

Integrated Water Cycle Management in Kazakhstan









Integrated Water Cycle Management in Kazakhstan

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Textbook developed in the TEMPUS IV – 5th Call of Proposals on Joint Projects



Almaty "Qazag university" 2014 Editors:

Burghard C. Meyer & Lian Lundy,

The publication should be citated as follows

Meyer B. C. & L. Lundy (Eds). 2014. Integrated Water Cycle Management in Kazakhstan. Al-Farabi Kazakh National University, Publishing House, Almaty, 320 pages ISBN: 978-601-04-0900-2

Published with active contributions of the TEMPUS IV IWEB-Project partner's institutions:

- Middlesex University, London, UK
- Al-Farabi Kazakh National University, Almaty, Kazakhstan
- Ahmed Yasawi International Kazak-Turkish University, Turkistan, Kazakhstan
- Kokshetau State University named after Shokan Ualikhanov, Kokshetau, Kazakhstan
- Universität Leipzig, Germany
- Universitat Politecnica de Valencia, Spain
- University of Cyprus, Nicosia, Cyprus
- Institute of Geography of the Republic of Kazakhstan, Almaty, Kazakhstan
- The Regional Environmental Centre for Central Asia, Almaty, Kazakhstan
- Kazakh Scientific Research Institute of Water Economy, Taraz, Kazakhstan
- Kazakh Research Institute of Fishery, Almaty, Kokshetau, Kazakhstan
- Institute of Professional Development and Retraining, Kokshetau, Kazakhstan
- Ministry of Education and Science Control Committee, Astana, Kazakhstan
- Center of Bologna process and academic mobility, Astana, Kazakhstan
- Fund Zhas Otan, Akmola region, Kokshetau, Kazakhstan

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Cover page photographs: Burghard Meyer

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Chapter 2

Methodologies and Supporting Tools for

Integrated Water Cycle Management

2. Methodologies and supporting tools for IWCM

2.1 Strategic risk management

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Introduction

As set out in the introduction to this textbook, modern frameworks of risk management facilitate an understanding of the relationship between those who manage (or make policy) and those who gather evidence to support that decision making. The key to the management of any risk is the requirement to make a judgement (e.g. how clean is clean enough? how safe is safe enough?). These judgements are based on the evidence gathered by the assessors of the risk but also need to reflect other criteria and values. One obvious consideration is cost since resources are finite but others may include differing objectives from stakeholders, implications for ethics or justice and perhaps even legality. In fact it turns out that managing the expectations of different groups of stakeholders can be as large a problem as acquiring the scientific and engineering evidence. In short, the process of managing risk almost always faces two huge challenges - not knowing enough (uncertainty) and facing differing interpretations of what is right (controversy).

Integrated risk management thus has to include economic, social, legal, psychological, ethical, and political dimensions, whereas risk assessment is, to some extent at least, an objective, technical function within the overall process. This chapter investigates the nature and relationships between these factors, at ways of communicating effectively with stakeholders about them, and at ways to make sustainable judgements that incorporate both evidence and values.

Understanding some fundamental principles of the risk management process enhances ability to make both day-to-day decisions and plan strategically with greater confidence. This will help risk management to move from being the province of specialists in different disciplines (e.g. water quality scientists, hydrologists, civil engineers etc.) to a situation in which decision makers are integrated in an approach that reflects the multidisciplinary nature of risk issues. At a societal, or government level, this can be broadly equated to setting policy to deal with the risk and establishing the political and social consensus to implement it, all of which entails a number of tasks:

- Setting objectives.
- Appraising risks that threaten achievement of these objectives (a task that will often encompass an evaluation of concerns about the risk from different stakeholder groups).
- Evaluation of the acceptability of the risk.
- Establishment of management actions (or policy) to control the risk.
- Communicating with stakeholders to enhance implementation of the policy. In fact, risk communication is an important component of risk management, with significant contributions to make throughout the process. Effective risk communication provides a forum for resolution of potential conflicts, allows stakeholders to have their say and creates trust in the institutions that manage the risk. It has come to play an increasing role over the last few decades.

Risk is socially defined.

At first it may seem counter intuitive that policy does not derive directly from science and, indeed, early models of the risk process are based on a belief that science dominates. Millstone *et al.* (2004) discuss three models. The first type of approach, shown in Figure 2.1.1, can be represented as a *'technocratic model'*, which



Figure 2.1.1 The "Technocratic" model (Millstone et al., 2004)

assumes, in effect, that science operates completely independently from social, political, cultural and economic conditions, and that science provides not just a necessary, but a sufficient basis for policy decision-making.

Amongst other difficulties, the technocratic model cannot explain policy development where there is acknowledged scientific uncertainty (Renn, 2008), and many public policy-makers and their expert advisors now represent the processes as what Millstone et al. (2004) call a 'decisionist model'. This corresponds closely to the US National Research Council (NRC) 'Red Book' model (NRC, 1983) and suggests that policy requires inputs other than science and is, and indeed should be, the product of a two-stage process. The first of these is purely scientific, often called 'risk assessment', and can be supplemented later by social and political considerations, which are known as 'risk management'. Thus, in this approach, risk assessment is seen as preceding, and being entirely independent of, risk management decision making. As Figure 2.1.2 shows, in this model there is a clear division of function between the scientific community, which is represented as assessing risks in a socially and ethically neutral way, and risk managers (policymakers) who then utilise the social and/or commercial benefits to offset the risks and their attendant uncertainties.

• The breadth and scope of scientific risk assessments.

- The ways uncertainties should be handled by risk assessors, and the significance that should be ascribed to them.
- The benchmarks by reference to which the available evidence is interpreted.
- The 'chosen level of protection' i.e. the extent to which those risks and uncertainties are socially acceptable (the how safe is safe enough question).

They therefore suggest a third approach, which they call a '*transparent*' model, or '*inclusive governance* model' (after NRC, 2003), which assumes that:

'Science-based risk assessments play a key role in policy-making processes, but that they are routinely and inevitably influenced by the socio-economic and cultural contexts in which they are developed'.

The 'transparent' model (Figure 2.1.3) assumes that risks are given a context specific frame that shapes the ways in which risk assessments are constructed and conducted. Risk management is seen as a holistic process (Renn, 2008), framed in a way that means that risk assessors are not expected to take responsibility for non-scientific judgements but to return their findings to a political or managerial process to make decisions. The 'transparent' model implies that disputes are more likely to be resolved if the existence and importance of risk assessment policy considerations are acknowledged and consistently deployed in a transparent fashion.



Figure 2.1.2 The "Decisionist" model (Millstone et al., 2004)



Figure 2.1.3 The "Transparent" model (Millstone et al., 2004)

This evolution reflects the idea that risk is not an objective, measurable entity (although some of the evidence may be - it is possible to measure salinity or faecal contamination in water for example) but is socially defined by what people value and prioritise.

An integrated approach to risk governance

Risk governance, in this context, may be defined as a framework within which policy and science interact in pursuit of an objective, for example to establish 'safe' concentrations in water, below which pollutants do not have adverse effects. In a number of instances it has been established that there is a number of different levels that policy might set as standards - based on widely differing characteristics of the pollutant material and different societal values placed on the outcome (for example people might tolerate different levels of contamination if the water was to be used for drinking, for irrigation or for recreation). In these cases policy makers need to seek to establish a 'tolerable' or 'acceptable' level. Identification of such acceptable values is a key function of risk management in every field and is usually a combination of technical evidence and societal values. The risk management process, as therefore has to address both discussed. uncertainty and conflict and the concepts may be used to examine some of the relationships between governments and related authorities, the scientific community and other stakeholder groups. The approach combines both evaluation of scientific technical and evidence and consideration stakeholder of concerns. Sometimes solutions are largely technical and are delivered by appropriated skilled (and mandated) professionals and sometimes decision making requires stakeholder engagement, including public

engagement. Understanding some key challenges to risk appraisal is very helpful in selecting the appropriate tools to use.

Figure 2.1.4 shows a modern transparent model (IRGC, 2005) that contains a number of characteristics that help to discuss some of the key features of the challenges faced in the development of an integrated approach to the management of water quality. The first thing to notice is that communication is placed at the heart of the process, which implies that there are many types of risk communication depending on context and what the stakeholder is being asked to do. In fact the entire framework can be viewed as a conversation between two sides - managers (or policy makers) and those that gather the necessary evidence (scientists, engineers etc.). The two most obvious collaborative steps are jointly undertaken - setting the context, including objectives (known as pre-assessment) and making the acceptability judgement (presented here as two linked steps characterisation which presents the technical profile of the risks and evaluation, which reviews this evidence in the light of stakeholder values). Evidence from risk appraisal (which includes risk and also stakeholder assessment concern assessment) is acquired by specialists who then pass it over to managers to implement solutions. This idea of a conversation between these two sides provides useful clarity on their respective roles and the placement of communication in the centre shows that this conversation flows in many directions throughout the process.

