Meta-tools:
Helping engineers select adequate modelling methods

Watermatex2011

San Sebastian
Spain

20 June 2011

Peter VANROLLEGHEM

Canada Research Chair in Water Quality Modelling

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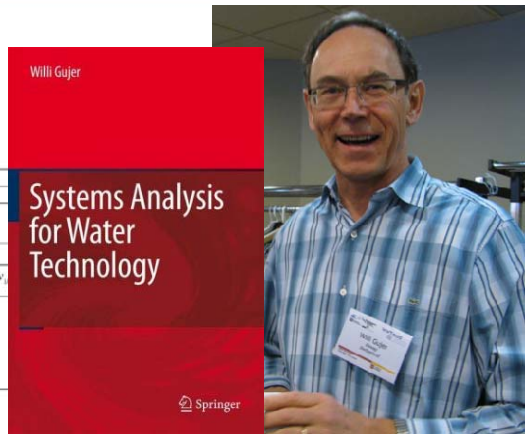
modelEAU

A tribute ...

- Willi Gujer: eawag, Zurich

Compound →	i	1	2
j	Process ↓	X_B	S_S
1	Growth	1	$-\frac{1}{Y}$
2	Decay	-1	
Observed Conversion Rates M L^{-3}T^{-1}		$r_j = \sum_i r_{ij} = \sum_i \nu_{ij} \rho_j$	
Stoichiometric Parameters: True growth yield: Y		Biomass M$_{COD}$ L^{-3}	Substrate M$_{COD}$ L^{-3}



A tribute ...

- Willi Gujer @ LET2005
  Sapporo, Japan, June 2005:

eawag aquatic research

Activated Sludge Modeling:
Past, Present and Future

Willi Gujer
Swiss Federal Institute of Technology, ETH, and
Swiss Federal Institute of Aquatic Science and Technology, EAWAG

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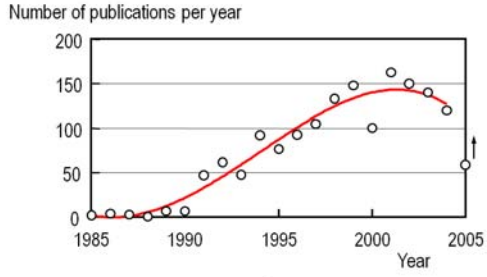
A tribute ...

- Willi Gujer
  @ LET2005:

ASM is not leading edge any more!



Total number of papers 1503 in 30 yrs
Key words in *Web if Science*®:
activated AND sludge AND model

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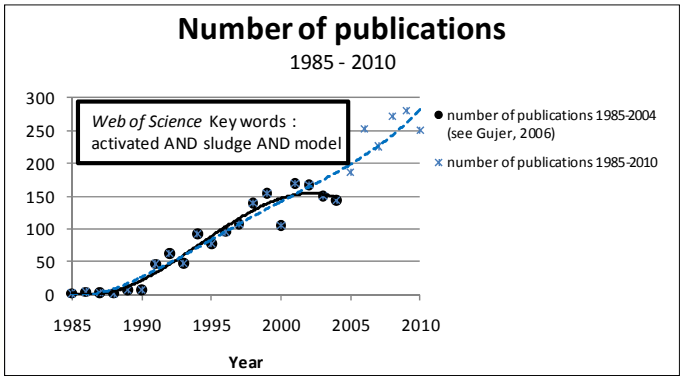
A tribute ...

- A little side note: The GMP Task Group STR:



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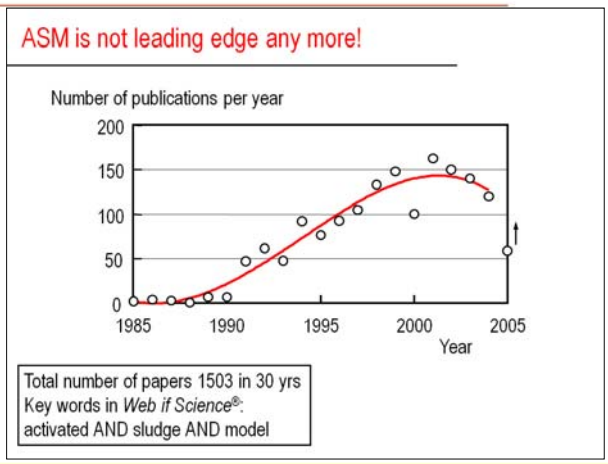
A tribute ...

