Applications of optimization

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Contents

- What is relevant in solving practical problems?
- Examples from the latest issues of *Optimization and Engineering* journal
- Different phases of solving practical problems
  - Example: wastewater treatment plant design & operation

Topology optimization in micromechanical resonator design

- Micromechanical resonators are important elements in the design of on chip signal processing systems
- The central task in topology optimization is to determine which geometric points in the design domain should be material points and which points should contain no material (i.e., are void)
  - Large scale integer optimization problem → converted into a continuous problem that is easier to solve by material interpolation functions
- Design goal: to control the first several eigen-frequencies of a micromechanical resonator using topology optimization

He et al., Topology optimization in micromechanical resonator design, *Optimization and Engineering*, **13**, 271-292, 2012

Optimization problem

- Modelled by PDEs
- ω_k are the eigen-frequences, $\bar{\omega}_k$ are pre-specified target eigen-frequencies
- $0 \le p_i \le 1$ are design variables (element-wise constant in a finite element discretization)
- Number of variables depends on the discretization

$$\min_{\substack{p_i \\ i=1,nelt}} \sum_{k=1}^{n} \left| \frac{\omega_k(p_i) - \overline{\omega}_k}{\overline{\omega}_k} \right|$$

$$g = \sum_{i=1}^{nelt} \theta_i (1 - \theta_i) = 0.$$

$$H(\boldsymbol{p}) = 0,$$

$$H(\boldsymbol{p}) = \sum_{i,j} h(\theta_{i,j}, \theta_{i+1,j}, \theta_{i,j+1}, \theta_{i+1,j+1})$$

He et al., Topology optimization in micromechanical resonator design, *Optimization and Engineering*, **13**, 271-292, 2012

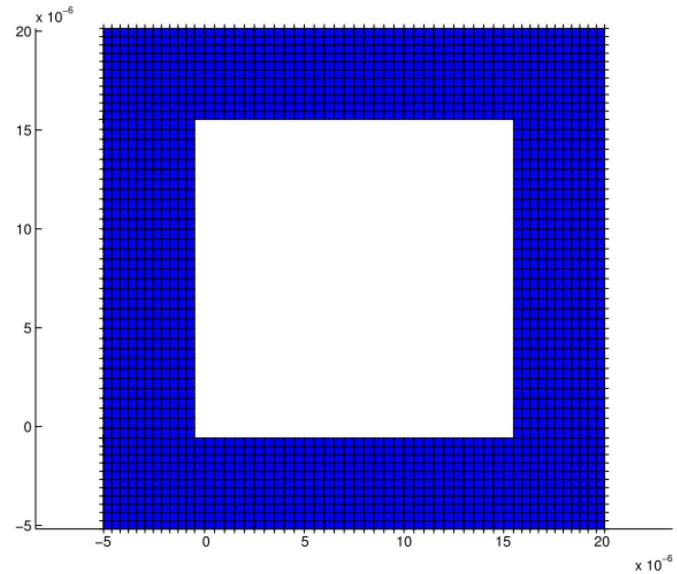
Methods

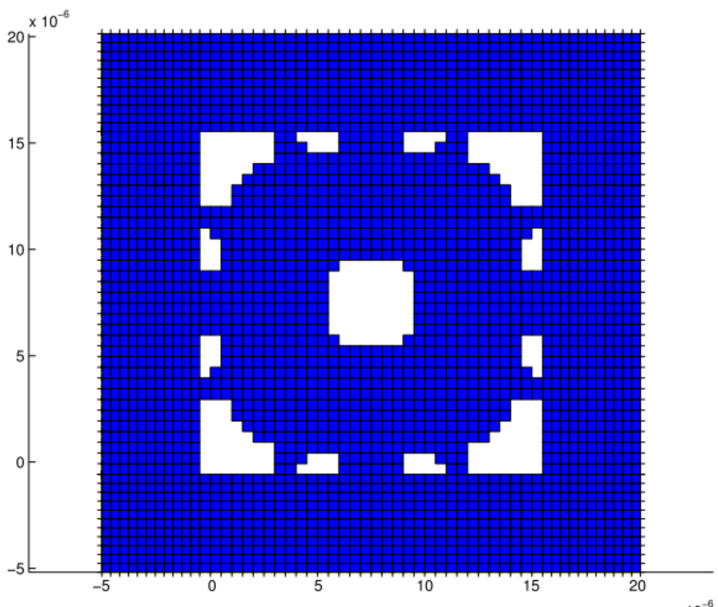
- Two methods used
  - Hybrid genetic algorithm (GA)
  - Method of moving asymptotes (MMA)
- Hybrid GA (Matlab utilized)
  - GA hybridized with a quasi-Newton method (BFGS)
  - Constraints handled by penalty function
  - Global optimization method
- MMA (developed for structural optimization)
  - Solves a sequence of convex approximating subproblems
  - Subproblems convex and separable → can be efficiently solved by a dual method
  - Local optimization method