Figure 2.1.4 identifies a number of challenges to the risk appraisal process that can be linked to different approaches to management and Figure 2.1.5 shows that differing stakeholder response to each. Many risks can be thought of as being 'simple' risks, which does not mean that they are not important and can be ignored but rather that they are relatively well understood and may already have well developed regulations and codes of practice. Typically they are wholly managed by technical specialists (with the authority do so delegated from the to management). The three challenges require the of development differing approaches to management. The first, complexity, occurs when a number of simple risks interact together in ways that may not wholly be predictable. It suggests a situation in which technical specialists may still be responsible for management but may require additional external advice, perhaps from other specialists or consultants in related fields. Where residual uncertainty remains high, for example where a new technology or pollutant has emerged, there may be insufficient evidence available to make a science based judgment. In this case it may be necessary to consider actions ahead of having reliable data because of stakeholder concern or other pressures in which case adoption of some level of precaution is required. Overzealous adoption of the precautionary principle (if you don't know it is safe, assume it is dangerous), has the potential to stifle innovation

and development and so it is necessary to consult key stakeholders to reach consensus on an appropriate level and to establish a management approach based on increasing resilience. The final challenge to risk appraisal, ambiguity, describes the situation in which there may be fundamental disagreement about the merit of a development on grounds other than the extent of the risk. Highly contested technologies, such as nuclear power, require a societal endorsement before they can be licensed. This means that the management process includes a stakeholder consultation at societal level. Actually nuclear power is a good example to consider as it can be seen that the challenges (and managerial responses) may evolve. An initial societal debate may lead to a country agreeing at government level to develop a nuclear power programme after a process that addresses the ambiguity. This is followed by a period of high uncertainty as differing technologies and precautionary levels are evaluated by stakeholders including communities, after which a particular technology is selected and risk management becomes an increasingly technical matter undertaken by nuclear specialists overseen by specific regulations.



Figure 2.1.4 IRGC Framework for risk governance annotated to show the challenges for risk appraisal and the implications for risk management



Figure 2.1.5 The 'Risk Escalator' showing the relationship of the challenges to risk appraisal and the management responses (Bunting, 2007)

Conclusion

A social definition of risk has been presented that highlights the requirement to relate assessment of risk to the value placed on them by stakeholders. This definition gives insight into the source of one of the major challenges to risk management of any type of risk, the controversy associated with any judgement which results from the widely differing ambitions, expectations and values of different stakeholder groups. This forces decision makers to move away from a purely technical approach to the management of risk that simply seeks to reduce uncertainty towards one that involves stakeholders to develop an inclusive and responsive risk handling process that maximises the effectiveness and acceptability of the judgements made. Careful selection of risk management practices attuned to an analysis of the specific challenges to risk appraisal in a given situation will avoid common pitfalls such as accidental (or deliberate) exclusion of stakeholders and/or their views or "paralysis by analysis" where too much consultation is applied where it is simply not required.

2.2 Risk assessment methods for land use optimisation using simple predictive models

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Introduction

The use of digital data and of models for land use decision making for multiple purposes is widely accepted and applied in practice. Land use is an integral of human activity on the basis of natural and cultural/economic conditions. The same land use type (e.g. forest) is different in different geographical regions or landscapes. Methods first developed in science in the context of the assessment of landscape functions have been further developed into detailed model systems. The methodological problems of scaling between different levels of investigation and of the integration of often conflicting different aspects e.g. by aggregative rules, decision trees, causal chains, spatial optimisation models, fuzzy logic,



Figure 2.2.1 Procedural steps of the method MULBO (Meyer & Grabaum 2008)

cellular automata etc. are multiple. New research lines e.g. for the ecosystem services assessment, often using the knowledge and the experiences from landscape risk assessment science, developed in landscape ecology in the last 50 years.

The article gives some insights about recent methodological developments in the assessment of landscape functions and landscape risks by using simple predictive risk models included in the Framework of multifunctional land use assessment and optimisation model MULBO.

MULBO - Model framework for multicriteria landscape assessment and optimisation – A support system for spatial land use decision (Meyer & Grabaum 2008)

Model framework

The model framework MULBO is a spatially explicit decision support method using risk evaluations for landscape functions. Its principal purpose is the establishment of optimal land use patterns as scenarios, which are balanced compromises between conflicting goals for the reduction of assessed risks.

A user manual for MULBO has been developed and includes the model descriptions of assessment tools. It is online available at www.mulbo.de; the landscape optimisation method LNOPT 2.0, is used on the basis of digital information in GIS. MULBO has been applied in several rural research landscapes. In this article, results of its application in the southern part of Saxony-Anhalt (Germany), a test area of 4800 ha in size, are presented.

The MULBO framework consists of and integrates several procedural steps, from goal definition to applied landscape planning activities (Figure 2.2.1). The framework is methodologically open for the integration of diverse spatial risk assessment methods, which means the integration of the new methods of landscape assessment. A landscape assessment is made for economic, social or environmental landscape functions. Results of such functions are assessment classes in form of landscape risks and the optimisation method calculates the best spatial distributions for a compromise to address the problems analysed for each landscape function by land use change. Table 2.2.1 gives an overview about the landscape functions run with MULBO.

Simple predictive assessment models

The MULBO landscape optimisation software LNOPT 2.0 runs with simple predictive model results. These types of models use diverse landscape parameters, landscape data and knowledge from different sciences in combination to predict a landscape function based on decision rules. An example is given in Figure 2.2.2 for the landscape water retention capacity.

Туре	Function	Assessment method/model	
	Groundwater recharge	Renger and Strebel (1980)	
	Groundwater protection	Zepp (1989)	
	Climate function	Alexander (1988)	
	Nitrate leaching	Frede and Dabbert (1999)	
Abjectic (regulation function)	Landscape water retention	Zepp (1989)	
Abiotic (regulation function)	Soil erosion by water	Schwertmann, Vogl, Kainz (1990)	
	Soil erosion by wind	Smith et al. (1992)	
	Infiltration capacity	Altmann, Schreiber, Thöle	
	initiation cupacity	(1992)	
	Habitat suitability of the corn	Meyer, Mammen, Grabaum	
	bunting	(2007)	
Biotic (habitat function)	Habitat suitability of the hara	Grabaum and Meyer (2002)	
	Habitat suitability of the hare	(internal report)	
	Habitat suitability of the red kite	Grabaum (2003)	
	A grigultural production function	Scheffer and Schachtschabel	
Socio-economic	Agricultural production function	(1994)	
	Recreation function	Marks et al. (1992)	

 Table 2.2.1 Functions included into the assessment of MULBO (Meyer & Grabaum 2008)



Figure 2.2.2 Data combination to analyse and to evaluate the water retention function according to Zepp (1989); (Meyer & Grabaum 2008; nFK = usable field capacity)

The example of the index of land quality generated in the investigation area Barnstädt (Figure 2.2.3) gives an indication of the type of input layers utilised in the optimisation process. The detailed interpretation of a fine grained soil map of German Soil Taxation at a scale of 1:10.000 was used as basis for developing the index. land quality Essentially different information layers are combined through the use of rule based interpretations or combining of information levels which result in a spatialised differentiation of the indicator under development. It is obvious that the integration of different aspects using models leads to high complexity. The optimisation models illustrated in this article are using only the assessment classes as input data for the optimisation. A discussion about the related complexity problems is found in Meyer et al. (2008). The optimisation process links land use decision making by the spatial distribution of potential land uses (e.g. forest, grasslands, arable land, settlements etc.) to the site assessments of all of the included assessment layers (see Table 2.2.1). A compromise optimisation example is demonstrated in Figure 2.2.4.

Optimal distribution of linear landscape elements (Meyer et al. 2011)

The importance of linear landscape elements is the topic of a wide-ranging discussion. A methods framework for the modelling and visualisation of optimal allocation of linear elements by multifunctional risk assessment was developed. We use the example of hedgerows to describe an optimisation technique for planning purposes.



Figure 2.2.3 Index of land quality in the investigation area Barnstädt (Meyer & Grabaum 2008)





Using the GIS tool "Line Generator", developed by the authors, a network of existing and new potential lines was defined and exemplified by hedgerows and rows of trees. A spatial risk assessment of the lines for selected landscape functions was then quantified. Goals of landscape development such as presetting the spatial orientation of linear elements are integrated into the framework. The authors developed the software LNOP 2.0, a linear programming software/tool combined with game theory. The methods were tested in an agricultural region in Saxony-Anhalt in Germany by integrating the opposing functions "wind erosion risk", "water erosion risk" and "habitat suitability for the farmland bird Corn Bunting (Emberiza calandra)". Results lead to optimisation of the benefits of a limited length of new linear elements. This combined method is a step towards

making both the planning and the integration of multi-functional assessments into land use decisions objective achievable using GIS (Meyer et al. 2011).

A framework for the optimal distribution of linear landscape elements was developed (Figure 2.2.5) by following main aspects shown in the Figure 2.2.1 and Table 2.2.1. Again, in an area of optimisation a set of map manipulation and assessments were adapted by adding e.g. a new line network for the potential orientation of new linear landscape elements. The line network solves the methodological problem that linear landscape elements are not included in spatial basic data and mathematically an indefinite number of lines can be arranged in the space.

Figure 2.2.6 gives an example of a scenario



distribution of linear landscape elements. Based on given lengths of landscape elements to be distributed throughout the area, the assessment maps of named landscape functions are interpreted here using the example of a reduction of wind erosion exposure. Again, LNOPT 2.0 has identified an optimal compromise to find the best places to reduce the landscape risks and to develop the best habitat configuration for an open farmland key species. optimisation "may pertain to the model itself, the data used, the knowledge and goals defined by actors, and the sampling representativeness in the same way as for autocorrelation problems. The definition of the test area and spatial units optimized should be organized in order to focus on the main problems to be solved. This also depends on the meaningful variables or model parameters integrated." This is acknowledged because integration is first of all limited by the



Figure 2.2.6 : Wind erosion risk by using the optimised landscape elements on the data set "line grid set 500" m (Meyer et al 2011).

Conclusion

The examples of risk assessments using simple predictive models and landscape optimisation approaches have shown the capability of GIS based approaches for land use decision making. This capacity, especially landscape assessment but also landscape optimisation or other methods to solve landscape pattern distribution problems, is still in scientific development and seldom used in application. When critically interpreting the different geospatial methods (i.e. predictive models for landscape assessment, data layers and the parameter integration rules) it is obvious that the methods developed are in their infancy and not vet fully available for practice as often mentioned in applied sciences. The examples given in this awareness-raising article lead to key aspects of integrated geography, human-nature interdependencies, landscape decision making and geo-informatics. Meyer et al. (2009) explain that uncertainties in model application for spatial

overall problem of complexity of a multi-criteria land use optimisation model.