- Willi Gujer @ LET2005:



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A tribute ...

- Willi Gujer @ LET2005:

Conclusion

- Activated sludge modeling is a mature technology
- Research now concentrates on scientific resolution
- Activated sludge modeling was leading edge in the 1980ties and 1990ties
- Return on research money is decreasing

In view of the global challenge to provide water and sanitation for all, I call for the liberation of scarce intellectual resources and therefore I call for an
Activated sludge model development moratorium

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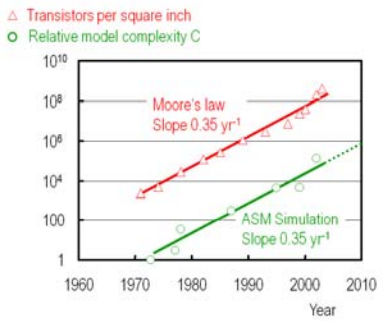
A tribute ...

- Willi Gujer @ LET2005:

Computing power determines model complexity



1965:
Gordon Moore
Director of an IT company

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A tribute ...

- Willi Gujer @ LET2005:

The future is where computational power is required!

Parameter identification (multiple computations)
Partial differential equations (local resolution)
Uncertainty propagation (MC)
Expert knowledge and Bayesian statistics (MCMC)
Single organism behavior
Model based process control (on line)

A tribute ...

- Peter Vanrolleghem @ Watermatex2004:

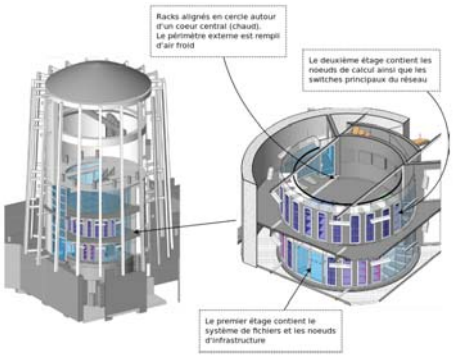
A tribute ...

- Peter Vanrolleghem
  @ model*EAU*

- Access to Laval's Colosse
  - Cluster computer
    97th in world Top 500 (Jun11)
  - 8000 compute cores
    24 TB RAM
    HDD: 4 DVD/s (17 GB/s)
  - In an old particle accelerator
  - Water & Energy ...

A tribute ...

- Peter Vanrolleghem
  @ model*EAU*

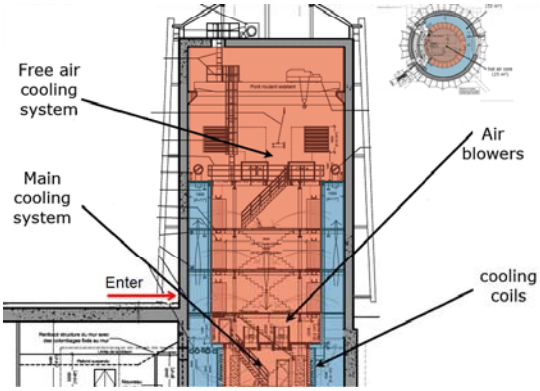


A tribute ...

- Peter Vanrolleghem
  @ model*EAU*

A tribute ...

- Peter Vanrolleghem
  @ model*EAU*



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Introduction

- Willi Gujer's favourite question to his students:

AND

WHAT ABOUT

THE FISH?

