WP5.2: Combination of MAR and adjusted conventional treatment processes for an Integrated Water Resources Management

Deliverable 5.2.12

State-of-the-art of well field optimization modelling

© 2010 TECHNEAU
TECHNEAU is an Integrated Project Funded by the European Commission under the Sixth Framework Programme, Sustainable Development, Global Change and Ecosystems Thematic Priority Area (contractnumber 018320). All rights reserved. No part of this book may be reproduced, stored in a database or retrieval system, or published, in any form or in any way, electronically, mechanically, by print, photoprint, microfilm or any other means without prior written permission from the publisher

Summary

Work package WP 5.2 "Combination of Managed Aquifer Recharge (MAR) and adjusted conventional treatment processes for an Integrated Water Resources Management" within the European Project TECHNEAU ("Technology enabled universal access to safe water") investigates bank filtration (BF) + post-treatment as a MAR technique to provide sustainable and safe drinking water supply to developing and newly industrialised countries.

One of the tasks within the project was the identification of state-of-the-art tools in the field of well field optimization modelling. Most of the currently used tools are process-driven simulation models like MODFLOW or FEFLOW. These are sometimes also combined with optimization models to reduce the computational demand and are utilized as strategic planning tools for water supply managers. However, in case of optimizing well field operation (i) under relatively constant boundary conditions and (ii) enough field data (temporal and spatial resolution dependent of the dynamics of the state parameter of interest, e.g. groundwater table, contaminant concentrations) data-driven approaches like support vector machines (SVM) can be used instead. If the water manager's key interest is only a good predictive capability in combination with low computational demand, the application of this approach is more goal-orientated to simulate the dynamics of well field performance indicators efficiently.

The contents of this report were presented to possible end-users, experts from Berliner Wasserbetriebe and Veolia. In agreement with their recommendations it was decided to focus further research within TECHNEAU on the empirical, data driven modelling approach. The selected approach is currently tested in the framework of a diploma thesis for a Berlin waterworks with the objective to analyse available production and observation well hydrographs by using modern statistical methods like principal component analysis and SVM (www.support-vector-machines.org).

Contact

Michael Rustler, Dipl.-Geoök., KompetenzZentrum Wasser Berlin gGmbH
Email: michael.rustler@kompetenz-wasser.de
Phone: +49 (0) 30 536 53 825

Dr. Gesche Grützmacher, KompetenzZentrum Wasser Berlin gGmbH
Email: gesche.gruetzmacher@kompetenz-wasser.de
Phone: +49 (0) 30 536 53 813

TKI Categorisation

Classification									
Supply Chain		Process Chain		Process Chain (cont'd)		Water Quality		Water Quantity (cont'd)	
Source		**Raw water storage**		**Sludge treatment**		**Legislation/regulation**		- Leakage	
- Catchment	X	- Supply reservoir		- Settlement		- Raw water (source)		- Recycle	X
- Groundwater	X	- Bankside storage	X	- Thickening		- Treated water			
- Surface water	X	**Pretreatment**		- Dewatering		**Chemical**			
- Spring water		- Screening		- Disposal		- Organic compounds			
- Storm water		- Microstraining		**Chemical dosing**		- Inorganic compounds			
- Brackish/seawater		**Primary treatment**		- pH adjustment		- Disinfection by-products			
- Wastewater		- Sedimentation		- Coagulant		- Corrosion			
Raw water storage		- Rapid filtration		- Polyelectrolyte		- Scaling			
- Supply reservoir		- Slow sand filtration		- Disinfectant		- Chlorine decay			
- Bankside storage	X	- Bank filtration	X	- Lead/plumbosolvency		**Microbiological**			
Water treatment		- Dune infiltration		**Control/instrumentation**		- Viruses		Consumers / Risk	
- Pretreatment	X	**Secondary treatment**		- Flow		- Parasites			
- Primary treatment	X	- Coagulation/flocculation		- Pressure		- Bacteria		**Trust**	
- Secondary treatment		- Sedimentation		- pH		- Fungi		- In water safety/quality	X
- Sludge treatment		- Filtration		- Chlorine		**Aesthetic**		- In security of supply	X
Treated water storage		- Dissolved air flotation(DAF)		- Dosing		- Hardness / alkalinity		- In suppliers	X
- Service reservoir		- Ion exchange		- Telemetry		- pH		- In regulations and regulators	
Distribution		- Membrane treatment		**Analysis**		- Turbidity		**Willingness-to-pay/acceptance**	
- Pumps		- Adsorption		- Chemical		- Colour		- For safety	X
- Supply pipe / main		- Disinfection		- Microbiological		- Taste		- For improved taste/odour	X
Tap (Customer)		- Dechlorination		- Physical	X	- Odour		- For infrastructure	X
- Supply (service) pipe		**Treated water storage**						- For security of supply	X

Internal plumbing		- Service reservoir				**Water Quantity**		**Risk Communication**	
- Internal storage		**Distribution**						- Communication strategies	
		- Disinfection				**Source**		- Potential pitfalls	
		- Lead/plumbosolvency				- Source management	X	- Proven techniques	X
		- Manganese control				- Alternative source(s)	X		
		- Biofilm control				**Management**			
		Tap (Customer)				- Water balance	X		
		- Point-of-entry (POE)				- Demand/supply trend(s)	X		
		- Point-of-use (POU)				- Demand reduction			

TKI Categorisation (continued)

Contains		**Constraints**		**Meta data**					
Report	X	Low cost	x	*Michael Rustler, Gesche Grützmacher*					
Database		Simple technology	x	*KompetenzZentrum Wasser Berlin*					
Spreadsheet		No/low skill requirement	x	*Michael Rustler*					
Model		No/low energy requirement	x	*michael.rustler@kompetenz-wasser.de*					
Research		No/low chemical requirement	x						
Literature review	X	No/low sludge production	x						
Trend analysis		Rural location	x						
Case study / demonstration		Developing world location	x						
Financial / organisational									
Methodology	X								
Legislation / regulation									

Colophon

Title
State-of-the-art of well field optimization modelling

Author(s)
Michael Rustler (KWB), Céline Boisserie-Lacroix (KWB),
Gesche Grützmacher (KWB)