The MULBO framework can be adopted to land use topics related to global change issues. landscape planning. restoration ecology. conservation ecology or water catchment issues for policy, planning or management purposes. The framework is well suited for understanding ecological, economic and social interrelationships in the landscape. Wu and Hobbs (2002), in discussing the 10 key issues and research priorities in landscape ecology, note that the optimisation of landscape patterns (also related to landscape optimal management, optimal landscape design and planning) ought to be considered for its significant influence over flows of material, energy and information (Meyer & Grabaum, 2008). Meyer at al. (2011) has explained that in scientific and applied practice, the implementation of the methods (such as the distribution of linear landscape elements using assessment and optimisation) "should be based on discussions, analysis and assessments carried out with land owners and stakeholders. The only restrictions or assumptions needed when running the optimisation are a maximal length of the proposed linear elements. The number of lines could be modified with the tool "Line Generator", e.g. by setting the desired maximal length. By demonstrating that the framework was applicable to the case study area, the example highlights the expected ability to find and to integrate best solutions to land use compromises which include several landscape functions."

2.3 Models and simulation methods in IWCM

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Introduction

Presently, mathematical models and simulation approaches have improved water cycle systems knowledge and the capacity to resolve environmental problems. Moreover, in the last years, society and stakeholders have come closer to scientific and technical studies related to water and its cycle. However, the complexity of the hydrological cycle creates the necessity of applying different modelling techniques for different processes and parts of them. Additionally, integrated water cycle management should consider several aspects such as water quantity and quality, environmental assessment, and economics. In this subchapter, several models are discussed to represent the different water cycle factors and the importance of their integration. However, the combined use of different models has been shown to optimally resolve integrated water cycle management problems.

The recommended approach to solve Integrated Water Cycle Management (IWCM) problems is to follow the Systems Analysis Approach, which consists of several steps: (1) definition of the problem, (2) collection of useful data and system (and subsystems) identification, (3) definition of goals and objectives, (4) definition of quantitative measures and indicators to evaluate different alternatives, (5) generation and evaluation of feasible alternatives, (6) selection of the best alternative, (7) final design and implementation of the selected alternative, and (8) review, update and feedback (in order to incorporate new information, learn about the real performance of the alternative and improve the system in future). In most of these steps, if not in all, tools for data management and analysis (as for instance, Geographical Information Systems), and models are needed in order to cope with the complexity, the basin scale scope, and the huge amount of information, alternatives and scenarios (Andreu et al., 2008). If the models used are the adequate ones, and they are well used, they constitute essential tools to perform the analysis in the most objective, reliable and replicable way.

Mathematical modelling simulation and approaches are currently used tools in the analysis of IWCM. This analysis contributes to a better understanding of the system, and the interconnections with other systems and enlarges the available background information. It also enables the prediction of the consequences of different alternatives, and allows the selection of the approach that best meets a particular function.

Definition and types of models

In a broad sense, a model of an element of the water cycle, or of an ensemble of elements, is a conceptualization of the real element preserving its essential features to the desired aim. With this definition there can be many types of models, such as: descriptive, graphical, experimental, mathematical, etc. All these models can be used in the decision making process. However, some of them are more complete in qualitative terms, and others (such as mathematical ones) are more quantitatively accurate.

Mathematical models are the easiest ones to transmit to others without losing information, and along with the fact of being the most accurate quantitatively, they are usually the most used. However, we must remember that they are only tools at the service of the analyst (either researcher, scientist, or professional) and not a substitute of the expert.

Usually, mathematical models consist of three components: parameters, variables and constraints. Parameters are fixed numerical values that describe properties of the system, and they are supposedly known, or estimated, for what they are usually called data. By contrast, variables are values that reflect the behaviour of the system during the runs of the model (e.g. results are variables of a model). Finally, constraints are mathematical expressions that describe the relationships between variables and between these variables and the parameters.

Mathematical models have certain qualities that make them suitable for analysis in IWCM. Some of these properties are, for example, enlarging their use because of their simple transmission (using mathematics) and rate of use (thanks to computers). These models, and partly also Developing a mathematical model implies a process in which the reality has to be abstracted into a conceptual model that intends to capture the functioning of the real system. This model is, in turn, transformed into a set of mathematical relationships that need to be solved by means of numerical algorithms, which in turn are programmed and compiled in order to run in a given computer environment (see figure 2.3.1).



Figure 2.3.1Example of the process to pass from reality to the mathematical relationship that will be solved by numerical algorithms to constitute a rainfall-runoff model

computers, allow the organization of data, results and alternatives. They can also evaluate different alternatives (applying repeatedly to different scenarios), so they are ultimately contributing to decision making.

These models can be classified according to various concepts, for example depending on the modelling process (rainfall-runoff, flooding, groundwater flow, reservoir management, etc.); on the consideration of random variables or not (stochastic, or deterministic); on its basis on actual observations (empirical) or, on some basic theory or without empirical coefficients (conceptual); on the type of mathematical relationships (linear, nonlinear, etc.); on the consideration of the spatial distribution of the physical characteristics of the system (distributed) or not (aggregated).

Simulation and optimization approaches

In addition to the previously mentioned type of models, an important distinction is made depending on the purpose of its use being descriptive (simulation) or prescriptive (optimization); and also on the time horizon and scope of the analysis (planning, management, etc.). Simulation models are used to assess the system status for given scenarios, while optimization models modify the parameters and/or variables to achieve the optimal value of a predefined objective function.

The use of simulation or optimization models will depend on which approach we prefer to find the solutions, the simulation or the optimization approach. Both techniques require the development of a model (simulation model and optimization model respectively). With the simulation technique the model is run using a set of controllable values of the operating data, then the results are analysed, and if necessary, the controllable inputs are changed, and the model run is repeated, expecting better system performance. On the contrary, and in theory, the optimization technique requires only one run of the optimization model to find the solution.

For real world problems, both techniques have their advantages and disadvantages. On the one hand, the advantage of the optimization is that, once assumed that the model represents the system precisely, it obtains optimal solutions, while the simulation, being a trial and error technique, depends on the skill of the analyst to find the optimum. However, optimization being a very laborious mathematical process, in many cases the system requires major simplifications, as mathematical models used in IWCM are shown, such as rainfall-runoff models (Patrical), groundwater flow model (MODFLOW), management simulation (SIMGES), and evaluation of water quality (GESCAL).

Patrical (Ferrer, 2012) enables the construction of hydrological cycle and water quality spatially distributed models, with monthly time step simulation. The constructed models perform the simulation of the hydrologic cycle in a natural regime or altered by human activity, applying the formulation in each small element (e.g. resolution of 1 km x 1 km) in the discretized watershed (see figure 2.3.1). Used as data maps of soil and groundwater characteristics, as well as maps of precipitation, temperature, and pollutants loads, the model provides as output, maps of real evapotranspiration, soil moisture, surface runoff, groundwater storage, and water quality for some constituents (see figure 2.3.2).



Figure 2.3.2 Example of results from Patrical. (a) Maps of monthly temperature and precipitation and results of water flows in the drainage network (Júcar Basin Organization District, in Spain) and (b) flux diagram of Patrical model (from Ferrer et al., 2012).

will be mentioned in subchapter 2.4, so that their level of detail is usually much lower than the one used in a simulation model, with the danger of not being realistic enough.

Given the above, it is desirable to use a problem solving approach combining adherence and flexibility of simulation models with the efficient exploration of mathematical optimization models (Wurbs, 1993).

Examples of models used in IWCM

The complexity of the hydrological cycle creates the necessity of applying different modelling techniques for different processes and parts of them. In this section several examples of SIMGES (Andreu et al., 1996) is a general tool to develop models to simulate the quantitative management of complex Water Resource Systems (WRS). The WRS is conceptualized as a flow network which includes all the relevant elements that constitute the WRS, such as surface storage (reservoirs and lakes), subsurface storage (aquifers), and elements for collection, transport, use and/or consumption (water demands) (see figure 2.3.3). Using as data the physical characteristics of the elements and also considering water rights, operating rules, and environmental objectives and restrictions, the model simulates each element (with specific submodels), as well as the relationships between the elements, at a monthly scale and renders as results the water flows and storages through the system at any spatial scale the user prefers. The model admits any configuration and, therefore, can be used in any WRS. both. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through river beds, can be simulated. Hydraulic conductivities or



Figure 2.3.3 Schematic of SIMGES model for the simulation of the management of the Júcar river water resource system, in Spain

MODFLOW-2005 (Harbaugh, 2005) is a tool to develop groundwater flow models that simulate steady and nonsteady flow, and also water quality, in an irregularly shaped aquifer whose layers can be confined, unconfined, or a combination of transmissivities for any layer may differ spatially and be anisotropic, and the storage coefficient may be heterogeneous.

GESCAL (Paredes-Arquiola et al., 2010) is a tool to develop mechanistic models to evaluate the



Figure 2.3.4 Example of the concentrations of a pollutant in a coastal aquifer in Spain, simulated with MODFLOW

water quality in the elements of a Water Resource System at a basin level. It includes the calculation of all the processes of water quality modification, both in rivers and in reservoirs. These calculations are done at every element of the river basin scheme defined for the previously mentioned that, in order to facilitate the use of models, and also to close the gaps between model developers and practitioners, and between technicians and stakeholders, it is currently recommended to integrate models in Decision Support Systems, at it will be demonstrated in subchapters 2.5 and 2.6.



Figure 2.3.5 Example of results from GESCAL. Compared conductivity of the Llobregat River, in Spain

SIMGES, connecting them according to the calculated flows. Therefore, applying the model to different decision alternatives in the river basin management, it is possible to evaluate the consequences for the water quality in the entire WRS.