Meta-tools:
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Introduction

- Observation (both in my own work and in literature):
  - Much recent research in the modelling field deals with method comparison
- Hypothesis:
  - Water industry appears in need for help in choosing the right method for modelling work
  - Water industry is NOT in need for new methods

Content

- My observations:
  - Control strategy development (*BSM TG*)
  - Verification of model implementation (*Hauduc, 2010*)
  - Process Monitoring methods (*BSM TG*)
  - Life cycle assessment (*LCA papers, Watermatex*)
  - Quality evaluation of models (*Hauduc, Watermatex*)
  - Optimization methods (*PVR & Keesman, 1996*)
  - Numerical solvers for ODE models (*Claeys, 2008*)
  - Sensitivity analysis methods (*Mannina, Watermatex*)
  - Uncertainty analysis methods (*DOUT TG*)

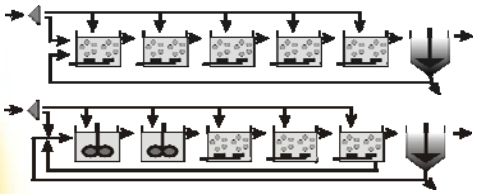
Control strategies

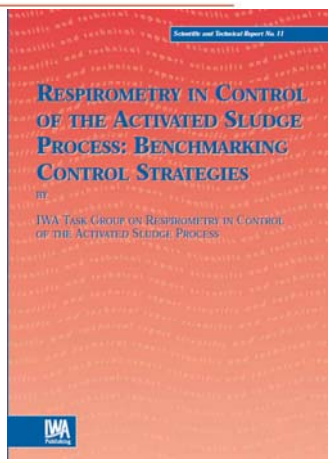
- Bibles of control theory (Levine, 2000+ pages)
- Is wastewater treatment that special that we need new control theory?
- PID, On/off, Cascade, Rule-based control does the job !

- Which control strategy to use ?
- Difficult to compare in full-scale !
- TG Respirometry → Benchmarking (Carlsson, '93)

Control strategies

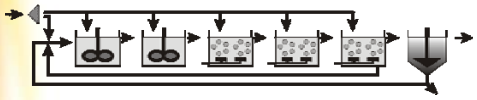
- IWA STR (Copp et al., 2002)
- CAS, NAS, BNR systems

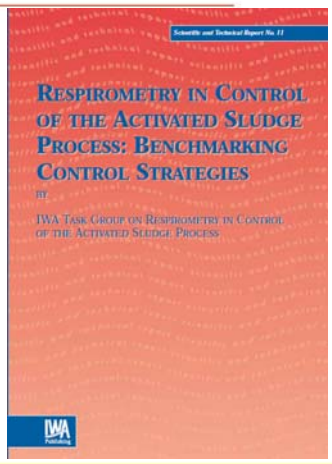




Control strategies

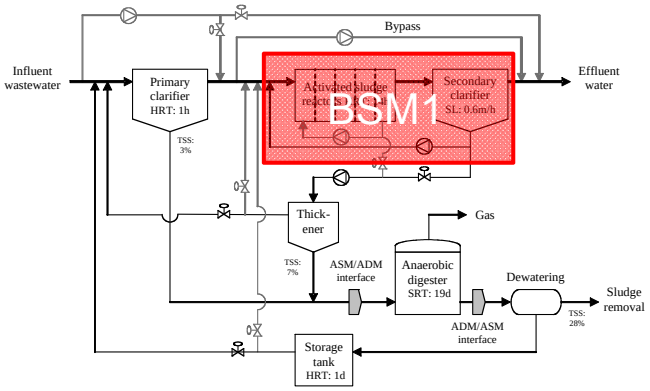
- IWA STR (Copp et al., 2002)
- CAS, NAS, BNR systems
- Evaluation of strategies
  - 3 on Energy Savings
  - 3 on Effluent Quality
  - 3 on Variability Reduction
  - 5 on Toxicity Protection





Control strategies

- Benchmark Simulation Model No.1 and 2



Control strategies

- BSM model evaluation and selection
  - ASM1 (Henze et al., 1987)
  - Secondary settler (Takacs et al, 1991)
  - ADM1 (Batstone et al., 2002)
  - Primary settler (Otterpohl & Freund, 1992)
- These models got increased credibility and use
- Implementations were verified (Copp et al. 1998)
- They were scrutinized for errors