Quality Assurance
By Katia Besnard (Veolia Environnement),
Dörte Siebenthaler (BWB), Gunnar Lorenzen (FUB),
Christoph Sprenger (FUB)

Deliverable number
D 5.2.12

This report is: PU for public

Contents

© TECHNEAU

1 Introduction

Context

The work package WP 5.2 "Combination of Managed Aquifer Recharge (MAR) and adjusted conventional treatment processes for an Integrated Water Resources Management" within the European Project TECHNEAU ("Technology enabled universal access to safe water") investigates bank filtration (BF) + post-treatment as a MAR technique to provide sustainable and safe drinking water supply to developing and newly industrialised countries. One of the tasks within this work package is to review existing tools for well field modelling in order to optimize the operation of well fields supplied by BF or MAR. This report summarizes the outcomes of this analysis and serves as a basis for the decision, which model approach can be tested for applicability in the further course of the project.

Background

A conceptual framework for well field optimization modelling is illustrated in Figure 1, which defines the main steps for the development and application of combined simulation-optimization models as described in Chapter 2.2.

In the first step the decision makers have to specify their management problem. For this they need to determine the key objectives (e.g. minimum raw water quality) and the constraints (e.g. maintaining predefined minimum groundwater levels) for the well field management. Subsequently either data-driven or process-driven simulation modelling (see Chapter 2.1) is used for the assessment of the impacts of different operational management plans on the groundwater system (state parameters e.g. groundwater levels, contaminant concentrations).

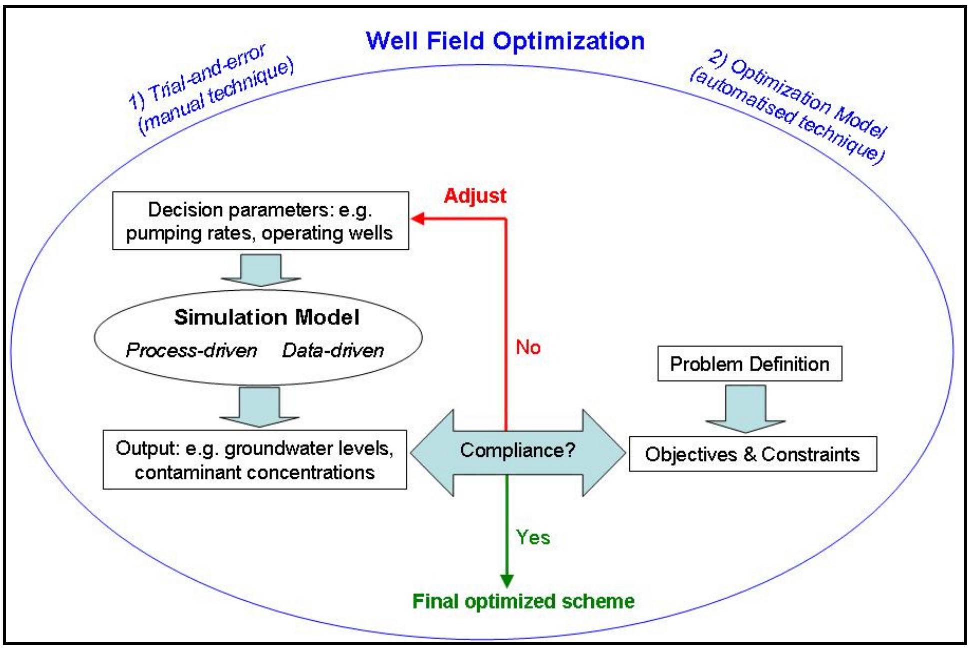

Figure 1 Conceptual framework for well field optimization modelling

Finally the optimal operational parameters are derived either by using mathematical optimization modelling (see Chapter 2.2) to identify the optimal values of operational decision parameters (e.g. pumping rates) or by using a simple trial-and-error technique (applicable for less complex management problems, where few management objectives shall be optimized).

The aim of this report is to give an overview of the current state-of-the-art tools for well field optimization management and answer the following questions:

- What is the difference between optimization and simulation modelling? What are these tools useful for?
- Which simulation approach (process-driven vs. data-driven) is more goal-orientated for a given problem at hand?
- Which simulation approaches and management tools are currently used by water suppliers (e.g. BWB, Veolia)?

2 Well Field Optimization Modelling

2.1 Simulation Modelling

Simulation modelling helps in answering 'what-if' questions through scenario modelling. One question may be for example what will happen to the pumped raw water quality at a bank filtration site if the sulphate concentration in the nearby surface water body rises. This can be evaluated through simulation modelling. For this purpose at least two model scenarios using different initial sulphate concentrations in the surface water body are computed and the impact on the pumped raw water quality is compared.
According to Figure 2 simulation models can be purely data-driven, purely process-driven or a mixture of both. In this report we will focus only on the two extremes.