Besides the examples provided herein, many other models can be found in the literature (Berhe et al., 2013; Loucks and Beek, 2005; Halwatura and Najim 2013; Mays 1996, Francés et al., 2007) with respect to specific phases of the water cycle, or integrating several phases, or integrating several aspects of IWCM, such as water quantity, water quality, environment and economics.

Conclusion

It has been stated that mathematical models enable us to solve real problems in a scientific way, helping us to analyse the water cycle and water resources systems. Several examples of models that can be used in IWCM have been shown. Besides these, many other models can be found in the literature with respect to specific phases of the water cycle, or integrating several phases or aspects of IWCM. However, there is no universal model that solves all the problems, but rather different models better suited for different aspects and phases of IWCM. The appropriate choice of the models used in IWCM is a key factor in the successful assessment of the effectiveness of proposed solutions for problems under given scenarios. Finally, it must be said

2.4 Optimization of Water Resources Systems

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Introduction

A water resources system, from the management point of view, can be considered to be a combination of different sources of water, multiple reservoirs, natural and artificial conveyance facilities, among other elements, which is operated to supply water for different existing uses, taking into account environmental necessities. Optimization of such systems consists of finding the decisions about resources allocation, flow regulating strategies and reservoir operation rules development, and real time decision-making about water withdrawals from different sources.

To achieve these objectives, the use of mathematical models that allow (or facilitate) carrying out the optimization process results are of great help. This chapter reviews the existing techniques that have been used for water resources systems optimization and gives some examples of their application in literature. Finally, it reviews the most common optimization problems in water resources systems analysis and shows different approaches for solving them.

As mentioned in subchapter 2.3, the analysis of problems related with Integrated Water Cycle Management (IWCM), can be facilitated by the use of models, mainly in the phases of identification and assessment of alternative solutions, and selection of the best alternative. We also commented that, in order to resolve these phases of the analysis, simulation or optimization approaches could be followed, with the final recommendation to follow а combined simulation-optimization approach. Optimization models are the tool used in the optimization approach, as well as in the combined simulationoptimization approach.

An optimization problem consists of obtaining the best value (maximum or minimum) of a function of the so-called decision variables. This function is called the objective function and it is the heart of any optimization technique (Wurbs 1993). Additionally, optimization problems can be classified with regard to their characteristics, commonly being classified as constrained and unconstrained problems. Other classifications exist with respect to the linearity or not of the objective function and/or the problem constrains, or whether the problem is continuous or discrete.

However, in real world problems of IWCM, the combination of the decision variables must be "feasible", and therefore, must comply with a series of restrictions, such as, for instance, mass balance equations, or maximum and minimum limitations. Therefore, the flow kind of optimization problems usually posed in IWCM fall into the constrained optimization, being the constraints of many types (e.g., equality, inequality, or even logical constraints in some cases), and, as it will be shown later, the number of decision variables can be huge, especially in dynamic problems, when variables are also function of time, hence multiplying the number of variable by the number of time periods considered in the problem (e.g., by 240, if optimizing a time horizon of 20 years in a monthly basis). As a result, analytical methods given by classical calculus approach are not useful to solve the problems, and numerical optimization models are the most used tools to solve real word cases.

Thus, we will usually face constrained optimization problems with the form:

 $min/\max f(\vec{x})$ subject to

$$\begin{cases} h_i(\vec{x}) = 0 & i = 1, 2, ..., m \\ g_i(\vec{x}) \le 0 & j = 1, 2, ..., r \\ \vec{x} \in S \end{cases}$$

where \vec{x} is a vector with n dimensions containing decision variables x_1, x_2, \dots, x_n , $f(\vec{x})$ is the objective function; $h(\vec{x})$ and $g(\vec{x})$ are equality and inequality restrictions respectively; and S is a subset of the n dimensional space.

In the present subchapter, we will focus mainly on the use of optimization models for Integrated Water Resource Systems Planning and Management (IWRPM).

Optimization in Water Resource Systems Planning and Management

A Water Resources System (WRS), from the planning and management point of view, can be considered to be a combination of different sources of water, multiple reservoirs, natural and artificial conveyance facilities, among other elements, which is planned and operated to supply water for the different existing uses, taking into account environmental, social and economical aspects related to the basin(s) and society(ies) where the WRS is located.

The optimal management and operation of a water resources system involves allocating resources, developing stream flow regulation strategies and operating rules for reservoirs, and making realtime decisions within the guidelines of the operating rules (Wurbs 1993). The objectives of water resources system optimization can be to maximize benefits, minimise costs, and/or meet the various water demands (e.g., minimizing deficits, or maximizing reliability, or minimizing vulnerability, etc.), subject to the mass balance equations and other constraints related to priorities and water rights, water quality and environmental considerations, etc. (Rani & Moreira 2010).

Materials and methods

The most common methods among numerical optimization techniques to solve the above problem described in the scientific literature are:

Linear programming: This methodology considers both the objective function and problem constraints to be linear. It is easily applicable to large problems, there is no need to supply any initial feasible solution and the solution always converges to a global optimum. Additionally, results of sensitivity analyses are very easy to apply since there are a large number of available tools to solve these kinds of problems.

Non-linear programming: Sometimes. linearization produces a solution that falls outside what would be acceptable in reality. Thus, the problem must be directly approached from a nonlinear point of view. Some robust and powerful algorithms that allow solving this are namely (Labadie 2004): sequential linear programming: sequential quadratic programming; augmented Lagrange method; or the reduced gradient generalized method. All these methods require that both the objective function and the problem constraints are derivable. The most important disadvantage of non-linear programming is the high computational requirements of the algorithms, so the most common application of these techniques is in implicit stochastic optimization.

Dynamic programming: This optimization method solves multi-stage decision processes. The most attractive characteristic to apply dynamic programming in water resources optimization is that a complex multi-stage problem can be decomposed into a series of simpler sub-problems that can then be solved in a recursive form (Rani & Moreira 2010), using the solution of one problem to obtain the solution of the next one. A general problem of this technique is the huge storage requirements of the algorithms since they need all the results from previous stages, which may be an issue in highly-dimensional problems.

Computational Intelligence: All the above optimization methods are algorithmic processes. This means that they all use well-structured procedures that converge to a certain quantitative solution. Computational intelligence is the term used to define a wide range of techniques such as evolutionary computation, fuzzy logic and artificial neural networks. These methods do not even guarantee achieving a local optimum, but try to find acceptable or satisfactory solutions. Nevertheless, they can deal with many complexities present in water resources systems that limit the use of traditional optimization methods. Generally, techniques belonging to this group are computationally demanding but provide an important range of modeling capabilities. Optimization models can be used to analyze problems in IWCM, as for instance prediction of water resource variables, optimal design of water

distribution networks, or design of optimal operating rules for WRS.

Applications

Application to optimal water allocation

In IWRPM, a common problem we will want to solve is the efficient operation of a complex multireservoir system for which we will need to define a series of operation rules to best meet all the water needs within the system, also known as the water allocation problem.

An optimization technique that adapts especially well in these cases among others is network flow programming, which is a particular case of linear programming. This method takes advantage of the particular distribution of water resources systems to use very efficient algorithms. Several commercial models for water resources systems optimization, such as OPTIGES (Andreu et al 1992) and MODSIM (Labadie 2000) use this method. Figure 2.4.1a shows a simple water resources system with one reservoir and two demands; we can assimilate this system to the graph in figure 2.4.1b that corresponds to the network flow expanded for an optimization period t.





With network flow programming we can calculate the optimal water allocation in the system during a determined optimization horizon. So, the main use of this optimization problem would be to know the yield of the system when it is operated optimally. Used in this way, it can be a very useful tool to preliminary design of WRS (e.g., sizing of demands, or sizing of reservoirs, or sizing of water transport facilities). Figure 2.4.2 shows a scheme of a real system where this optimization approach was followed to assess the optimal yield of the Segura River WRS, in Eastern Spain, including water transfer from the Tagus River system. Also, an operating policy could be inferred from the optimal results provided by the network flow problem, for instance, by doing a linear regression of the results to find the relation between some state variables (e.g., reservoir volumes) and some decision variables (e.g., water releases).

Despite the extensive use of linear programming, many aspects within water systems have a strong non-linear behavior such as aquifers, evaporation or demands returns. These aspects have been traditionally solved by simplifications, approximations or iterations (Haro et al. 2012, Fredericks et al. 1998).

Application to the design of operating rules

When looking for optimal operating rules, one can express the operating rule in an explicit manner within the constraints of the optimization problem and find the optimal parameters, for instance, as it is done in the linear operating rule. But this approach is very limited in practice since the form of the operating rule is usually very simple.

Figure 2.4.2. Scheme of the Segura River WRS to

assess its optimal yield including a water transfer from another WRS

Another possible approach to this problem is coupling a simulation and an optimization model. First, creating a simulation model of the system (e.g., using a simulation shell as SIMGES, which will be shown in subchapter 5.6) and, second, finding the best operation rule by recursively varying its parameters until obtaining the best value of the objective function with an optimization technique like genetic algorithms. This approach was successfully applied in Lerma et al (2013a & 2013b) in a form similar to the one shown in figure 2.4.3.

Other applications

The amount of problems in water resources planning and management for which an optimization approach might be necessary is very broad. There are simple problems such as sizing a reservoir capacity or determining the maximum obtainable yield, and there are more complex issues like optimal multi-reservoir operation, conjunctive use of surface and groundwater, optimal water quality management, hydroeconomic modeling of WRS, or optimal water resources system expansion. In either case, the techniques described above can be used alone or combined to find a proper solution to any of these problems. Several additional examples can be found in Loucks and van Beek (2005).

Finally, another application of optimization techniques within the scope of IWCM and IWRS warranting consideration is the calibration of complex simulation models, so they match reality in the best form. In this case, the problem is finding the best combination of parameters of one particular model so its results match the observed



data. This is important because a calibration process normally involves changing the values of the model parameters in a recursive way until finding the best combination, and evolutionary algorithms are particularly applicable in perform this task.