Model verification

- Method for verification of model correctness

825 © IWA Publishing 2010 Water Science & Technology—WST | 61.4 | 2010

A systematic approach for model verification: application on seven published activated sludge models

H. Hauduc, L. Rieger, I. Takács, A. Héduit, P. A. Vanrolleghem and S. Gillot

ABSTRACT

The quality of simulation results can be significantly affected by errors in the published model (typing, inconsistencies, gaps or conceptual errors) and/or in the underlying numerical model description. Seven of the most commonly used activated sludge models have been investigated to point out the typing errors, inconsistencies and gaps in the model publications: ASM1; ASM2d; ASM3; ASM3 + Bio-P; ASM2d + TUD; New General; UCTPHO+. A systematic approach to verify

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Model verification

- ASM-type models
- Continuity check (Excel)
  → Stoichiometry correction

ASM1 Composition matrix

		Elements		
		COD	N	Charge
1	S_I	1	0	0
2	S_S	1	0	0
3	X_I	1	0	0
4	X_S	1	0	0
5	$X_{B,H}$	1	0.086	0
6	$X_{B,A}$	1	0.086	0
7	X_P	1	i_{XP}	0
8	S_O	−1		0
9	S_{NO}	−4.57	1	−0.071
10	S_{NH}	0	1	0.071
11	S_{ND}	0	1	0
12	X_{ND}	0	1	0
13	S_{ALK}	0	0	−1
14	S_{N2}	−1.71	1	0

ASM1 Gujer matrix
(S_{N2} has been added for continuity)
i: state variable
j: process
v_{ij}: stoichiometric coefficient (calculated from parameter values of Henze *et al.*, 2000)

i	1	2	3	4	5	6	7	8	9	10	11	12	13	14	
j	S_I	S_S	X_I	X_S	$X_{B,H}$	$X_{B,A}$	X_P	S_O	S_{NO}	S_{NH}	S_{ND}	X_{ND}	S_{ALK}	S_{N2}	
1	Aerobic growth of heterotrophs		−1.49			1			−0.49		−0.09			−0.006	
2	Anoxic growth of heterotrophs		−1.49			1				−0.17	−0.09			0.006	0.172
3	Aerobic growth of autotrophs						1		−18.04	4.17	−4.25			−0.50	
4	Decay of heterotrophs				0.92	−1		0.08					0.081		
5	Decay of autotrophs				0.92		−1	0.08	v_{ji}				0.081		
6	Ammonification of soluble organic										1	−1		00.07	
7	Hydrolysis of entrapped organic		1		−1										
8	Hydrolysis of entrapped organic N											−1	1		

10^{-15}	10^{-15}	10^{-15}
10^{-15}	10^{-15}	10^{-15}
10^{-15}	10^{-15}	10^{-15}
10^{-15}	10^{-15}	10^{-15}
10^{-15}	10^{-15}	10^{-15}

$\Sigma_i\ v_{ij} \cdot i_{iC} = 10^{-15}$

Model verification

- ASM-type models
- Four questions to find kinetic inconsistencies
  - Consumed components → limitation function
  - Involved biomass → biomass in rate
  - Environ. conditions (e.g. DO) → limitation function
  - Inhibitory components → inhibitory function

Model verification

- ASM-type models

Modèle	Stoichiometry	Kinetics
ASM1(Henze *et al*., 2000)	1	2
ASM2d (Henze *et al*., 2000)	3	4
ASM3 (Gujer *et al*., 2000)	0	0
ASM3+BioP (Rieger *et al.*, 2001)	2	6
Barker & Dold (Barker and Dold, 1997)	16	12
UCTPHO+ (Hu *et al.*, 2007)	50	20
ASM2d+TUD (Meijer, 2004)	1	7

Process monitoring

- Fault-detection and diagnosis for robust or fault-tolerant control
- Same problem as for control strategy choice:
  - Many methods exist
  - No objective way to asses their performance