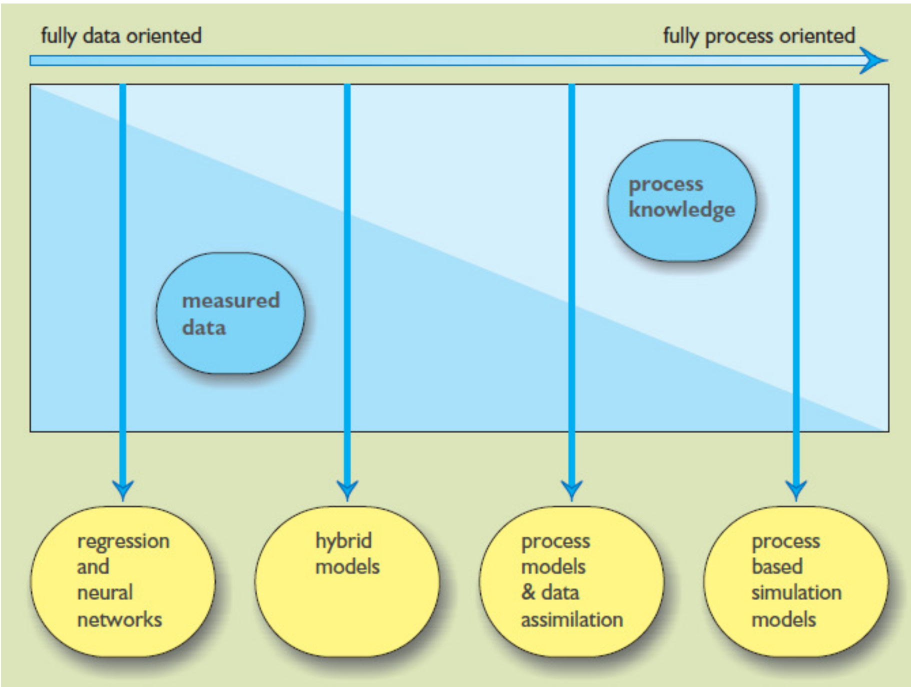

Figure 2 Overview of simulation techniques (LOUCKS & VAN BEEK 2005)

1) Process-driven or deterministic models utilize parameters whose values are usually determined from observed data (field measurements) during model calibration. The modeller attempts to incorporate what he or she believes to be the most important aspects of the conceptual model into a model so that it will provide useful information about the system. Deterministic groundwater models are based on knowledge of the fundamental processes like conservation of mass, momentum and energy ('white box' models).
The resulting partial differential equations can be solved analytically, but an analytical model like for example the Bank Filtration Simulator (HOLZBECHER et al. 2008) requires that the parameters and boundaries are highly idealized (e.g. homogenous aquifer & constant flux boundary). This is illustrated in

Figure 3, where different operational scenarios (pumping rates) were calculated considering the inherent uncertainty with the parameterisation of the clogging parameter (at an exemplary bank filtration scheme). The results show that the operational management decisions are very sensitive to the parameterisation of the clogging parameter, which in turn is highly variable in time and space (e.g. WIESE & NÜTZMANN 2009) and thus difficult to specify.

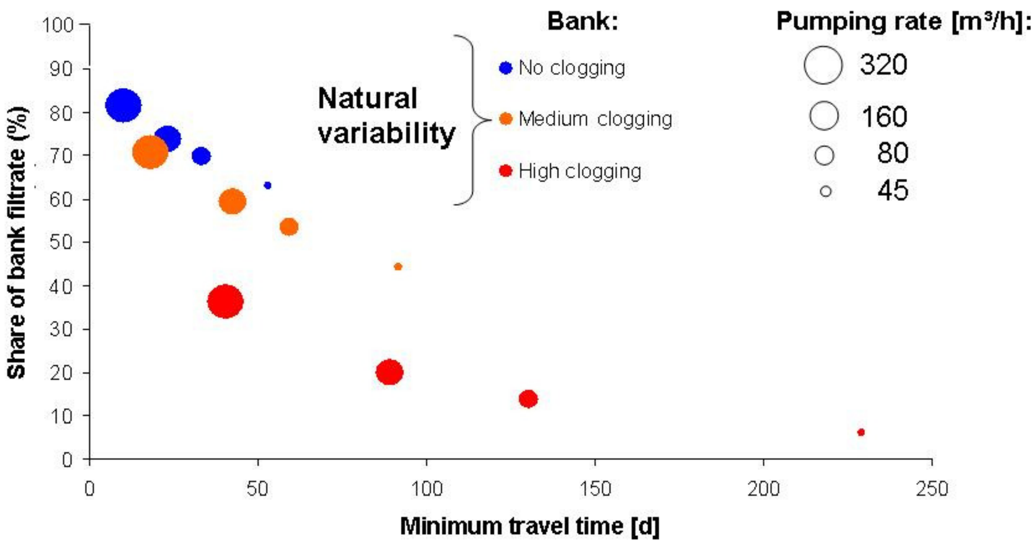

Figure 3 *Process-driven simulation model (Bank Filtration Simulator): Impact of different pumping rates under uncertain clogging parameter (no clogging: no difference in hydraulic conductivity between aquifer and bank; medium clogging = 100 times lower hydraulic conductivity in bank than in aquifer; high clogging = 5000 times lower hydraulic conductivity in bank than in aquifer) on both, bank filtration share and minimum travel time.*

For most real-world problems the simplified assumptions (e.g. homogenous aquifer) of analytical models are insufficient approximations. KALBUS et al. (2009) investigated the influence of heterogeneous and homogenous streambed conductivities on the groundwater discharge for an effluent (or gaining) river reach and concluded that the homogeneity assumption leads to an underestimation of groundwater discharge variability by a factor of ten compared to measured values. Numerical groundwater models like MODFLOW (HARBAUGH 2005) or FEFLOW (DIERSCH 2009) are able to simulate complex, steady-state and transient 3-D-flow and (reactive) transport processes in heterogeneous river-aquifer systems, but at the expense of longer simulation times (sometimes hours to days). In addition, the higher the included complexity of these numerical groundwater models the more model parameters are needed, which can easily lead to (i) over parameterisation (and thus a lower predictive model capacity) and (ii) higher data demand for calibration. A further difficulty is the inherent uncertainty of parameter estimation, due to an effect called 'equifinality' (BEVEN 2006). This means that two different parameter sets are able to produce exactly the same hydraulic heads. For example if the hydraulic conductivity for the aquifer and streambed are increased simultaneously by the factor ten, the hydraulic head at an observation well near the river will be the same for both scenarios. However, the total mass flux through the aquifer is ten times larger for the latter scenario. Subsequently a good model fit concerning the hydraulic heads is not a sufficient indicator for the adequacy of the model as a predictive tool. Nevertheless, process-driven simulation models are the only strategic (long term) planning tools available which are able to analyse the effects of significantly changing boundary conditions (e.g. impact of new well field on catchment's water budget). Thus water suppliers commonly order the application of process-driven models from environmental or hydrogeological consulting firms as done by BWB (e.g. GCI GMBH 2002) and Veolia (BURGEAP 2009).