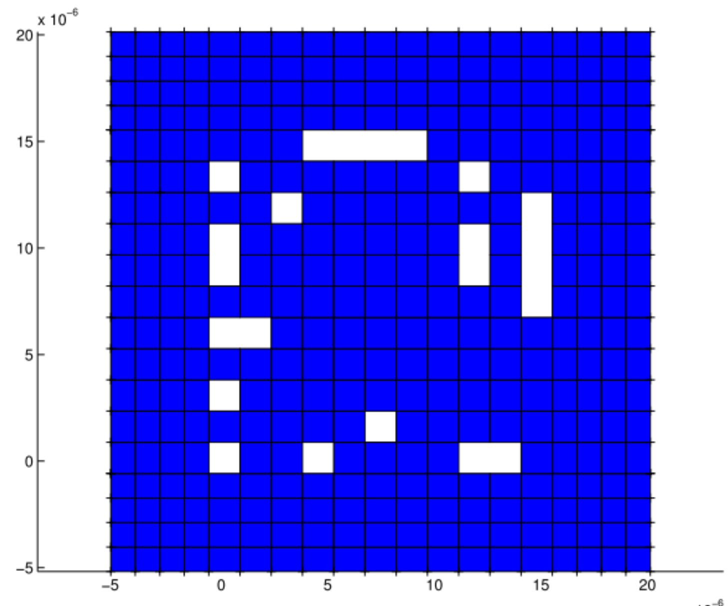
He et al., Topology optimization in micromechanical resonator design, *Optimization and Engineering*, **13**, 271-292, 2012

Results

- Top: design domain
- Bottom: optimal topology for the first two eigen-frequencies around 1.04 GHz
  - left: MMA (1024 variables)
  - right: hybrid GA (121 variables)







He et al., Topology optimization in micromechanical resonator design, *Optimization and Engineering*, **13**, 271-292, 2012

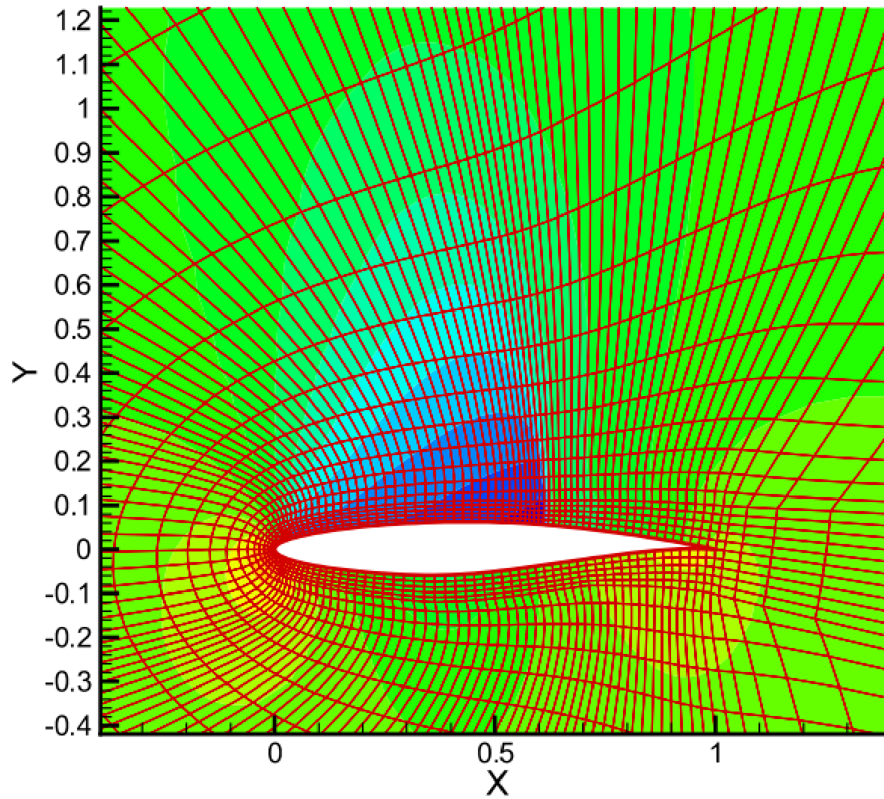
Efficient aerodynamic shape optimization by structure exploitation

- Optimization problem for the complete design chain of an airfoil
- Drag (C_D) and lift (C_L) important properties in airfoil design
  - Drag needs to be minimized
- Model based on Computational Fluid Dynamics (CFD)

Gauger et al., Efficient aerodynamic shape optimization by structure exploitation, *Optimization and Engineering*, **13**, 563-578, 2012

Example of an airfoil

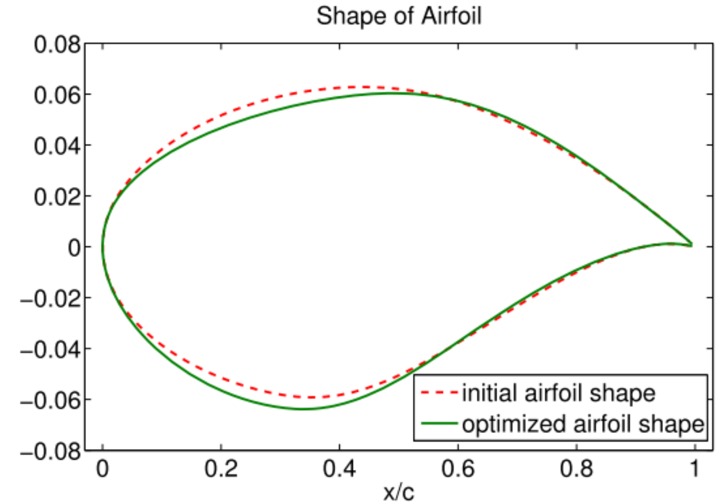
- Evaluating the objective function
  - Generate a grid around the airfoil
  - Compute the flow around the airfoil
  - Compute the objective
- Gradients computed by automatic differentiation
  - Other options: finite differencies or adjoint approaches



Gauger et al., Efficient aerodynamic shape optimization by structure exploitation, *Optimization and Engineering*, **13**, 563-578, 2012