Conclusion

We presented the problem of water resources optimization in this subchapter. We saw that both objective function and constrains in this kind of problem are usually complex and there is not a single algorithm that warrants achieving a global optimum. Nevertheless, if we take certain precautions, we can normally reach values very close to optimum. The continuous evolution of computer technology offered new chances to computational and detail limitations of models make that results are not as good as operators are willing to accept; (3) optimization models are more mathematically complex, what makes them more difficult to understand than simulation models; (4) many optimization models cannot include risk or uncertainty in the calculations; (5) there is a large quantity of options among which to choose and sometimes it is difficult to decide which is the most appropriate one; and (6) it is not possible to generalize all of the described methods what will require a specific formulation in each case.

Including optimization models in decision support systems (see subchapter 2.5), such as OPTIGES in AQUATOOL (Andreu et al., 1996), may help users "lose their fear" to use optimization as a



solve problems previously impossible to solve.

Optimization techniques will allow us to approach a complex decision making problem in which a number of values must be chosen for a number of interrelated variables paying attention to one or several objectives designed to measure the results and the quality of the decisions made. Thus, it is essential to find a proper objective function. However, this is not an easy task in any kind of problems nor it is representing in a complete form all the complexities within the system to optimize. Therefore. optimization results must he considered as approximations and not as exact solutions.

Water resources systems optimization is one of the knowledge areas in which more different optimization techniques have been previously applied (Labadie 2004). Despite this, there is still a big difference between theoretical applications and real life ones. Some of the reasons for this are: (1) the skepticism of many operators with regard to model results, preferring to place their confidence in their own experience; (2) method to solve many problems currently present in the field of WRS management. However, it is necessary to improve the representation of models as well as their generalization so it is not necessary to particularize the formulation of problems for each different case.

An additional recommendation is that, once we reach the optimal solution, it is interesting to perform a sensitivity analysis. This refers to the changes of the optimal solution if we introduced variations in the model parameters. These changes refer to both the value of the objective function and the variables of the problem. With this analysis we can identify the most critical parameters and the need of their better estimation if there was some uncertainty on their appropriate value.

Acknowledgements

The authors want to thank the Spanish Ministry of Economy and Competitivity (Comisión Interministerial de Ciencia y Tecnología, CICYT) for funding the projects **INTEGRAME** (CGL2009-11798) SCARCE (CSD2009-00065) and NUTEGES (CGL2012-34978). Also thanks to the European Commission (Directorate-General for Research & Innovation) for funding the projects DROUGHT-R&SPI (FP7-ENV-2011, 282769) and ENHANCE (FP7-ENV-2012, 308438).

2.5 Decision Support Systems For Integrated Water Resources Planning And Management: Water Quality And Environmental Issues

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Introduction

Multidisciplinary models are useful tools to combine different disciplines when addressing Integrated Water Resources Planning and Management. This sort of model facilitates the construction of a shared vision of the river basin among the actors, and provides results to analyse the trade-offs between the alternatives to solve existing problems. The Decision Support System Shell AQUATOOL allows the building of such an integrative model. It includes tools for water resources management, water quality and habitat analysis, amongst others. By coupling them together, it is possible to optimise environmental flows regimes while considering the real constrains in river basins. As an example of its use, we propose a methodology in which the water allocation model solves the allocation problem through network flow optimisation, and considers the environmental flows in selected river stretches; the water quality model performs the water quality evolution in rivers and reservoirs; and the habitat model provides Habitat Time Series for each available Weighted Usable Area-Flow curve. This approach was applied to the Tormes Water Resources System. The results demonstrate the potential of the methodological

framework to reach a balanced solution for the key aspects of the river basin, by defining water management rules that simultaneously maintain water supply, aquatic ecosystem and water quality legal standards.

The current framework for water planning and management in Europe is the Water Framework Directive (EP, 2000), which aims to achieve good status in all water bodies. It sets the river basin as the appropriate unit of analysis and for developing solutions. Referring to surface water, this includes reaching good ecological and chemical status. Further to this, the satisfaction of water demands should also be a main target in the long term (planning) and short term (management). In order to cover so many aspects at river basin scale, tools for data management and analysis, and integrative models are needed to cope with the complexity, the basin scale scope, and the huge amount of information, alternatives, and scenarios (Andreu et al., 2008). As mentioned in sub-chapter 2.6, Decision Support Systems (DSS) are suitable platforms to organise, summarise and analyse data from different models to support decision-making. Moreover, DSS are essential for the purpose of providing integration, easiness of use by actors involved in the decision making process and in developing a shared vision for conflict resolution (Andreu et al., 2008).

The establishment of environmental flows (the stream flow regimes needed to maintain the structure and functionality of aquatic ecosystems and the associated terrestrial ecosystems) in river systems with water scarcity requires an agreement among the different uses because it influences many variables, like water availability for economic uses or water quality. In this chapter, we propose an integrated methodology consisting of three linked models for water resources management, water quality modelling and habitat availability. Whilst each of these models could work independently, the analysis is much simpler if they work under a common DSS. Thus, the data transfer is immediate in that the outputs of one model are inputs for others. To illustrate the potential of the AQUATOOL DSS for Integrated Water Resources Planning and Management, we describe, reason and solve the establishment of environmental flows regimes by means of a scenario approach in the Tormes Water Resources System (TWRS) in Spain.

Material and Methods

Methodology

The AQUATOOL DSS Shell (Andreu et al., 1996) includes, among others, the module SIMGES (Andreu et al., 2007) which addresses the water quantity allocation problem through network flow optimisation, and considers the environmental flows in selected river stretches; the module GESCAL (Paredes-Arquiola et al. 2010) that performs water quality evolution aspects in rivers and reservoirs; and the module CAUDECO (Paredes-Arquiola et al., 2011) based on the Instream Flow Incremental Methodology (Bovee et al., 1998), which determines Habitat Time Series (HTS) using flows in rivers and Weighted Habitat-Flow curves resulting from specific habitat studies (see Figure 2.5.1).

Figure 2.5.2 shows a diagram of the proposed methodology. First, the three models have to be built, calibrated and validated. The construction of

the model includes the visual diagram of the river system and the data introduction. All this is done AQUATOOL. The calibration using and validation of the models consists in changing the different parameters to achieve an acceptable similarity between simulated and observed variables. Then, the integrated model is ready to be used. SIMGES is run with certain management assumptions, providing time series about the water supply to demands, flows in rivers and volumes in reservoirs, amongst other results. This information is used as input for GESCAL which provides time series of concentrations in rivers and reservoirs for some selected pollutants, and CAUDECO which produces HTS for the studied aquatic species, like the Luciobarbus bocagei.

Case study: The Tormes Water Resources System (TWRS)

The TWRS is a multipurpose water system where agricultural, urban and hydropower demands account for most of water resources. The annual



Figure 2.5.1 Conceptual diagram of CAUDECO



Figure 2.5.2 Integrated methodology diagram (Paredes-Arquiola et al., 2013).

water demand is 60% of the annual renewable resources, what leads to water stress problems during drought periods. Moreover, water quality is affected by urban discharges in the lower part of the basin, with high dependence on river flows. The critical site of the system is point 4, just upstream the Almendra Reservoir (see Figure 2.5.3).

the maximum value of the range in all the control points, but reduces them in dry years.

To conduct the trade-off analysis, several indicators were obtained from each simulation: maximum annual deficit of agricultural demands, 80% percentile of the HTS for the "Large *Luciobarbus bocagei*" fish species, maximum ammonium concentration and minimum dissolved



Figure 2.5.3 Location and main elements of the TWRS



Figure 2.5.4 Scenarios analysed.

We conducted a scenario analysis with different environmental flows. They were established in four control points (see Figure 2.5.3), and they were simultaneously changed in all points from 0m³/s (PRESENT scenario), in steps of 10% increasing, to the maximum flow determined in biological studies (QECO-OPT scenario), 6m³/s in point 4, for instance. After a trade-off analysis to agree on a final environmental flows regime, an operation rule was defined to improve the system functioning in drought conditions, resulting in the Operation Rule scenario (OR scenario). This scenario establishes the environmental flows at oxygen concentration.

Results and Discussion

The trade-off graphic showed in Figure 2.5.5 represents, in a simple and clear way, the evolution of the selected indicators as the environmental flows change at point 4 (the critical point in the TWRS). In relation to the Spanish legal prescriptions (for water quality in water bodies, supply to demands and habitat availability) concerning the diverse scenarios analysed, the most adequate environmental flow is

6m³/s in point 4 (QECO-OPT scenario). It provides water quality values which accomplish the legal Spanish water quality standards for ammonium and dissolved oxygen concentrations and usable habitat values around 82% of the maximum weighted usable area for 80% of the simulated months. However, the water supply deficit of agricultural demands is higher than the threshold established by the Spanish legislation: 621.6Hm³versus 511.8 Hm³, respectively. This is mainly due to the selected simulation period, which includes a drought situation. If a high environmental flow has to be fulfilled, it is not way, it is possible to identify problematic periods with high supply deficits, and to define the best operation rule. The new indicators are the time series of the supply deficits with regard to meeting agricultural demands, ammonium and dissolved oxygen concentrations and the HTS of the Large *Luciobarbus bocagei*. It can be observed in Figure 2.5.6 that the water quality and the habitat availability have ideal values during the simulated period. On the other hand, the supply deficits are frequent and have significant magnitudes that represent the 60% of the total demand.



Figure 2.5.5 Curves for the trade-off analysis.

possible to meet all supply demands and hence deficits appear.