2) Empirical, data-driven models aim at deriving a relationship between input (cause) and output data (effect), without the attempt to define any physical basis for the relationship ('black box' models). This approach relies solely on measured data and its application is therefore only adequate if a high temporal and spatial resolution for the output variable of interest (e.g. water quantity, water quality) is available (BERTRAND-KRAJEWSKI et al. 2008). Once calibrated, the model can be used to estimate the output variable values as long as the input variable values are within the range of those used to calibrate the model (Figure 4).

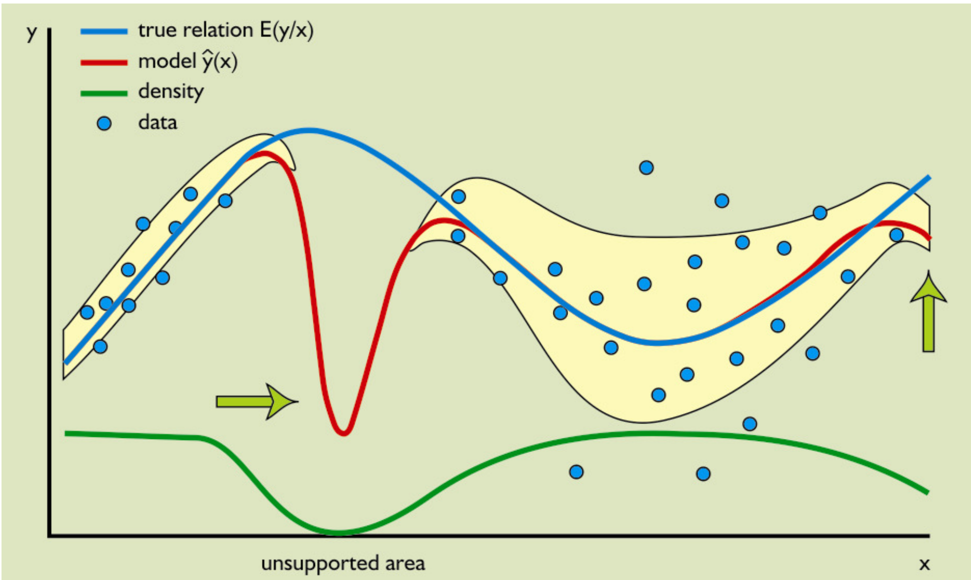

Figure 4 Data-driven simulation model: impact of data resolution (density) on the predictive model accuracy (arrows indicate weak model performance due to missing data values), (LOUCKS & VAN BEEK 2005)

Modern statistical modelling techniques are for example artificial neural networks (DREYFUS 2005) or support vector machines (www.support-vector-machines.org, WANG 2005, HAMEL 2009). Both are machine learning methods that can be used for classification (unsupervised learning) or prediction (supervised learning). KHALIL et al. (2005) showed that statistical learning algorithms can be used as efficient, fast computing proxy for the more complex, time demanding numerical groundwater models without loosing the predictive capability. Hence, statistical learning methods constitute a valuable means for saving effort in groundwater modelling and improving model performance at the same time. The major advantage of support vector machines (SVM) is the fact that they are less susceptible to overfitting than artificial neural networks (ANN), uniquely solvable and there is no need to train them in a repetitive manner (KHALIL et al. 2005). Thus the application SVM is highly recommended if fast (results usually within a few minutes) and robust model results with good predictive capability are required. In contrast to process-driven models, where the required input data is known a priori, this is not the case for data-driven models. Thus it is a precondition to identify the input parameters which are highly correlated with the desired model output in a first step, which means a significant effort in data pre-selection (pattern recognition). This task can be accomplished by using a model-free tool that needs no prior assumptions about key properties of the data, such as dominant processes but preserves a maximum amount of information (LISCHEID 2009). Principal component analysis (for details, see REIMANN et al. 2008) is such a tool that was successfully used to identify (i) the key processes that drive groundwater level fluctuations in a lowland groundwater-surface water system and (ii) their quantitative contribution (LEWANDOWSKI et al. 2009). Hence, as the most important processes and thus input parameters are identified, the principal component analysis effectively helps to minimize the structural model uncertainty which in turn leads to more reliable predictions of the data-driven simulation model.

3) Which is the optimal model approach for simulation modelling?
Consecutively there are some questions that may help in deciding whether a process-driven or data-driven modelling approach is more goal-orientated for a given well field management problem:

- For what purpose will the model be used? Is the main interest to get good predictive capacity or process knowledge? In the former case a data driven is adequate but a process driven approach is required for the latter case.
- Is a distributed model representation (e.g. water balance for different sub-watersheds) or is a lumped model (e.g. groundwater dynamics of observation wells) sufficient? In the first case a process-driven model is needed, in the second case the data driven model is sufficient.
- Are there time constraints? If yes, how long is the maximum acceptable computation time for one model run? Keep in mind that the execution time of transient process-driven models usually is much larger (depending of the complexity: groundwater flow, advective transport, biogeochemical reactions) compared to data-driven models.
- In the case of a process-driven model: Is there enough hydrogeological information available to develop a conceptual model of the system of interest? Is the model parameterisation supported by field data to specify them in realistic boundaries? Is the temporal and spatial variability of the clogging layer negligible? If yes, then the process-driven model is adequate. If the contrary is true, a non-parametric, data driven approach is required.

- In the case of a data-driven model: Is the data resolution sufficient to adequately describe the dynamics of the system of interest (depends on temporal and spatial variability of the process of interest, see e.g. BERTRAND-KRAJEWSKI et al. 2008)? Are the boundary conditions for calibration and prediction period approximately the same? If yes, this model is well chosen to solve the problem.