Results

- Shape is updated by a parameterized deformation
  - 20 parameters are variables of the optimization problem
- Gradient-based optimization
  - IPOPT interior point method from the COIN-OR webpage



$$\min_{p} J(x) = C_D \quad \text{s.t.} \quad C_L \geq C_{Li},$$

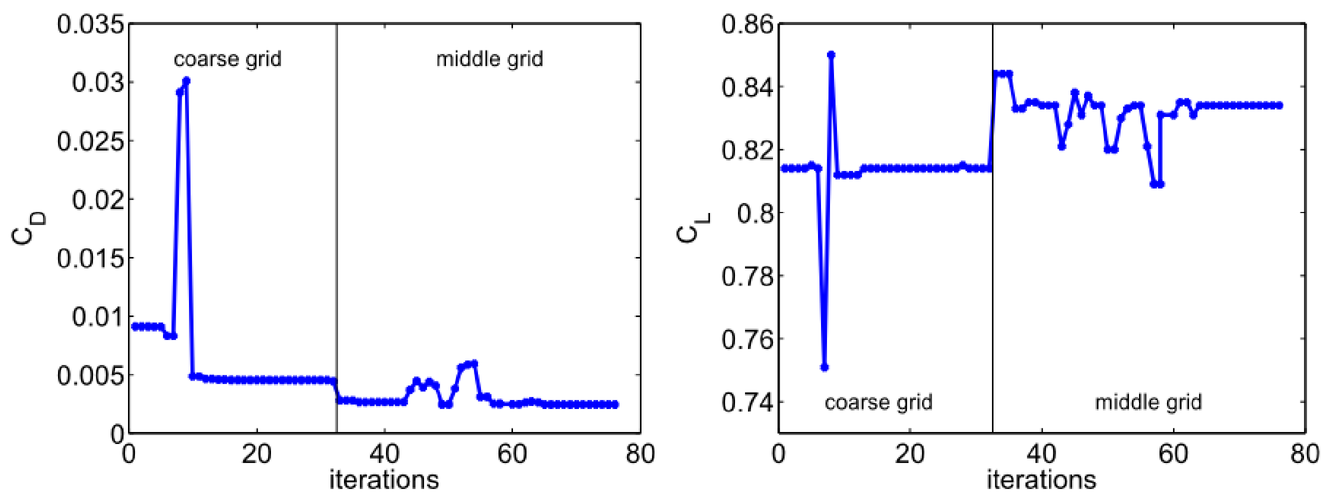
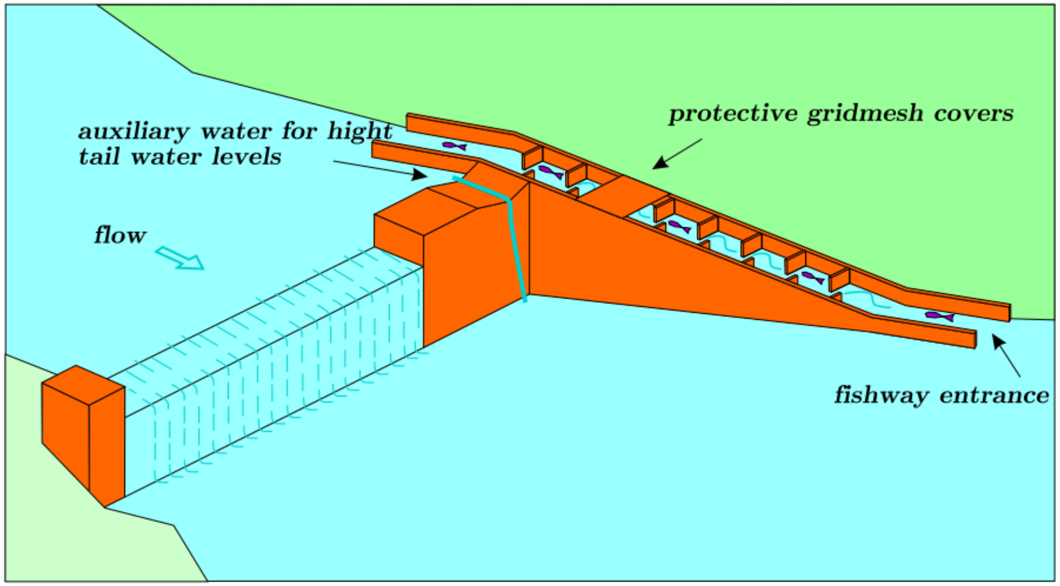


Fig. 11 Optimization history of drag (C_D) and lift (C_L) coefficient during optimization using multilevel approach

Gauger et al., Efficient aerodynamic shape optimization by structure exploitation, *Optimization and Engineering*, **13**, 563-578, 2012