According to the results presented above, it is necessary to design an operation rule to balance the system functioning in dry years to ensure the proper water supply to demands. To do so, a detailed assessment of the selected environmental flows regime effects has to be undertaken. In this In order to address this problem, the OR reduces the environmental flows in dry years to diminish the impact on water demands. Every month it compares the inflows to the head reservoir with the historical inflows; then, a different restriction coefficient is applied to the environmental flows regime in control point 3 depending on the relation between both inflows. Figure 2.5.7 shows



the final operation rule.

Figure 2.5.6 Evolution of indicators in the QECO-OPT scenario.



Figure 2.5.7 Operation rule to reduce environmental flows in dry years.

The OR scenario presents a more balanced result among the different variables. In this case, the agricultural demands deficit accomplishes the legal specifications. In turn, as depicted in Figure 2.5.8, the habitat availability maintains high values and only falls to 50% of the maximum habitat in dry years, which is considered satisfactory. The same occurs with the dissolved scenario would be suitable to be established in the TWRS.

Conclusion

In the process of decision making, information must be managed and analysed in relation to the feasible alternatives, their impact on the multiple objectives, the trade-offs among them, and the associated risks (Andreu et al., 2008). DSS are useful to support complex assessments. DSS such as AQUATOOL are appropriate tools to develop and apply methodologies which link different kinds of models together at a river basin scale to support the development of Integrated Water Resources Planning and Management strategies. These methodologies are very useful to evaluate the relationships among key aspects of water resources systems. Moreover, they provide results which can be used in participatory processes to achieve consensus among all actors of the river basin.



Figure 2.5.8 Evolution of indicators in the OR scenario.

oxygen concentrations. In contrast, the ammonium concentration is more affected by the environmental flow reduction, although most of the time the concentrations are under the legal threshold, 1mg/L.

In summary, the OR scenario is considered a good solution to ensure a good environmental and water quality situation in normal and humid years, while in dry years the impact is distributed among all the considered aspects (water supply, water quality and habitat availability). Thus, this In this sub-chapter, we have presented a scenario approach to define an environmental flows regime in the Tormes Water Resources System that simultaneously satisfies the legal requirements for water supply demand, river water quality and habitat availability. Moreover, a set of trade-off and simulation indicators have been proposed. They show in a simple and clear way the evolution of the target variables, contributing to achieving more integrated, efficient and equitable solutions.

Acknowledgements

Authors would like to thank the Spanish Ministry of Economy and Competitiveness for its financial support through the project SCARCE (Consolider-Ingenio 2010 CSD2009-00065) and NUTEGES Nacional de I+D+i 2008-2011, (VI Plan CGL2012-34978). Besides, we are grateful to the European Commission for funding the research projects DROUGHT-R&SPI (FP7-ENV-2011, 282769), ENHANCE (FP7-ENV-2012, 308438), WAMCD (EC-DG Environment No. 07.0329/2013/671291/SUB/ENV.C.1) and LIFE ALBUFERA (LIFE12 ENV/ES/000685).

2.6 Decision Support Systems For Integrated Water Resources Planning And Management: Water Quantity Issues, Conflict Resolution, And Drought Risk Assessment

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Introduction

New water policies around the world are demanding more integrated, participatory, sustainable, efficient, and equitable planning and management of water resources. All these considerations introduce a higher degree of complexity into the already complex task of integrated water resources management. In the process of making good decisions, information must be managed and analyzed about the feasible alternatives, their impact on the multiple objectives, the trade-offs among them, as well as risks associated with them (Andreu *et al.*, 2008).

To elaborate and analyse such information, sound science, technology, and expertise have to be involved. But, as noted by Andreu *et al.* (2008), decision makers, stakeholders and general public, that is, Policy Making Actors (PMA), are not prepared to produce and understand such information. Therefore, a transfer of technology and ideas from scientist to PMA is needed. This has to be an effective transfer in the sense that PMA must be able to apply the technology easily and in a repeatable and scientifically defensible manner (NRC, 2000). One of the best ways to conduct this transfer, and to build a shared vision of the basin, is through the joint development of Decision Support Systems (DSS).

A Decision Support System (DSS) is a computer tool developed to help in the process of making decisions. They are essential for the purpose of providing integration, sharing vision for conflict resolution and implementing sensitivity analysis and risk assessment. Many examples of DSS development are presented and/or reviewed by Reitsma *et al.* (1996), Giupponi *et al.* (2006) and Palaniappan *et al.* (2008).

We should differentiate between DSS with specific purpose, and integrative DSS (Andreu et al., 2008). The first ones are required during the basin identification phase in order to study the physical and other aspects of the basin, and its management. Even though this step might seem as not requiring participation of stakeholders and public, but only of experts in the subjects, experience shows that a great effort has to be devoted to transparency, and to education and diffusion of the modelling activities. One of the most important goals of this step is to get the confidence and trust of the PMA about the basic data and models that will be used during the policy making process. Furthermore, it is essential to have an integrative DSS at basin scale. This means that there must be a DSS integrating, in a single model and for the entire basin, all the relevant surface water elements, aquifers, environmental infrastructures, water uses, requirements on flows, water rights and priorities, and operating rules for the system. The purpose of this model is to simulate the management of the basin. Once the system is completely defined, the user can perform simulation runs of the management for multiple different alternatives, time horizons and scenarios, using different hydrological data and also different operating policies.

For over 35 years, researchers and technicians in information systems have been dedicated to the development of DSS. As a result, several DSS are currently being used in the analysis of water resource systems in various parts of the world. Some examples of these tools are:

- ModSim, from the Colorado State University (USA) (Labadie, 2007)
- WEAP21, from the Stockholm Environment Institute (United States) (Yates, 2005)
- MIKE Basin, the Danish Hydraulic Institute (Denmark) (DHI, 1997)

- REALM, developed at the Victoria University (Australia) (Victoria University, 1997)
- Ribasim, from Delft Hydraulics (Netherlands) (DHL, 2002)
- Waterware, developed during the European research project Eureka- EU497 (ESS, 1995)
- IRAS, from Cornell University (United States) (Loucks et al., 1995)
- AQUATOOL, from the Polytechnic University of Valencia (Spain) (Andreu et al., 1996)

In this subchapter, two real cases of use of DSS in participatory decision making processes for the Jucar River Basin, in Spain, are presented. The DSS for these purposes was developed using AQUATOOL DSS shell (Andreu *et al.*, 1996), facilitating the development and use of the water resource system, conflict resolution and drought management. More details about AQUATOOL are given in subchapter 2.5.

The Jucar River Basin, in Spain

Spain is an EU country characterised by presenting a high irregularity in temporal and spatial distribution of water resources, with numerous areas affected by water scarcity and frequent droughts (MIMAM, 2000). The Jucar Basin Agency (Confederación Hidrográfica del Júcar, CHJ) manages a basin with an total surface of 42,989 km², including areas within several adjacent basins which flow to the Mediterranean Sea in eastern Spain (see figure 2.6.1).

Participatory analysis has been implemented in the Jucar River Basin for over a decade, not only in the tasks related to the River Basin Management Plan, but also in the design phase of some projects, or in the management conducted during the drought episode that lasted from 2005 to 2008.



Figure 2.6.1 Location of the basins that constitute de CHJ territory

Conflict resolution with DSS: The Jucar-Vinalopo Project

In the year 2004, a Group of Study (GS) was established to study the feasibility of the Jucar-Vinalopo Project (JVP), which is a transfer of water from the Jucar River Basin to the Vinalopo-Alacanti-Marina Baja area. This GS was composed of the main representatives of the several groups involved in the planning and management of water resources, experts, and stakeholders, and was working for four months in the development of a water resources management model applied to the Jucar River Basin, in order to have a common objective tool to analyze the viability of the project. Moreover, this model was made available to all members of the GS, so they could perform simulations on their own, either to check results offered by other parties, or for their own analysis (see figure 2.6.2).

Scenarios and alternatives were identified (Andreu *et al*, 2009a): hydrological scenarios to use in the analysis, water needs for the different water uses, environmental requirements at several places in the Jucar River Basin, operating rules to be adopted in order to reflect legal priorities among sectors of water uses, among users in each sector, and between environmental requirements and water uses in normal and drought situations and technical measures that could be included in the management of the system in order to improve reliability of water uses and environmental requirements.

Finally, the simulations were run for all scenarios considered and the corresponding results were obtained, which provided valuable information for the decision making process. From these results a complete report, which agreements, disagreements, and simulation results were reflected, along with summaries and synthesis was developed. In order to facilitate decision making, graphs showing the trade-offs between objectives were produced, as the one shown in figure 2.6.3, were trade-offs between potential transfer to Vinalopo-Alacanti-Marina Baja (y axis), environmental flow requirements at Jucar River (x axis), and Albufera wetland inflow are displayed (each group of lines corresponds to a different level of total inflows to the lake). Besides to helping in the analysis of the problem at hand, an important achievement of this GS was to transmit to stakeholders a filling of transparency in the resources management, getting them water familiarized with the tools of analysis, thereby achieving the transfer of knowledge and acceptance and confidence in results. Finally, it became a very useful experience for future issues, such as the drought in the CHJ in the period 2005-2008.

"Permanent Drought Committee" (PDC), with special powers to administer the basins of CHJ



Figure 2.6.2 Schematic of the Water resources management model for the Jucar River Basin, developed with AQUATOOL



Figure 2.6.3 Synthesis graph to display trade-offs between ecological flows, wetland inflows, and water transferred to Vinalopo-Alacanti-Marina Baja area.

Drought management with DSS: The 2005-2008 drought in the Jucar River Basin

During the hydrological year 2004/05, a severe meteorological drought started within the Jucar River Basin. In fact, it led to one of the more intense hydrological droughts registered in the basin in the recorded history (since 1940). This particular hydrological year from 2004 to 2005 was ranked third, in terms of lowest total inflows to the ensemble of Alarcon, Contreras and Tous reservoirs; 2005/06 was ranked the lowest (Andreu *et al.* 2013), as shown in figure 2.6.4.