Process monitoring

- BSM1_LT (long-term) with:
  - Sensor/Actuator and fault models (including toxicity)
  - A monitoring performance index (punishment for false alarms, false acceptance)
  - Performance of univariate fault detection methods

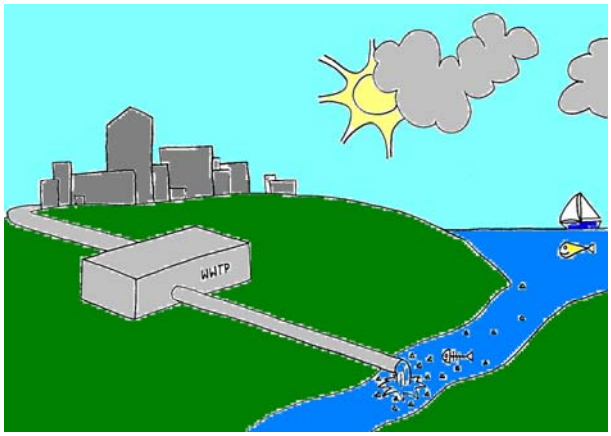
ARTICLE

BIOTECHNOLOGY AND BIOENGINEERING

Performance Evaluation of Fault Detection Methods for Wastewater Treatment Processes

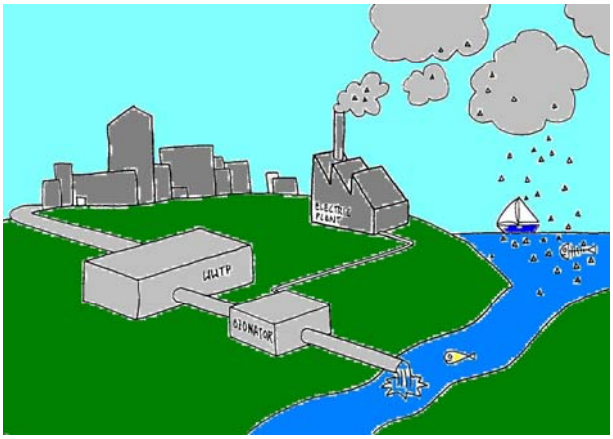
Lluís Corominas,[1] Kris Villez,[1,2] Daniel Aguado,[3] Leiv Rieger,[1] Christian Rosén,[4] Peter A. Vanrolleghem[1]

Life Cycle Assessment (LCA)



Peter
Augusto
Hansen

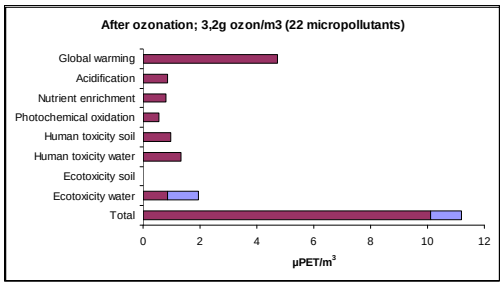
Life Cycle Assessment (LCA)



Peter
Augusto
Hansen

Life Cycle Assessment

- Multiple methods (even though ISO 14040)
- No consensus on criteria to evaluate
  - Global warming
  - Acidification
  - Eutrophication
  - Human toxicity
  - Ecotoxicity
  - ...



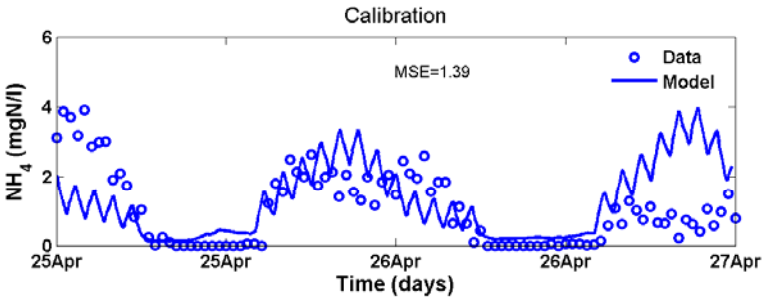
Life Cycle Assessment

- Multiple methods (even though ISO 14040)
- No consensus on criteria to evaluate
  - Global warming
  - Acidification
  - Eutrophication
  - Human toxicity
  - Ecotoxicity
  - ...