On the optimal design of river fishways

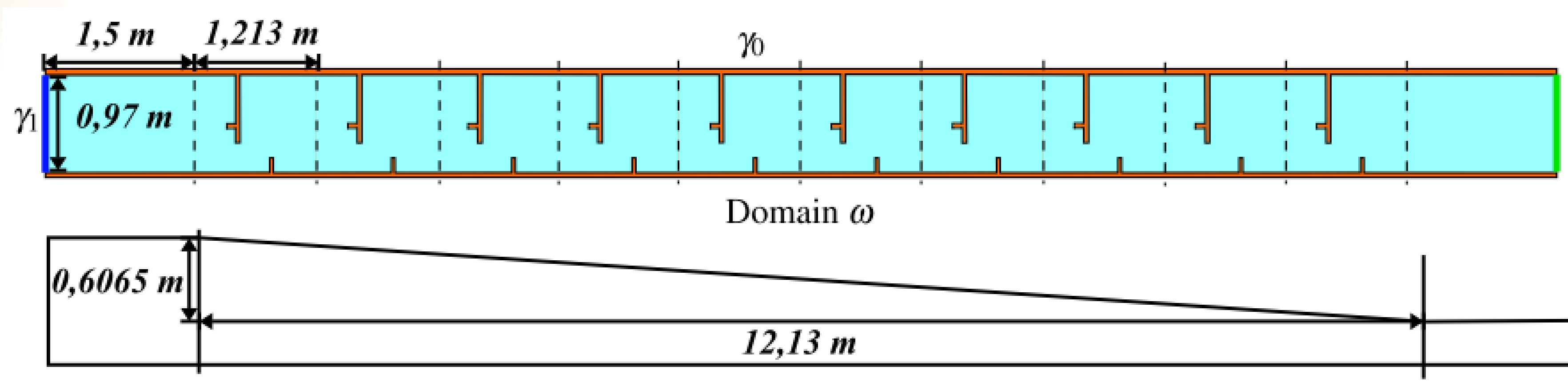
- A river fishway is a hydraulic structure enabling fish to overcome stream obstructions such as dams in hydroelectric power plants
- Aim: present an application of mathematical modeling and optimal control theory to an ecological engineering problem related to preserve and enhance natural stocks of fish migrating between saltwater and freshwater



Alvarez-Vazquez et al., On the optimal design of river fishways, *Optimization and Engineering*, **14**, 193-211, 2013

Task

- Optimal shape of the fishway can be used to directly control the water velocity
- Model based on CFD (2D shallow water equations)
- Flow turbulence must be minimized
- The velocity of the water must be close to a target velocity
- Shape of the fishway is controlled by six design variables



Alvarez-Vazquez et al., On the optimal design of river fishways, *Optimization and Engineering*, **14**, 193-211, 2013

Problem

- Min $J=\frac{1}{2}\int_0^T\int_\omega\left\|\frac{\mathbf{Q}}{H}-\mathbf{v}\right\|^2+\frac{\xi}{2}\int_0^T\int_\omega\left|curl\left(\frac{\mathbf{Q}}{H}\right)\right|^2,$

$(s_1,s_2,s_3,s_4,s_5,s_6)^T\in\mathbb{R}^6$

- s.t.

$$\begin{cases}\dfrac{\partial H}{\partial t}+\nabla\cdot\mathbf{Q}=0 & \text{in } \omega\times(0,T),\\ \dfrac{\partial \mathbf{Q}}{\partial t}+\nabla\cdot\left(\dfrac{\mathbf{Q}}{H}\otimes\mathbf{Q}\right)+gH\nabla(H-\eta)=\mathbf{f} & \text{in } \omega\times(0,T),\end{cases}$$

$$\begin{cases}H(0)=H_0,\quad \mathbf{Q}(0)=\mathbf{Q}_0 & \text{in } \omega,\\ \mathbf{Q}\cdot\mathbf{n}=0,\quad curl\left(\dfrac{\mathbf{Q}}{H}\right)=0 & \text{on } \gamma_0\times(0,T),\\ \mathbf{Q}=q_1\,\mathbf{n} & \text{on } \gamma_1\times(0,T),\\ H=H_2 & \text{on } \gamma_2\times(0,T).\end{cases}$$

$$\begin{cases}x_{min}=\frac{1}{4}1.213\le s_1,s_3,s_5\le\frac{3}{4}1.213=x_{max},\\ y_{min}=0\le s_2,s_4,s_6\le\frac{1}{2}0.97=y_{max}.\end{cases}$$

$$\begin{cases}\Delta_1=s_3-s_1\ge 0.1=h_1,\\ \Delta_2=s_2-s_4\ge 0.05=h_2.\end{cases}\qquad\begin{cases}\Delta_3=s_1-s_5\ge\frac{1}{2}0.0305=d_1,\\ \Delta_4=s_6-s_2\ge\frac{1}{2}0.0305=d_2.\end{cases}$$

Alvarez-Vazquez et al., On the optimal design of river fishways, *Optimization and Engineering*, **14**, 193-211, 2013

Results

- Methods
  - Nelder-Mead (NM)
  - Spectral Projected Gradient (SPG)
- NM (99 hours of CPU time in a laptop with two Intel Pentium 4 microprocessors)
  - 167 function evaluations
- SPG (27.4 hours)
  - Gradients by finite differences
- Starting point had an effect → non-convex problem
- Cost: NM=240.4255, SPG=242.6674

Fig. 7 NM algorithm: Optimal fishway and corresponding water height at final time $T = 300$ s for optimal point: $a_{NM} = (0.7248, 0.1573)$, $b_{NM} = (0.9169, 0.0494)$, $c_{NM} = (0.4450, 0.4727)$. Height values: 0.26 (*blue*), 0.38 (*green*), 0.46 (*yellow*), 0.50 (*orange*), 0.54 (*red*)

Fig. 10 SPG algorithm: Optimal fishway and corresponding water height at final time $T = 300$ s for optimal point: $a_{SPG} = (0.7032, 0.1593)$, $b_{SPG} = (0.9002, 0.0633)$, $c_{SPG} = (0.4076, 0.4238)$. Height values: 0.26 (*blue*), 0.38 (*green*), 0.46 (*yellow*), 0.50 (*orange*), 0.54 (*red*)

Alvarez-Vazquez et al., On the optimal design of river fishways, *Optimization and Engineering*, **14**, 193-211, 2013

Solving optimization problems in practice

- In practice, the following issues need to be considered
  1. **Modelling of the problem**
  2. **Modelling of the optimization problem**
  3. **Choosing an appropriate optimization method**
  4. **Coupling of optimization software and a modelling tool**
  5. **Optimization and analysis of the solution obtained**
- *We go through these steps with the help of an example*