At the end of the 2004/05 hydrological year, the

under emergency situations was set up (Andreu et al. 2009b). The PDC was composed of the PMA, with representatives of the Ministry of Agriculture, the CHJ, regional governments, the agricultural, industrial and urban uses, the Spanish Geological Institute, labour unions and non-governmental environmental organizations. Its missions were (Andreu et al. 2013): to take decisions on water management during the drought; to perform a continuous monitoring in order to control the efficacy of decisions; to follow the evolution of the drought, and its impacts on users, on water quality environment; and to and on the authorize emergency works.

In March 2006, the forecast provided by the previously mentioned DSS for the Jucar River was that, if no additional measures with respect to the





ones taken in the previous year were undertaken, reservoir storage would reach values bellow 55 hm³ (minimum environmentally and technically admissible value) (see figure 2.6.5). In figure 2.6.5, we also can see a probabilistic forecast given by the DSS, which gave only a 20% of probability of ending the campaign with more than 100 hm³ in the reservoirs. These figures built up a perception of risk in the body of the PDC, leading to anticipation measures in order to reduce the risk. So, surface water allocated to irrigation was reduced to 50% of normal supply in traditional users, and to 30% of normal supply to junior water rights. Supplementary supplies from groundwater of about 40 hm³ were mobilized, as well as 60 hm³ from recirculation of water in the rice fields in the wetland area (Andreu et al., 2009b).

2006/07 and 2007/2008. The abundant rainfall received in the hydrological year 2008/09 brought the basin back to normality.

The implementation of the PDC became a very useful experience for other issues such as the review of the operating rules, the design of the Special Drought Plan (MMA, 2007), and subsequent new versions of the Basin Plan.

Conclusion

According to the authors' experience, participatory analysis is part of the planning and management of water resources, not only because it is a requirement of the Spanish and EC directives, but also because it has become a necessity. In this



Figure 2.6.5 Deterministic (left) and probabilistic (right) forecast for the reservoir storage evolution in 2006 campaign (Andreu et al., 2009b)

It was agreed to take to reduce the supply to the metropolitan area of Valencia from the Jucar River, and to increase the amount of water supplied from the Turia adjacent basin in 50 hm³/vear approximately. As а partial compensation, it was also agreed to supply over 35 hm³ of adequately treated waste water to traditional agricultural users in the Turia basin. Furthermore, CHJ temporarily purchased 50 hm³ of water rights from other agricultural users to avoid extracting from groundwater, which resulted in lower abstraction from the middle Jucar River and an improvement in environmental flows. The design of these measures was based on the results of the DSS (Andreu et al., 2013 showing the improvements provided by the measures (see figures 2.6.5). As shown, with the application of the measures, the deterministic forecast gave a value storage at the end of the campaign of 143 hm³, and the probabilistic forecast gave a 90% of probability of ending the campaign with more than 100 hm³. So, the measures were implemented, and similar analysis and actions were performed in hydrological years

chapter we have shown two examples of active, effective, informed and responsible participation. We have noted that participation of all stakeholders allows a participatory management being more effective and sustainable, solving problems and conflicts and requiring transparency, technology transfer, effort and patience.

The use of DSS enables the integration of planning (long term) and management (short term), and, as it has been shown DSS can be very useful for the real time management basins, for instance, during drought episodes and their associated conflict situations. Efficient water management becomes a fundamental requirement, always oriented to drought management and requiring anticipation and permanent savings.

Acknowledgements

Authors would like to thank the Spanish Ministry of Economy and Competitiveness for its financial support through the project SCARCE (Consolider-Ingenio 2010 CSD2009-00065) and NUTEGES (VI Plan Nacional de I+D+i 20082011, CGL2012-34978). Besides, we are grateful to the European Commission for funding the research projects DROUGHT-R&SPI (FP7-ENV-2011, 282769), ENHANCE (FP7-ENV-2012, 308438) WAMCD (EC-DG Environment No. 07.0329/2013/671291/SUB/ENV.C.1) and LIFE ALBUFERA (LIFE12 ENV/ES/000685).

2.7 Sampling strategies

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Introduction

In reporting results for chemical, physical or biological parameters for water quality/quantity assessment and awareness should always be made that empirical findings can only be estimates of true population parameters. As such reporters must always ensure that measures of both location (central tendency) and dispersion are reported in parallel. While estimates of population parameters conventionally use the mean as a measure of central tendency, skewed data sets may render the mean an unreliable measure of central tendency thus researchers must consider and test the underlying distribution of such parameters before undertaking statistical testing of data. In particular the median and accompanying measures of dispersion such as the inter quartile range should be considered where data are skewed

Confidence intervals for population parameter estimates should be given at all times which serve to acknowledge the uncertainty associated with laboratory and in particular, field measurements. Acknowledgement of uncertainty must also be incorporated into experimental design – for example sample size calculations using sample variation, and effect sizes will be provided for effective experimental design.

Planning of sampling

The research question and the chosen target analyte(s) inform the sampling strategy. Depending on the input paths, distribution and fate of the substance(s) to be monitored different sampling strategies are required. If these processes are not fully understood it can be useful to undertake a pilot study in order to identify variations and limiting factors and to develop an appropriate sampling strategy. The sampling of surface waters, for example, will vary depending on which water phase is required, if suspended particulate matter (SPM) is to be separated, or if biota (see chapter 4) are of interest.

For different monitoring strategies, different sampling approaches are required and three main types are differentiated:

- Snapshot sampling: a single sample is collected to provide information at a single time point and location. This can be useful if an acute situation requires monitoring or if conditions are known to be very stable.
- Selective sampling: the location(s) at which samples are collected are chosen based on an informed judgement, considering, for example, sites of pollutant entry or sites of increased exposure of the public to a water body.
- **Repeated sampling**: defined timing of sampling to monitor levels at a locale at adequate intervals.

When it is necessary to take samples for returning to the laboratory, there are basically three types of sample:

- ٨ Grab or spot sample: sample taken over a short period of time from a river or lake using a glass or plastic (usually polyethylene) bottle of 1 1 or 2 1 capacity depending on requirements. This obviously allows only the determination of water quality at the moment of sampling and says nothing about the quality before or after sampling. Spot samples may be taken at a specific depth by lowering the stoppered bottled into the water and removing the stopper with a string. It is possible to obtain an integrated sample between the water's surface and bottom by lowering the bottle at a controlled rate, avoiding contact with sedimentary material and any consequent disturbance. In deep waters (the oceans), special oceanographic samplers e.g. Knudson & Van Doom samplers, are specifically designed to collect a water sample at a specific depth using a messenger system.
- Composite sample: involves taking a series of grab samples and mixing them together to give a more representative sample. Such samples are usually collected (either manually or automatically) at regular intervals and pooled into a large sample prior to analysis. Composite samples are often used

to evaluate the efficiency of wastewater treatment facilities.

• Flow weighted composite sample: taken so that the volume of the sample is proportional to the flow at the time. This is particularly useful when loadings are required.

A more complete description of samplers is given in the ASTM Standards Book (American Society for Testing and Materials), which is published annually.

Time or flow proportional sampling (Ort et al. 2010)

Documentation of sampling strategy

A full documentation and justification of the sampling strategy is required. This is important to identify the rationale behind the chosen strategy, ensure that a full quality assessment is possible The following information should be collected and reported with different samples (Egli *et al.* 2003).

- Sampling location(s), including distance from shore for lake, river and sea water
- Sampling frequency and time(s)
- Sample size
- Sampling method
- Sample storage and treatment

Additional information needs to be provided depending on the nature of the water sample (Egli *et al.* 2003), this is summarised in Table 2.7.1.

Pre-analytical sample treatment and sample storage

The sampled water will often contain suspended solids which may require to be removed or measured separately. If so, filtration through 0.45 μ m membrane filters is required (0.45 μ m:

Table 2.7.1 Further parameters that should be recorded when sampling different water bodies (Egli *et al.*2003).

Type of information	Water temperature	Water pH	Weather conditions ²	Length of collection time	Depth of sample origin	Extraction method	Flow rate (actual & average)	Size of water body	Separation method ³	Other parame- ters ⁴
Rain water	\checkmark	\checkmark	\checkmark	\checkmark					\checkmark	\checkmark
Ground water	\checkmark	\checkmark			\checkmark	\checkmark				\checkmark
Inland surface water⁵	\checkmark		\checkmark		\checkmark		\checkmark	\checkmark	\checkmark	\checkmark
Sediment					\checkmark					\checkmark
Pore water		\checkmark			\checkmark					
Sea water ⁵					\checkmark				\checkmark	\checkmark

and to allow future adaptation of the strategy to new problems.

definition of soluble fraction). If the total sample, including the suspended solids, is to be analysed, this should be carried out as quickly as possible or preservatives added to reduce the chemical and

suspended particles, specific ion concentrations, DO, redox potential, specific information on the water body (including aquifer for ground water and sediment dry matter and content)

⁵ Including suspended matter

² at sampling time and during relevant time period before sampling, including times and volumes of precipitation

³ if dry deposit or suspended material is removed or statement that it was not separated

⁴ if known or assumed to impact the analyte or relevant for the specific research, e.g. DOC, conductivity,

biological processes which will continue in any natural water sample. There may also be interactions with the walls of the sample bottle by leaching of contaminants from the surface or "dirty" containers, leaching of organic substances from plastic or silica, Na+ etc from glass, adsorption of trace metals onto glass surfaces or organics onto plastic surfaces, or reaction of sample with the container material (e.g. fluoride may react with glass). Therefore analysts should use glass bottles when sampling for organics and plastic bottles when sampling for metals. Adjustment of pH to 2 can overcome these problems by inhibiting biological action and retarding ion adsorption to container surfaces. Refrigeration to 4^oC or below will further preserve samples if required. Because of the different sampling bottles and preservatives it may be necessary to collect several samples at each sampling point for determination of different parameters. Samples collected for the identification of biota (see chapter 4) can only be stored for short time periods and ought to be analysed as soon as possible.