- Different normalisation/valuation approaches
- Functional unit definition is critical, but unclear
- WWT is not positive (see Godin @15:30,OP.18,S.09)

Model quality evaluation

- Different objective functions are used for comparison of predicted and observed values

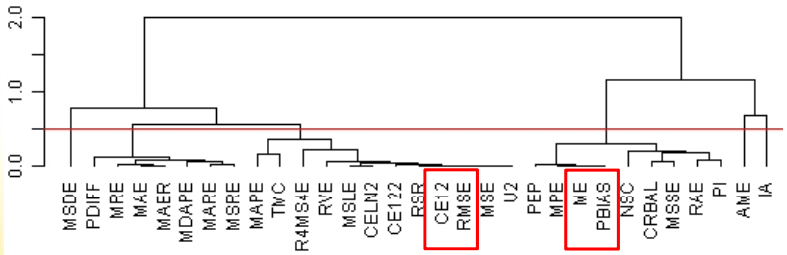


Model quality evaluation

- Multiple reviews (especially in hydrology) exist listing/comparing objective functions
- Still, the choice of objective function remains a problem for the water engineer:
  - ME: Mean Error
  - PBIAS: Percent Bias
  - RMSE: Root Mean Square Error
  - CE: Nash-Sutcliffe Efficiency
  - ...

Model quality evaluation

- Do these criteria express different objectives?
- No! (see Hauduc at 9:30, OP.03, S.03)



- Further work is required to help select criteria

Optimization methods

- Many books on numerical optimization
- Help may be useful for water engineers
  - Comparison of optimizers
    e.g. Vanrolleghem & Keesman (1996)

Table 4. NPE results for double Monod model to OUR_{ex} data-set (N=323, m=6)

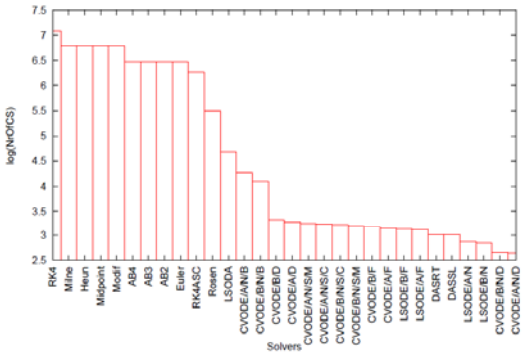
	μ_{max1} (/d)	K_{s1} (mg/l)	μ_{max2} (/d)	K_{s2} (mg/l)	$S_1(0)$ (mg/l)	$S_2(0)$ (mg/l)	MSE (*10^5)	Runs
BFGS	0.344	0.449	0.173	1.414	17.859	31.984	92.01	39
Brent	0.340	0.385	0.172	1.419	17.930	32.051	74.22	37
Simplex	0.358	0.603	0.171	1.423	18.387	31.771	111.86	26
Jackknife	0.337	0.358	0.171	1.361	17.823	31.948	75.59	37
Set-Memb	0.413	0.860	0.148	1.215	20.940	28.723	729.06	8

Numerical solvers for ODEs

- Many numerical solvers for ODEs
  - How to select them among the list ?
  - How to choose their settings ?
- May make quite a difference in time to get the answer to your question
  - Optimizations
  - Uncertainty analysis
  - Sensitivity analysis
  - Scenario analysis

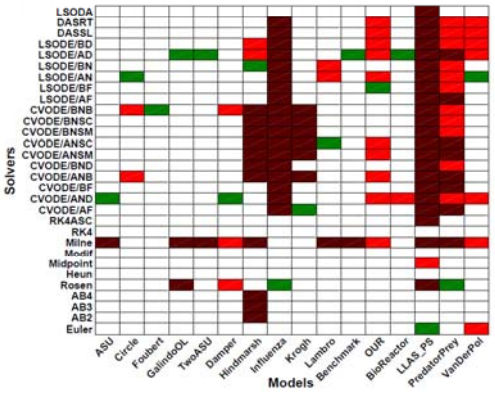
Numerical solvers for ODEs

- Many numerical solvers for ODEs
- Claeys (2008)
  - 30 solvers
  - Number of Compute states
  - 3 log scales speed-up !