2.2 Optimization Modelling

Optimization modelling addresses 'what should we do' questions, which means what are the best management options for the given objectives (e.g. economic, environmental) and constraints (e.g. technological, law restrictions). This does not mean that only one best solution is found, but instead a set of relatively small number of good alternatives that satisfy the above defined scope (objectives & constraints). If any feasible solution exists that satisfies the objective function it is called 'optimal'. The objective of using optimization is to reduce an initially large number of potential management plans to a few that can be later tested through simulation modelling. In the context of well field management optimization models have been used to identify optimal (i) pumping rates and (ii) allocation of pumping rates within the well field in order to minimize the up-coning of deeper saline water (e.g. (KINZELBACH et al. 2007, RAO et al. 2007) or (iii) pumping costs (e.g. SIEGFRIED 2004, DANSKIN et al. 2006).
The formulation of an optimization model is the most difficult part in the development process. WAGNER (1975) offers the following guidelines for this stage of the optimization analysis:

- What are the key decisions to be made? What problem is being solved?
- What makes the real decision environment so complex as to require the use of an optimization model? What elements of complexity are incorporated in the model? What elements are ignored?
- What distinguishes a practical decision from an unusable one in this environment? What distinguishes a good decision from a poor one?
- As a decision-maker, how would you employ the results of the analysis? What is your interpretation of results? In what ways might you want or need to temper the results because of factors not explicitly considered in the model?

A management objective can be the optimization of well field design and operation in order to pump a predefined minimum raw water quantity or quality. In this case the water resource managers' decision parameters can be either design (location of pumping wells within the well field) or operation (pumping schedules, pumping rates, allocation of pumping rates within the well field) variables. The latter has been theoretically tested for the Palla well field northern of Delhi (India) in order to identify operation schemes that achieve a predefined 'optimal' bank filtration share (RUSTLER & BOISSERIE-LACROIX 2010). This was done in a trial-and-error approach (see Figure 1) which is illustrated in Chapter 2.1. However, in a first step a conservative mixing model was used to identify the 'optimal' target bank filtration share range, which satisfies a predefined minimum water quality constraint. Thus in this application not decision parameters (e.g. pumping rates) are optimized, but optimization modelling was used for identification of optimal values for the bank filtration share (state variable) instead. This is also shown in Figure 5, where the feasibility space of 'optimal' solutions if further limited due to a minimum travel time constraint (from surface water to production well) of at least 50 days for guaranteeing good microbiological water quality.

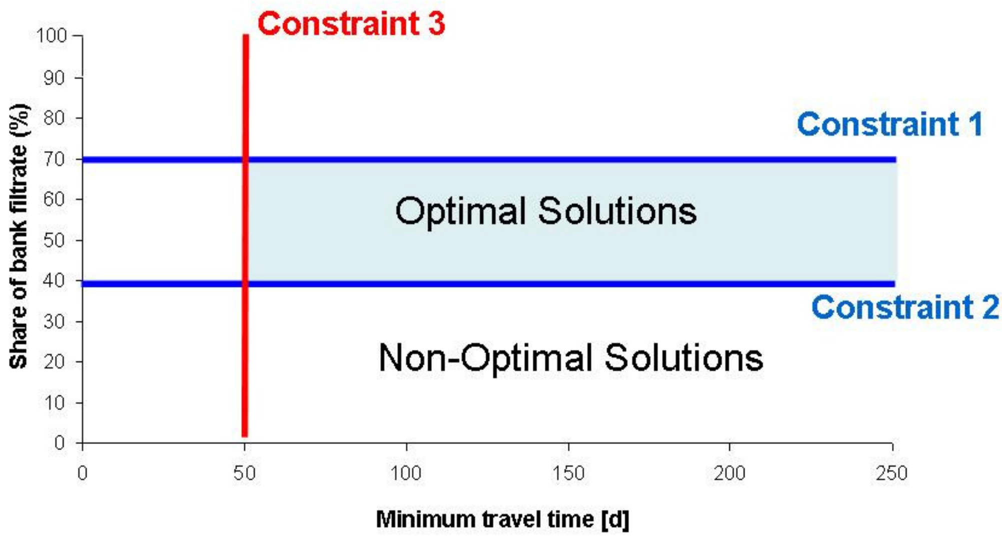

Figure 5 *Hypothetical multi-objective optimization model: Identification of target BF share range (constraint 1 & 2), including additional constraint for maintaining a pre-defined minimum travel time of 50 days (constraint 3)*

A simple operational well field optimization problem is presented below, which is slightly modified from DANSKIN et al. (2006). The defined management goal is the maximization of the pumping rate from two wells. Thus the objective function (Z) can be written as:

$$\text{maximize}\ Z = Q_{\text{Pump1}} + Q_{\text{Pump2}} \quad (1)$$

where the value of Z should be maximized and the decision variables Q_{Pump1} and Q_{Pump2} represent the pumping rate in m^3/s for production well 1 and 2, respectively. However, due to high fluoride concentrations (1.8 mg/L) at production well 1 the pumped raw water needs to be blended with the pumped raw water of production well 2, which contains less fluoride (0.8 mg/L). This can be expressed mathematically as the first constraint:

$$1.8mg/L \cdot Q_{Pump1} + 0.8mg/L \cdot Q_{Pump2} \leq 1.4mg/L \qquad (2.1)$$

The second constraint is due to limited maximum pumping capacity at each production well of 100 m^3/h (Q_{Pump1}) and 150 m^3/h (Q_{Pump2}), respectively.

$$Q_{Pump1} \leq 100m^3/h \quad (2.2)$$
$$Q_{Pump1} \leq 150m^3/h \quad (2.3)$$

© TECHNEAU

And a third constraint is due to the fact that the pumping rate cannot be negative:

$$Q_{Pump1}, Q_{Pump1} \geq 0 m^3 / h \quad (2.4)$$

For the management problem described above linear algorithms are used for solving the equations, e.g. LINPRO (SIMONOVIC 2009), since the all objectives and constraints of the optimization model are linear. However, in general the procedure (or algorithm) most appropriate for solving a particular optimization model depends on the particular mathematical structure of a model. Thus there is no single universal solution procedure that will efficiently solve all optimization models. For more details about the theoretical background on current state-of-the-art optimization techniques and easy hands-on examples for water resource management problems the reader is referred to LOUCKS & VAN BEEK (2005), HAIMES (2009) or SIMONOVIC (2009).