Case study

Wastewater treatment plant design and operation

TIES483 Nonlinear optimization

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Wastewater treatment

- Mathematical modelling of Wastewater treatment plants (WWTPs) began gaining ground in the 1990s
- Majority of modelling considers the activated sludge process (ASP), globally most common process
  - biomass suspended in the wastewater to be treated is cultivated and maintained in an aerated bioreactor
  - wastewater is purified, i.e. organic carbon, nitrogen and phosphorus are removed, during its retention in the bioreactor
  - followed by a clarifier basin, in which the biomass is separated by gravitational settling and returned to the bioreactor
  - treated wastewater is directed as overflow to futher treatment or to discharge

Wastewater treatment plant design

- Nowadays WWTP design faces several challenges
  - operational requirements (notably the effluent limits of nitrogen and phosphorus) more and more strict
  - economical efficiency (e.g., minimizing plant footprint as well as consumption of chemicals and energy) is required
  - operational reliability should be emphasized
- More complex wastewater treatment processes are gaining ground

→ Multiple conflicting evaluation criteria!

The PROSIM project

- Headed by Pöyry Finland Oy (Ltd) in the Modelling and Simulation technology programme of *Tekes, the Finnish Funding Agency for Technology and Innovation*
- The aim is to model some Finnish WWTPs
  - simulation models as a result → can be used to support design and optimization
- Additional aim: find out how multiobjective optimization could benefit design of WWTPs

1. Modelling of the problem

- Collaboration with expert in the application field essential
- Mathematical modelling of the phenomenom → approximating reality
- Numerical simulation model by using a simulator or other modelling tool → enables numerical simulation with fixed values of the decision variables
- **Extremely important for getting reliable results!**

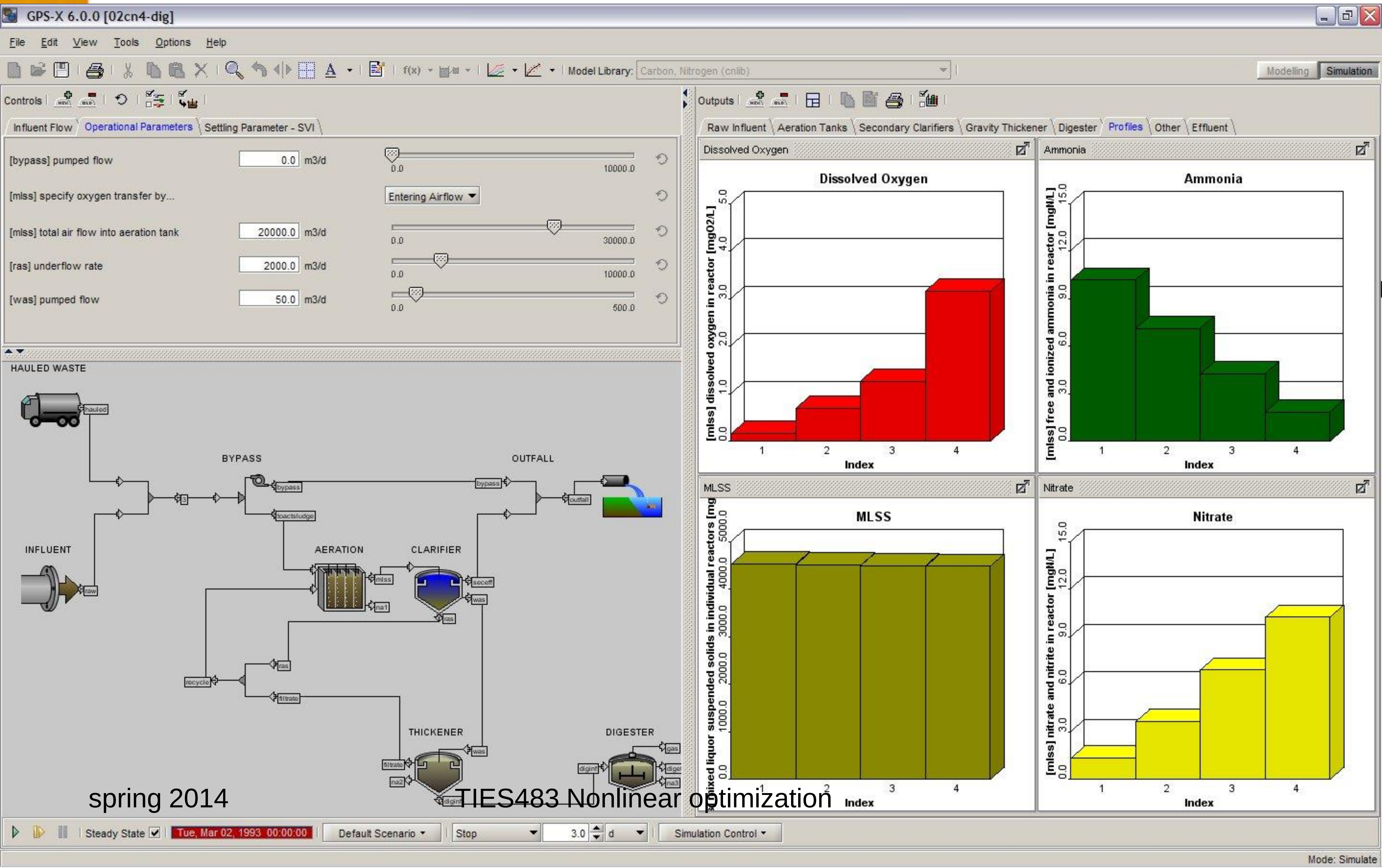
Modelling in the project

- Model was created by an expert in WWTP design in Pöyry
  – had experience in simulation but not in multiobjective optimization
- A commercial simulator was used (GPS-X)
- Two cases: simple one for testing followed by a more realistic one