Numerical solvers for ODEs

- Many numerical solvers for ODEs
- Study by Claeys
  - 30 solvers
  - Correct solution? (16 models tested)
    - Failure
    - Anomaly
    - Best solver
    - OK solver



Sensitivity analysis

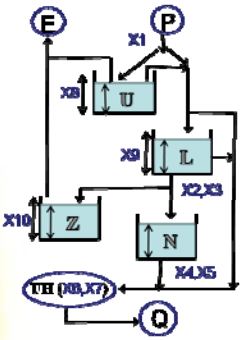
- How much does a variable change when I change a factor of the model (parameter, input)?
- Local sensitivity analysis
  - For the nominal value of the parameters
  - Numerical or symbolic derivation → Different methods
- Global sensitivity analysis
  - For a range of parameter values
  - Numerical derivation → Different methods

Sensitivity analysis

- Studies of Global Sensitivity Analysis methods
  - Computational load (Nr of required simulations)?
  - Importance ranking of factors similar?
- Often compared methods:
  - SRC (standardized regression coefficients)
  - Morris screening method
  - FAST method
  - Sobol's method
- Example of comparison: Mannina, OP.66, S.25

Sensitivity analysis

- Manandraitsiory Randrianantoandro (2011)
- Mordor10 model



Parameters	SRC	MORRIS		FAST		SOBOL 2002	
		mu*	sigma	Elementary	Total	Elementary	Total
X1	0.5537	0.8259	1.0383	0.5174	0.7612	0.4715	0.7367
X2	0.0310	0.4335	3.4560	0.0028	0.0379	0.0052	0.0189
X3	0.1822	0.3199	0.9758	0.0546	0.2583	0.0642	0.2672
X4	0.1246	0.1688	0.3845	0.0130	0.0799	0.0260	0.0482
X5	0.1013	0.2013	0.4316	0.0405	0.2212	0.0325	0.2093
X6	0.1235	0.1579	0.3118	0.0200	0.0938	0.0167	0.0616
X7	0.0802	1.7063	50.6556	0.0160	0.1064	0.0172	0.0530
X8	0.0643	0.0609	0.0808	0.0043	0.0306	0.0027	0.0072
X9	0.0913	0.1309	0.2269	0.0118	0.0705	0.0103	0.0443
X10	0.0265	0.0436	0.0834	0.0010	0.0238	0.0017	0.0016

Uncertainty analysis

Benedetti, 2006

Uncertainty analysis

- Gets increasing attention in the water field
  - Has been covered for a long time in hydrology
  - EU Water Framework Directive
  - International Working Group on Data and Models (under Joint IWA/IAHR Committee Urban Drainage)
  - Design and Operations Uncertainty Task Group

Uncertainty analysis

- Different methods exist to:
  - Assess uncertainties in parameters, model structure
    - Bayesian vs. Frequentist approaches
    - Much development is still required
  - Propagate uncertainties into model predictions
    - Linear error propagation for moderately nonlinear models
    - Monte Carlo methods of different kinds
    - Mature technology, but no guidance exists really
- If you want to know more, come to OP.08, S.05

Take home

- Observation (both in my own work and in literature):
  - Much recent research in the modelling field deals with method comparison
- Hypothesis:
  - Water industry appears in need for help in choosing the right method for modelling work
  - Water industry is NOT in need for new methods

Take home

- Many methods are around
  - Both in each of the water fields
  - and in other water fields, ready to be transferred
- What we don't need:
  - Further method development (moratorium)
- What we do need:
  - Synthesis, comparison, consolidation, ...
  - Guidance to method users, Decision trees, ...

  One size fits all won't work

Take home

OFF YOU GO!

GO AND CREATE META-TOOLS (TOOLS ABOUT TOOLS)