Note that the 'optimal' solution of the mathematical optimization model is only optimal with respect to the included objectives and constraints. In addition, the 'optimal' solution is also dependent upon the chosen optimization technique (e.g. linear, nonlinear, dynamic programming, evolutionary algorithms) and the assumed values for the model parameters. The latter limitation is further intensified through the inability to quantify and express all objectives and constraints in a mathematically adequate way. For example different decision makers may have different priorities for performance objectives or specific target values. A method which is able to take this uncertainty into account is the fuzzy set theory (SIMONOVIC 2009), which allows to define fuzzy membership functions for both, objectives and constraints. This method tolerates smaller violations (constraints do not need to be completely satisfied), but its application needs expert judgement about the specific qualitative value loadings.

In a nutshell the 'optimal' solution of an optimization model is only optimal with respect to included objectives and constraints, its specific structure and its assumed values, which may not always reflect the value loadings of each decision-maker. Nevertheless the application of optimization models is a valuable tool, as it enables to analyse the impacts of different management objectives and constraints in a systematic way. This may lead to the following benefits in the decision making process (PRODANOVIC 2008):

- Identification of trade-offs among different inherently competing management goals (e.g. high bank filtration share vs. long minimum travel time)
- Discussion and potential reconsideration of unrealistic target values for which no optimum solution is possible

As a consequence optimization modelling brings a higher transparency into the decision-making process. Thereby it further stimulates the identification of key management objectives in an open, goal-orientated dialogue and thus helps to manage well fields more efficiently.

2.3 Combining Simulation and Optimization Modelling

Simulation models are useful tools to assess groundwater flow systems, to test specific water-resource management plans, or even, in a trial-and-error approach, to select the plan that meets desired goals and constraints criteria best. They address 'what if' scenarios, that is, how does the well field system react if a certain scenario (e.g. clogging parameter) is assumed or a particular management decision (e.g. on pumping rates) is made. However, given the complexity of groundwater systems and the large number of decision-factors involved, the trial and error approach is insufficient to obtain overall optimal solutions (considering multiple management objectives and constraints). In particular this process can be very time-consuming. Thus simulation works well if only a few alternatives are taken into account. To address this difficulty simulation models are often linked and run in tandem with optimization models (Figure 6).

Since optimization models explicitly consider management objectives and constraints they can be efficient pre-screening tools to find 'optimal' management plans or operating policies. The output of the optimization model is used as input parameter for the simulation model (see red text in Table 1). The subsequent model run enables to estimate the impacts that those 'optimal' management decisions may have on the state parameters of the well field performance (e.g. groundwater levels, pumped raw water quality, bank filtration share, travel time, drawdown).

For example combined simulation-optimization models are used for managing regional aquifer systems (BARLOW 2005), transboundary aquifer systems (SIEGFRIED 2004), the conjunctive use of surface water & groundwater (CZARNECKI et al. 2003) or energy demand and contaminant level optimization of well fields (DHI 2007-2010, MADSEN et al. 2009). For example the water supplier BWB has ordered such a tool for strategic planning purposes (GCI GMBH 2004).

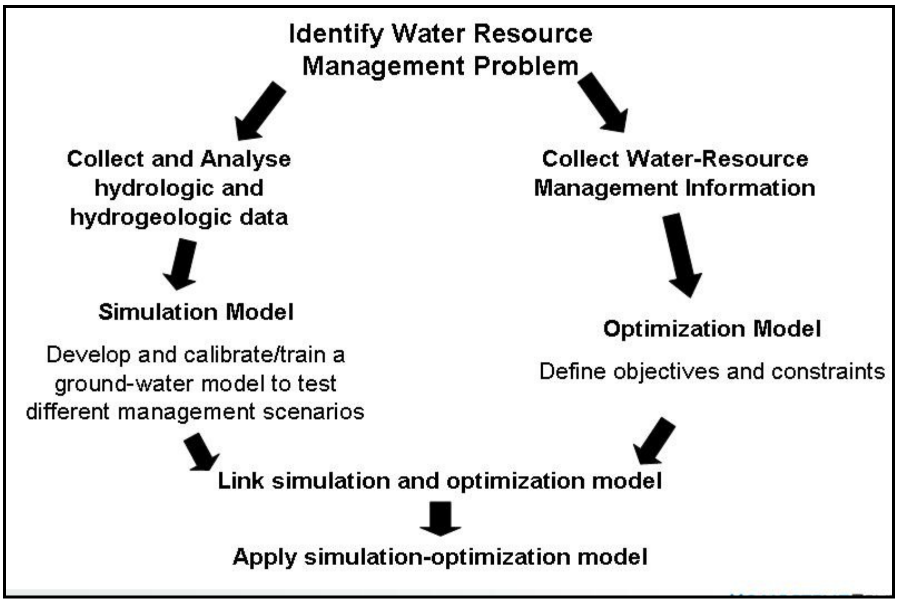

Figure 6 Development process of combined simulation-optimization models, slightly adapted from (BARLOW 2005)

© TECHNEAU

As mentioned above the main difference between simulation and optimization models is their scope. While optimization models need an explicit mathematical description of objectives and constraints, simulation models do not. Thus, the required model input and output parameters for both are quite different as illustrated in Table 1. Linking between both is established by using the output parameter of the optimization model as input parameter of the simulation model (red text in Table 1) and vice versa (green text in Table 1).

Table 1 Comparison of input-output data for simulation and optimization models

Tool	Technique	Input parameters	Output parameters
Simulation	**Process-driven (e.g. MODFLOW, FEFLOW)**	***a priori known input parameters*** *(for MODFLOW see e.g. REILLY & HARBAUGH 2004);* *System properties* : aquifer/riverbed transmissivity, effective porosity *Model discretization* (temporal & spatial); *Initial and boundary conditions:* no flow, constant head, constant flux or time varying head/flux boundary, initial hydraulic head distribution; Production well discharge: well locations, pumping rates (**>input from optimization model**);	Distributed model results (water budget for each model grid or mesh element) Groundwater levels (**>input for optimization model**), streamlines, drawdown Share of bank filtrate Minimum travel time (production well - bank) Infiltration Length
	Data-driven (e.g. ANN, SVM)	***a priori undefined input parameters (dependent on the modelling objective):*** *determination through pattern recognition techniques, e.g. principal component analysis; requires adequate temporal and spatial data resolution (depending on the dynamics of the output parameter of interest)*	Dependent on the modelling scope (e.g. groundwater levels, contaminant concentrations in pumped raw water), Lumped model results: only for locations used as input variables
Optimization	**General (e.g. linear, nonlinear optimization)**	*Decision parameters: e.g. pumping rate per well, allocation of active pumping wells within the well field* *Objectives:* minimum raw water quality (e. g. thresholds from drinking water guidelines), BF share *Objective function:* linear (e.g.: pollutants concentration value) or nonlinear (e.g. pumping costs with additional lift height due to interference of multiple production wells) *Constraints:*, minimum groundwater level (**>input from simulation model**), pumping capacity of wells, water demand	Optimal value(s) for decision parameter(s) (e.g. pumping rates) **(> input for simulation model)**