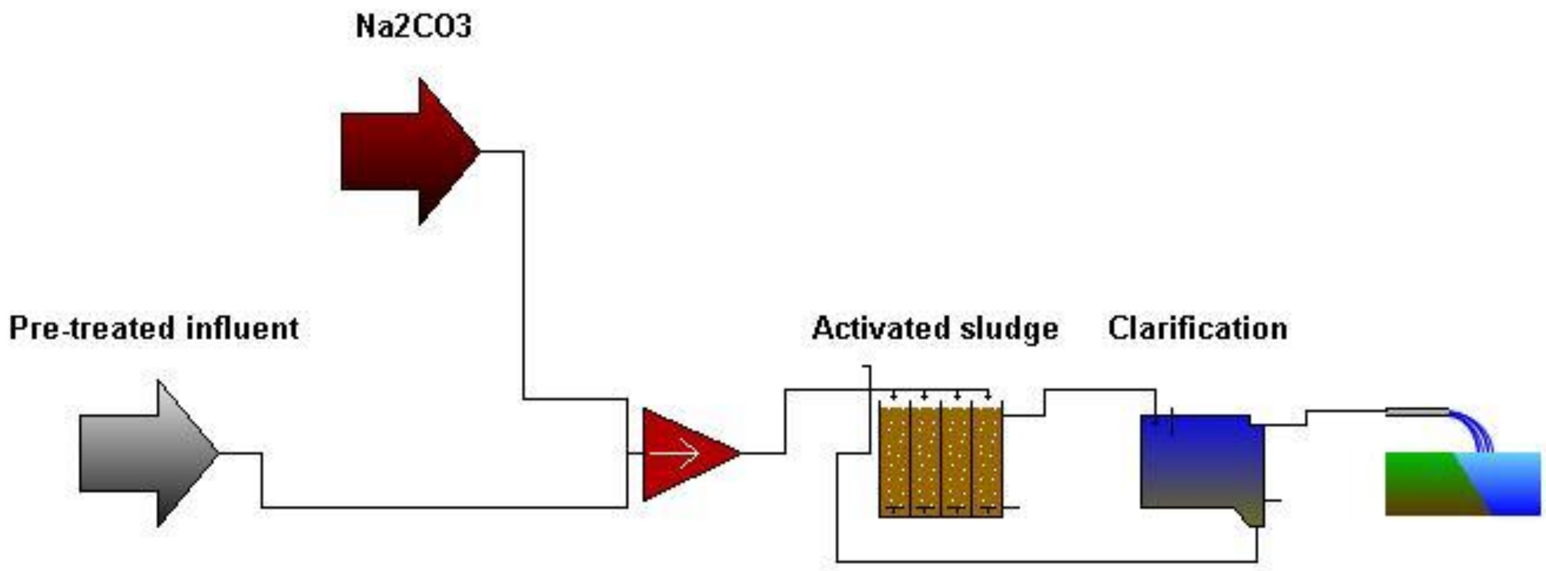
GPS-X

- Commercial process simulator designed for wastewater treatment
  - sold by Hydromantis (Canada)
- http://www.hydromantis.com/GPS-X.html
- Pöyry uses GPS-X in WWTP design
  - technical support available
- Single license about 17k$, academic license 2k$
  - includes technical support and updates for one year
- Pöyry provided JyU a license for the project

