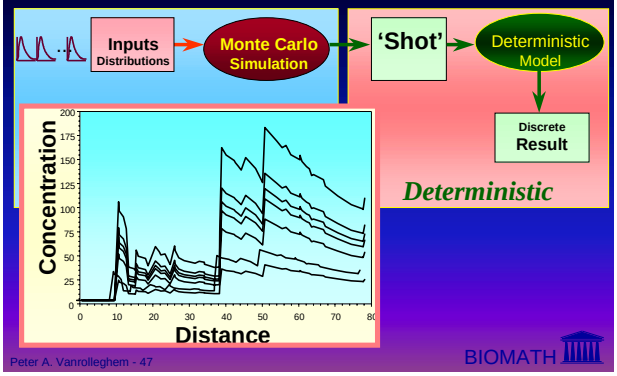


Stochastic simulation

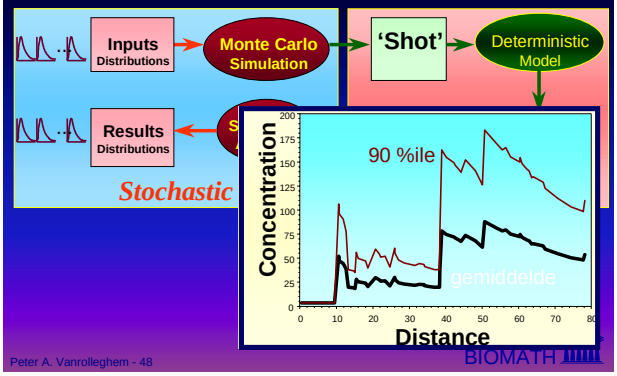
Monte Carlo simulation



Stochastic simulation

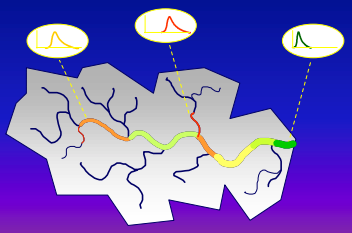


Stochastic simulation



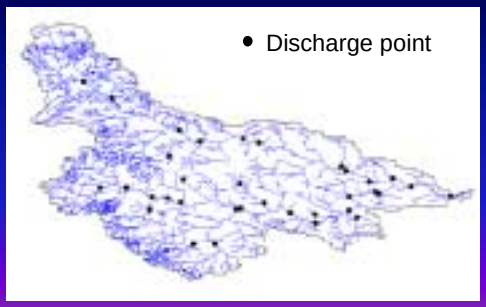
Analysis

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



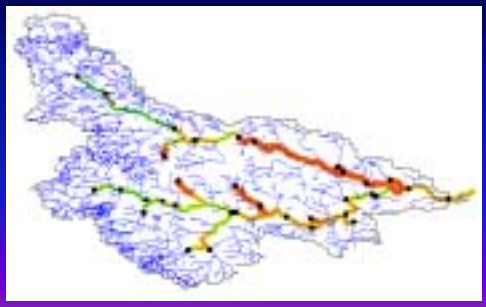
GREAT-ER Validation

Catchment in Yorkshire (UK)

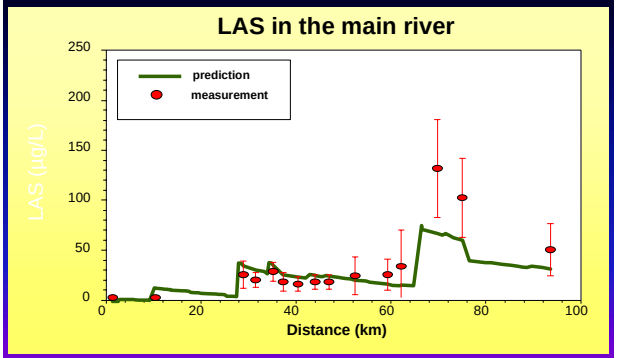


GREAT-ER Validation

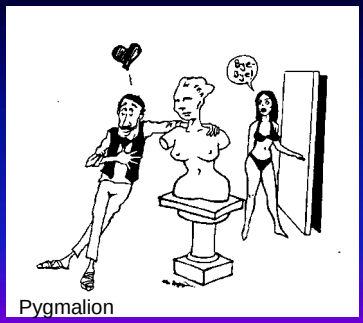
LAS concentrations in the river stretches



Validation of GREAT-ER



"Do not fall in love with your model"

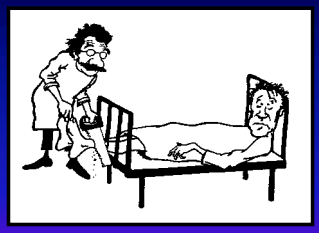


Pygmalion

Epilogue

Models are and can be very useful,
but they are only an approximate description of reality

Procrustes bed:
(Greek mythology)



"Do not adjust reality to the model"

Modelling should be done
with knowledge in the field !