The results for the combination of our hypothetical simulation-optimization model (see Chapter 2.2 and 2.1) are shown in Figure 7. Two 'optimal' out of four initially defined operational management options are identified in case of a single production well (45 or 80 m^3/h pumping rate), which work fine for zero or medium bank clogging.

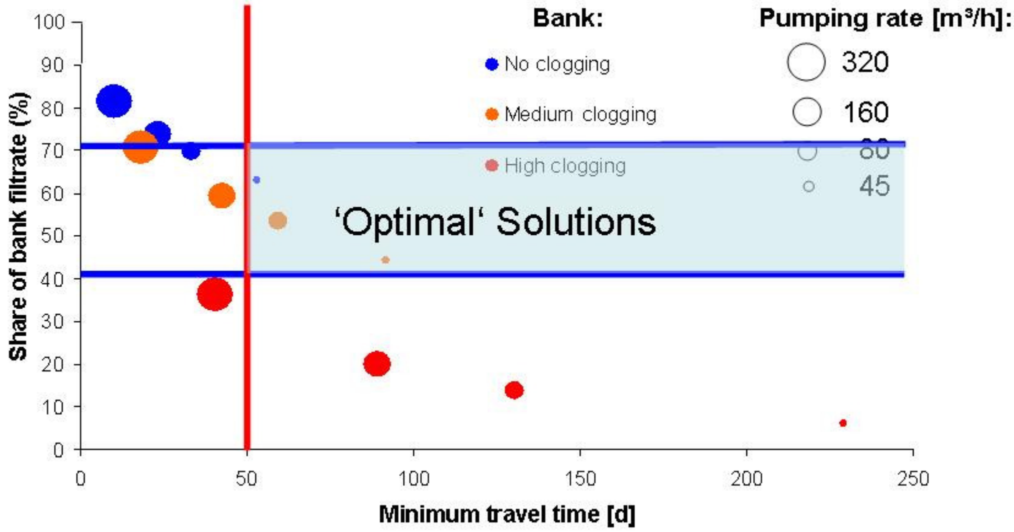

Figure 7 *Resulting 'optimal' management options for hypothetical simulation-optimization model. Note that optimization modelling is used in this context only for identifying the target values of the management objective BF share (see Chapter 2.2)! Subsequently the decision parameter (pumping rate) was not determined automatically through an optimization model, but by using a simple trial-and-error approach (see Figure 1).*

For more complex management problems (multi-objective optimization for many decision parameters: operating production wells, pumping rates) the benefit of joining simulation and optimization techniques will be much greater, since the potential well field operating schemes will increase according to the included decision parameters (production wells) by power two. As a consequence combined simulation-optimization models can greatly enhance the efficiency of simulation models alone by directly incorporating management objectives and constraints into the modelling process. This pre-screening of the most promising operational management plans helps to (i) minimize the computational effort of simulation models and to (ii) identify trade-offs among competing objectives, which adds transparency to the decision making process.

3 Conclusion

In a nutshell we identified that most of the well field simulation tools ordered by water suppliers from environmental or hydrogeological consulting firms are based on process-driven models like FEFLOW (for BWB e.g. GCI GMBH 2002). These are sometimes also combined with an optimization model to reduce the computational demand, so that they can be used as strategic planning tools (for BWB e.g. GCI GMBH 2004). Ongoing research activities in the field of combined simulation-optimization modelling for well field management are mainly focused on this approach (e.g. DHI 2007-2010, MADSEN et al. 2009). However, even if the burden of the high computational effort can be minimized, the application of these deterministic models still is based on the (i) integration of the conceptual hydrogeological understanding into the model and (ii) the selected model parameterisation (e.g. hydraulic conductivity, clogging layer, temporal and spatial model discretization). Subsequently wrong assumptions in both can easily lead to bad predictions, which in turn limit their usefulness especially for operational well field management.

In case of optimizing well field operation (i) under relatively constant boundary conditions and (ii) sufficient field data (temporal and spatial resolution dependent of the dynamics of the state parameter of interest, e.g. groundwater table, contaminant concentrations) data-driven approaches like support vector machines can be used instead of process-driven models. If the water manager's key interest is only a good predictive capability in combination with low computational demand, the application of these tools is orientated more towards the goal to efficiently simulate the well field dynamics.

The contents of this report were presented to possible end-users, experts from Berliner Wasserbetriebe and Veolia. In agreement with their recommendations it was decided to focus further research within TECHNEAU on the empirical, data driven modelling approach. This approach is currently tested in the framework of a diploma thesis for a Berlin waterworks with the objective to analyse available production and observation well hydrographs. These data will be used to develop an empirical model, which is able to derive the influence of the pumping regime on the groundwater levels within the well field. For this linear and nonlinear statistical methods like principal component analysis and Support Vector Machines will be applied. Under the constraint of the above mentioned boundary conditions it should be possible to derive optimal management options, which will be compiled in Deliverable 5.2.13.

4 References

BARLOW, P. M. (2005): Use of simulation-optimization modeling to assess regional ground-water systems. Fact Sheet 2005-3095, U. S. Geological Survey, http://pubs.usgs.gov/fs/2005/3095/pdf/factsheet.pdf

BERTRAND-KRAJEWSKI, J.-L.; FLETCHER, T. D. & MITCHELL, V. G. (2008): Spatial and temporal scale considerations Data requirements for integrated urban water management. Fletcher, T. D. & Deletic, A. Paris, UNESCO Publishing: 45-63 p.