Screenshot of GPS-X



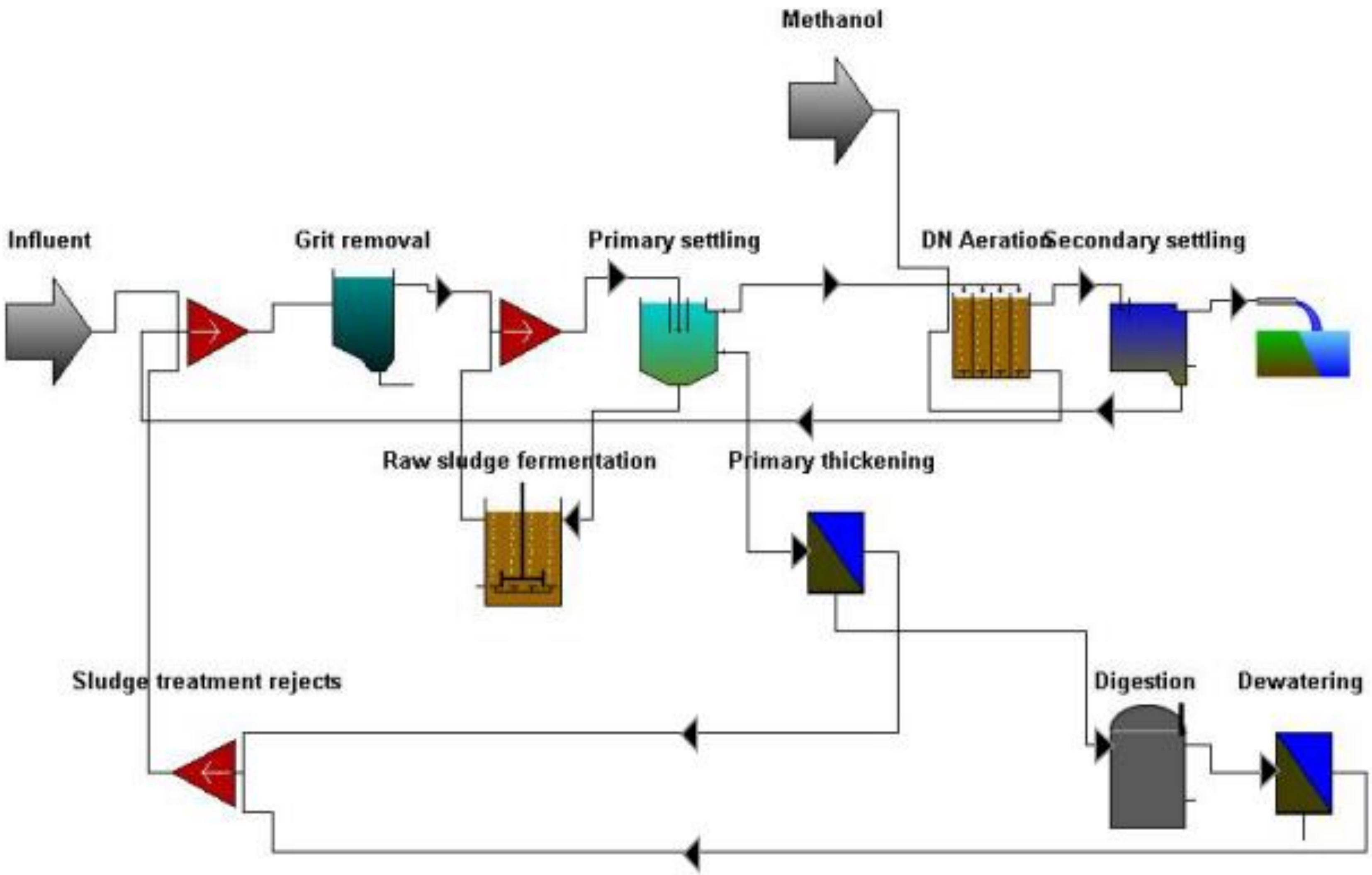
1. Activated sludge process



1. Activated sludge process

- Nitrifying activated sludge process (ASM3 model)
- Performs oxidation of ammonium nitrogen to nitrate nitrogen by biochemical reactions
- Wastewater treated corresponds to typical Finnish mechanically and chemically pre-treated municipal wastewater
- 1 simulation by GPS-X ≈ 5 seconds

2. Plant-wide optimization of operational settings



2. Plant-wide optimization of operational settings

- Model describes a modern WWTP; wastewater is treated chemically and biologically
  - pre-treatment (grit removal, solids separation)
  - nitrogen removal (nitrifying ASP)
  - sludge fermentation ($\rightarrow$ carbon sources for denitrification)
  - anaerobic digestion of sludge ($\rightarrow$ biogas for electricity and/or thermal energy)
  - excess sludge and reject from sludge treatment are recycled by mixing them into influent wastewater
- 1 simulation by GPS-X ≈ 11 seconds

2. Formulation of optimization problem

- Aim of optimization needs to be clear
  - – *what is really wanted from optimization?*
- Definition of the objectives
- Selection of the decision variables and bounds for them
  - – should define an interesting area
- Definition of constraints
- Collaboration between experts in optimization and application area

WWTP design and operation

- Traditionally, WWTP design has been realized
  - as comparing different process schemes using simulation and engineering judgement
  - or as a single objective optimization problem: all the criteria converted into money and total costs are minimized
- Drawbacks
  - first one is not systematic,
  - second one hides interdependencies and contains uncertainties
- Only few papers where multiple objectives have been considered, no interactive approaches

Formulation of the optimization problem in the project

- In collaboration with the expert from Pöyry
- Clear objectives for both cases
- Ranges of the decision variables were adjusted during the project
  – more realistic area in the decision space, makes optimization more efficient

1. Activated sludge process

- Biochemical reactions consume a lot of oxygen and alkalinity
- Oxygen is supplied by aeration compressors and alkalinity by influent wastewater & adding chemicals
- Aeration consumes energy and chemicals cost money
- Biomass concentration should be kept as low as possible

1. Activated sludge process

- Three objective functions to be minimized (conflicting)
  - **residual ammonium nitrogen concentration**
  - **dosage of alkalinity chemical**
  - **consumption of energy by aeration**
- Three decision variables
  - **biomass concentration**
  - **dosage of alkalinity chemical**
  - **O_2-concentration in the last section of the reactor**
- Constraint: alkalinity of treated wastewater should be between specified bounds

2. Plant-wide optimization of operational settings

- Overall idea is to minimize total amount of nitrogen in treated wastewater and minimize operational costs
- Operational costs consist of four different objective functions:
  – minimize need for aeration in the activated sludge process
  – minimize consumption of additional carbon source for denitrification
  – minimize amount of excess sludge produced
  – maximize biogas production

→ total of 5 objective functions

2. Plant-wide optimization of operational settings

- Five objective functions to be optimized (conflicting)
- Four decision variables
  - **pumping to fermentation**
  - **pumping of excess sludge**
  - **O_2-concentration in one of the sections of the reactor**
  - **dosage of additional carbon source (methanol)**
- Constraints for (lower and upper bounds)
  - effluent ammonia concentration
  - biomass concentration
  - total nitrogen removal rate (%)

3. Choosing an appropriate optimization method

- What is known about the properties of the problem?
- Are gradients available?
- Is problem potentially non-convex?
- Is obtaining function values (= simulation) time consuming?
- Multiple objectives, is decision maker available?