BEVEN, K. (2006): A manifesto for the equifinality thesis Journal of Hydrology 320(1-2): 18-36

BURGEAP (2009): Champ captant de Crépieux-Charmy - Comité de pilotage Rosalye

CZARNECKI, J. B.; CLARK, B. R. & STANTON, G. P. (2003): Conjunctive-use optimization model of the Mississippi River Valley alluvial aquifer of Southeastern Arkansas, U. S. Geological Survey

DANSKIN, W. R.; MCPHERSON, K. R. & WOOLFENDEN, L. R. (2006): Hydrology, Description of Computer Models, and Evaluation of Selected Water-Management Alternatives in the San Bernardino Area, California, U. S. Geological Survey

DHI (2007-2010): Well Field Optimisation - Research project on optimal real-time control of groundwater abstraction Retrieved 12.1.2010, http://wellfield.dhigroup.com

DIERSCH, H.-J. G. (2009): FEFLOW 5.4 - Finite Element Subsurface Flow & Transport Simulation System (User's Manual). Berlin, DHI-Wasy GmbH: 204 p., http://www.feflow.info/uploads/media/feflow_users_manual_54.pdf

DREYFUS, G. (2005): Neural networks. Berlin, Springer.

GCI GMBH (2002): Ständig verfügbares Grundwassermodell für das Wasserwerk Berlin-Spandau http://www.gci-kw.de/content/referenzen/referenz_0048.php

GCI GMBH (2004): Entwicklung eines Kontroll- und Steuerungsmodells (KSM) für das Wasserwerk Berlin-Spandau. http://www.gci-kw.de/content/referenzen/referenz_0047.php

HAIMES, Y. Y. (2009): Risk modeling, assessment, and management. Hoboken, NJ, Wiley.

HAMEL, L. (2009): Knowledge discovery with support vector machines. Hoboken, N.J, John Wiley & Sons.

HARBAUGH, A. W. (2005): MODFLOW-2005, The U.S. Geological Survey Modular Ground-Water Model—the Ground-Water Flow Process Techniques and Methods 6-A16, U.S Geological Survey: 254 p., http://pubs.usgs.gov/tm/2005/tm6A16/

HOLZBECHER, E.; GRÜTZMACHER, G.; AMY, G.; WIESE, B. & SHARMA, S. (2008): The Bank Filtration Simulator - a MATLAB GUI. Proceedings of EnviroInfo 2008: -.

KALBUS, E.; SCHMIDT, C.; MOLSON, J. W.; REINSTORF, F. & SCHIRMER, M. (2009): Influence of aquifer and streambed heterogeneity on the distribution of groundwater discharge Hydrol. Earth Syst. Sci. 13(1): 69-77, http://www.hydrol-earth-syst-sci.net/13/69/2009/hess-13-69-2009.pdf

KHALIL, A.; ALMASRI, M. N.; MCKEE, M. & KALUARACHCHI, J. J. (2005): Applicability of statistical learning algorithms in groundwater quality modeling Water Resour. Res. 41(5): 1-16

KINZELBACH, W.; BAUER, P.; SIEGFRIED, T. & BRUNNER, P. (2007): Sustainable groundwater management - problems and scientific tools. Groundwater Modeling for Arid and Semi-Arid Areas
(G-WADI Workshop, Lanzhou, China, 11-15 June 2007). Paris, UNESCO: 39-44.

LEWANDOWSKI, J.; LISCHEID, G. & NÜTZMANN, G. (2009): Drivers of water level fluctuations and hydrological exchange between groundwater and surface water at the lowland River Spree (Germany): Field study and statistical analyses Hydrol. Processes 23(15): 2117-2128

LISCHEID, G. (2009): Non-linear visualization and analysis of large water quality data sets: A model-free basis for efficient monitoring and risk assessment Stochastic Environmental Research and Risk Assessment 23(7): 977-990,

LOUCKS, D. P. & VAN BEEK, E. (2005): Water resources systems planning and management: An introduction to methods, models and applications. Paris, UNESCO.

MADSEN, H.; REFSGAARD, A. & FALK, A. K. (2009): Energy Optimization of Well Fields Ground Water 47(6): 766-771, http://dx.doi.org/10.1111/j.1745-6584.2009.00625_3.x

PRODANOVIC, D. (2008): Use of data to create information and knowledge. Data requirements for integrated urban water management. Fletcher, T. D. & Deletic, A. Paris, UNESCO Publishing: 139-169 p.

RAO, S. V. N.; KUMAR, S.; SHEKAR, S.; SINA, S. K. & MANJU, S. (2007): Optimal pumping locations of skimming wells Hydrol. Sci. J. 52(2): 352-361

© TECHNEAU

REILLY, T. E. & HARBAUGH, A. W. (2004): Guidelines for Evaluating Ground-Water Flow Models. Scientific Investigations Report, U. S. Geological Survey. 2004-5038: 30, http://pubs.usgs.gov/sir/2004/5038/

REIMANN, C.; FILZMOSER, P.; GARRETT, R. & DUTTER, R. (2008): Statistical data analysis explained - Applied environmental statistics with R. Chichester, Wiley.

RUSTLER, M. & BOISSERIE-LACROIX, C. (2010): Decision Support System for BF Systems. TECHNEAU Integrated Project. D5.2.11, www.techneau.org

SIEGFRIED, T. (2004): Optimal utilization of a non-renewable transboundary groundwater resource - Methodology, case study and policy implications Zürich, ETH Zürich

SIMONOVIC, S. P. (2009): Managing Water Resources - Methods and tools for a systems approach. Paris, UNESCO.

WAGNER, H. M. (1975): Principles of Operations Research. Englewood Cliffs, NJ, Prentice-Hall.

WANG, L. (2005): Support Vector Machines: Theory and Applications. Berlin, Springer.

WIESE, B. & NÜTZMANN, G. (2009): Transient leakance and infiltration characteristics during lake bank filtration Ground Water 47(1): 57-68,