Simulation-based optimization

- Closed (Black-box)
  - simulation first, then optimization
  - optimizer calls simulator which gives a (steady state) solution (all the constraints are satisfied)
  - time consuming, doesn't require much information about the model being optimized
- Open
  - simultaneous simulation and optimization
  - utilizes information about the model being optimized
  - steady-state solution (all the constraints are satisfied) only when optimal solution is found

Challenges for optimization of WWTPs

Characteristics of a WWTP design problem

- simulation-based (usually black-box)
- no gradients available
- computationally demanding (simulation takes time)
- includes continuous variables and nonlinear objectives and constraints
- needs to be considered from different perspectives (multiobjective)
- requires engineering judgement (decision maker)

→ **Need for efficient optimization tools for decision support**

Software used in the project

- Interactive approach was used
- Process was modelled by using the GPS-X process simulator
- GPS-X was combined with IND-NIMBUS
  – methods of global optimization were used in solving single objective subproblems
- DM was an expert in WWTP design

4. Coupling of optimization software and a modeling tool

- What software are available?
  – implementations of different optimization methods
- What information should be transferred between the software?
- What are the interfaces?
  – possibility to change the interfaces helps
  – coupling with commercial modelling tools often difficult, not possible to affect the interfaces
- Testing the coupling before optimization
  – e.g. with simple problems where the behaviour is known

Coupling in the project

- Commercial simulator (GPS-X) and optimization software developed in JyU (IND-NIMBUS)
- Possibility to affect only to the interface of IND-NIMBUS
- Information of the interface to GPS-X and how to use it from the technical support of GPS-X

Communication between GPS-X and optimizer

- Optimizer wants to know the function values (objective and constraint) with some fixed values of the decision variables
  - decision variables values are written in a text file (`values.in`) by using GPS-X naming convention for the variables
- GPS-X converts the simulation model into an executable file (`model.exe`)
- Input as a command file (`model.cmd`), which reads values of the decision variables from `values.in`
  - specific format for the command file for controlling the simulation

Communication between GPS-X and optimizer

- Simulation is started by executing a system call
- Output of the simulator can be extracted by reading the simulated values of the functions → a text file (`values.out`)
- Optimizer reads the values from `values.out` and uses them in optimization

5. Optimization and analysis of the solution obtained

- Definition of appropriate parameters (in modeling tool & optimization software)
- Utilize the knowledge of the expert in the application area (e.g. as a DM)
- Learning about the behaviour of the problem in optimization
- Optimization can also be used to test the model
- Analyze and verify that the solutions obtained make sense (together with the expert)

Decision making process

- Can be divided into two phases
  - learning phase
  - decision phase
- In interactive MO, different preferences are given in the learning phase and the obtained solutions are evaluated $\longrightarrow$ gives idea of what is possible to achieve, what are the interesting regions in the PO set
- In decision phase, the best compromise is identified in the interesting region with more focused preferences

1. Activated sludge process

Solution	N [gN/m^3], min	A [m^3/d], min	E [kW], min
Best	0.03	0.45	308
Worst	31.5	354	599
1	8.05	218	460
	$\downarrow$ 1.0	$\uparrow$ 330	$\approx$ 460
2	3.52	286	490
3	1.69	326	506
4	4.90	298	477
	$\downarrow$ 0.5	free	$\uparrow$ 510
5	1.11	336	515
6	0.55	347	528
	$\uparrow$ 1.0	free	$\downarrow$
7	9.36	246	448
8	30.2	7.23	308
9	0.90	333	519
	2 interm.	solutions between	5 and 6
10	0.92	336	519
11	0.72	332	524

1. Activated sludge process

- Altogether 11 PO solutions were computed
- Five of them were practically relevant (that is, the nitrification works)
- The solution with the lowest ammonium nitrogen concentration used too much energy and chemicals without sufficient improvement to the quality of treated wastewater
- The remaining 4 solutions were in practice equally good with respect to energy and chemical consumption (any of them could have been chosen)
- Among them, a solution with the lowest biomass concentration was chosen → better operability for the process

1. Activated sludge process

- Hakanen, J., Miettinen, K., Sahlstedt, K., Wastewater Treatment: New Insight Provided by Interactive Multiobjective Optimization, *Decision Support Systems*, 51, 328-337, 2011

2. Plant-wide optimization of operational settings

Solution	Total nitrogen [gN/m^3], min	Blower/aerator [kW], min	Methanol [g/m^3], min	Mass flow total [kgTS/d], min	total gas [m^3/d], max
Best	14.93	404	0.26	14426	10285
Worst	17.81	451	48.9	15885	8901
1	15.98	418	22.8	15026	9656
	↑	↑	↓ 20	↓	↑ 10000
2	16.25	421	0.64	14426	8901
3	16.21	424	3.51	14521	9053
4	16.18	425	5.96	14574	8915
	↑	↑	↓ 20	↓	↑ 10000
5	16.11	427	1.52	14444	8947
6	16.47	422	21.0	14976	9730
7	16.85	415	22.8	15003	9721
8	17.40	417	17.5	14971	9763
	≈ 16.11	≈ 427	↑ 14	↑ 14800	↑
9	16.01	425	8.04	14591	9132
10	16.08	425	11.0	14698	9265

2. Plant-wide optimization of operational settings

- Initially, DM used typical values based on engineering knowledge for the objectives (’initial reference point’)
- DM was able to investigate interrelationships between the operating costs (4 different objectives)
- Altogether 10 PO solutions were computed
- Global optimization methods in IND-NIMBUS were used in solving the single objective subproblems
- The best compromise had clearly better values for three objectives (11, 15 and 45%) and only slightly worse values the other two when compared to the engineering knowledge
- **The biggest improvement was in the usage of chemicals**

2. Plant-wide optimization of operational settings

- J. Hakanen, K. Sahlstedt & K. Miettinen, Wastewater Treatment Plant Design and Operation under Multiple Conflicting Objective Functions, *Environmental Modelling & Software*, **46**, 240-249, 2013.