Monitoring strategies that allow for testing on-site have the benefit that results are obtained quickly and transport and storage are cut out of the process. However, these are limited to certain analytical methods where the analytical equipment is portable.

Remote monitoring using satellites does not require collection of physical samples at all but it is still necessary to define the correct parameters for the imaging process.

Sample variations and sample size considerations

In addition to the criteria outlined above, researchers who wish to devise sampling regimes for hypothesis testing should always consider the sample size required for the investigation. Clearly, given that any sample measurement is an estimate of the parameters of the underlying population there may be a temptation to collect as many samples as possible in order to be very confident of the precision of the result. The danger of undertaking such an approach is that more samples than are actually required could be collected resulting in wasted expenses and time. On the other hand, the collection of too few samples may result in an inability to provide any meaningful conclusions about the data gathered.

Case study

Suppose a water resource is rated on a scale of 1-7 where 1 is considered excellent quality and 7 poor quality. New water management practices are being implemented and authorities wish to assess their effectiveness. Suppose a mean improvement of 2-points on this scale is deemed to represent a genuine and meaningful improvement in water quality. This is known as the effect size and should be determined before any intervention is investigated and be based on domain expertise, regulatory influence or perhaps a manufacturer's claim, but not on statistical knowledge. In order to calculate the sample size required, a total of 5 parameters are required:

- (1) The effect size being investigated i.e. what is deemed to be a meaningful shift in the parameter being investigated – for this case study we assume this is a shift of 2 points
- (2) The existing or expected variation e.g. in the form of a standard deviation in the parameter is being measured. This may be determined experimentally or estimated from relevant literature – for this example we will assume a standard deviation of 1.5.
- (3) The statistical significance required (e.g. α =0.05, the predetermined p-value for the significance test being undertaken, also known as the Type I [false positive] error rate).
- (4) The Type II error rate β conventionally set at 0.2. Thus, researchers set a 4:1 β : α risk based on α =0.05 and β =0.20.)
- (5) Statistical power: defined as $1-\beta$ and is therefore typically set at 0.8.

In reality only (1) (2) and (5) are required to be entered in statistical software since (5) is derived from conventional inputs of (3) and (4). Detailed descriptions of formulae and calculations can be consulted in Ryan (2013). If students do not wish to calculate sample sizes by hand a number statistical software packages can be used.

In all practice, researchers are advised to carefully implement statistical software or reputable sample size calculators to determine their sample size. Fig. 2.7.1 below shows a typical dialogue box (in Minitab 16 statistical software) for sample size calculation together with the generated output. In the example provided here, it can be seen that a difference of 2, a standard deviation of 1.5 and a power of 0.8 results in a mean sample size of 7 being deemed as acceptable.

ower and Sample	Size for 1	Sample t	
Specify values for a	ny two of t	he following:	
Sample sizes:			
Differences:	2		
Power values:	0.8		
Standard deviation:	1.5	Options	Graph
Help	[ОК	Cancel
	<u></u>		

Figure 2.7.1 Dialogue box for sample size calculation in Minitab 16.

Conclusion

Researchers should always bear in mind that sampling should be done with a purpose and should therefore design their sampling strategies carefully according to that purpose. Good design means not only selecting the relevant parameters to be measured but should consider how and where the samples should be taken as well as careful statistical analysis of the numbers required. Pre-planning the sampling strategy employed can save time and effort as well as producing more meaningful data for monitoring purposes, hypothesis testing and future management strategies.



Figure 2.7.2 Graphical output illustrating effect size, statistical power and required sample size of 7 for case study parameters

2.8 Monitoring of water quality and pollutant levels

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Introduction

This section will help the reader to relate their aims to the relationship between the environmental/ social/ regulatory context and the planned investigation. Reference to prior knowledge and data for target pollutants and how these may influence the choice of monitoring strategies will be explored.

Monitoring strategies, examples of monitoring techniques for specific pollutants (i.e. chemical/microbiological) and approaches for monitoring of specific sources (i.e. drinking water/ recreational water/wastewater etc) will be summarised. Readers will be provided with an understanding of pollutant indicators (chemical and microbiological). Appropriate laboratory methods for the analysis of these will be introduced. Monitoring systems that can be operated remotely and allow for frequent or continuous monitoring will be outlined, and compared with traditional approaches involving sampling and laboratory based analysis. Guidance

> will be given to the supporting data required when results are interpreted and reported.

> The section will address the process from identifying the problem, identifying the analytical method, planning appropriate sampling. interpreting the results and considering setting up a routine monitoring system. The potential for errors within each step that can impact on the results will be discussed.

Monitoring strategies

The qualitative and quantitative analysis of water quality and pollution indicators is an essential tool within environmental risk assessment processes. Decision making and implementation of regulations are directly related to the data available from monitoring programmes and thus depend on their reliability. The clear definition of monitoring aims and the development of a monitoring strategy as well as sound sampling protocol (see chapter 2.7) are of pivotal importance.

Monitoring strategies consist of defined monitoring objectives which are linked to appropriately designed sampling plans and analytical methodology as well as clearly formulated decision rules (Fig 2.8.1). analyzed and ultimately provide the baseline and information about the status of a specific environment.

Parameters to be monitored depend on the media is the subject of the particular which environmental study, and on the processes that influence material/ substance inputs that change the chemistry of that media. To determine the risk, measurement is usually aimed at the elements which are most likely to exceed accepted limit values and which therefore are believed to represent the main risks to human and environmental health. In relation to this, the data produced after the lab analysis has to be compared against the relevant limit values. These are different for each type of media and are presented in the relevant legal formats (for Europe, the EU Directives), or in other relevant standards (WHO



Figure 2.8.1 Monitoring strategy components (taken from EPA Guidance for the Data Quality Objectives Process).

Environmental monitoring is used in risk assessment and for the preparation of environmental impact assessments. Regulations often specify the requirements with regards to compliance assessment and for the reporting of emissions and discharges into the environment, be it domestic, agricultural or industrial.

The data collected from monitoring programmes as specified above can be reviewed, statistically or any other). In addition to limit values, there are also warning thresholds.

A flow scheme for policy-related monitoring investigations is shown in Figure 2.8.2. Policy, for example, could be Water Protection, where the relevant regulation in Europe is the Water Framework Directive (EU WFD)



Figure 2.8.2 Flow schematic for a monitoring investigation

Substance specific monitoring can be categorized into six groups by the primary objective of the monitoring.

- Investigative or snapshot monitoring, to get a first impression on the nature and extent of pollution of selected areas or input scenarios
- **Trend monitoring**, to trace the concentrations over a certain time period to detect seasonal variations, accidental inputs

or the effectiveness of measures by authorities

- **Spatial monitoring**, for sources identification or the study of the dissipation and fate of substances of concern carried out at different locations
- Retrospective monitoring, repeated samplings at well selected sites and adequate storage of samples to allow a future (trend) monitoring of appropriately archived material

- Compliance monitoring, to determine whether the quality or quantity of environmental parameters conform to legal requirements
- **Remote monitoring**, to determine qualitative or quantitative parameters without the need for sampling or local access

Planning and management

Planning is the most important step for implementation of a monitoring program. Aspects not covered at this stage appropriately may jeopardize the whole effort. This includes:

- definition of objectives and responsibilities
- Selection of sampling sites according to objectives and financial budget, and representativeness (see Section 5.8)
- long term observation periods vs. short-term projects
- spatial vs. temporal monitoring

The planning phase will be affected by many factors which include socio-economic and financial factors but also those which are substance and/or media related.

If possible, the sampling and monitoring strategies should not focus on a single substance group. Other substances may become important in the future and thus the stored sample of a monitoring campaign should be appropriate for the analysis of these substances. Furthermore, utilising a previously developed strategy provides a quick and cheap approach. To achieve these goals a thorough documentation and quality assurance for sampling, sample preparation, (long-term) storage and analysis is required. Basic data sets to be elaborated and important on-site data for later interpretation of analytical data need to be clearly defined. A number of questions may usefully be addressed at this stage:

What is the context of the monitoring investigation?

What is the ultimate purpose of the study (e.g. if a trend should be detected: how much change in how many years should be identifiable; in other cases the identification of the background concentration of a chemical could be the aim)? What are the target compounds? Are certain methods obligatory?

What is already known for a target compound and what can be expected?

Before starting a monitoring study it is essential to gather as much information as possible for consideration in the planning. All information on substance properties should be considered since these can help to identify the most likely environmental compartment for the occurrence of a substance (intrinsic and extrinsic substance properties; fate of the substance including accumulation processes and disappearance).

How the target substances do enters the environment and does the monitoring strategy depend on input scenarios?

The possible sources of contamination should be studied, for example the importance of sewage treatment plants and effluents as a point source or diffused sources such as agricultural and urban run-off.

Analysis of pollutant indicators

In addition to minimal reporting, as in Section 2.7 Documentation of sampling strategy, researchers should carefully consider which particular parameters are of interest to their monitoring programme in light of experimental design and legislative requirements.

Water quality parameters can generally be divided into seven categories outlined below, all of which may be considered for investigation. For a number of physic-chemical parameters, field test kits are provide increasingly reliable and sensitive means of measurement.

Subjective impression

Characteristics which are subjective include colour, turbidity (cloudiness), taste and smell. These characteristics are difficult to quantify but nevertheless important to the public who would probably object to e.g. drinking water which was murky or malodorous. EEC Directive 80/778/EEC defines guide levels for organoleptic parameters such as turbidity in drinking water and indicates the desired analytical techniques.

Other subjective factors which are often associated with water quality include the amount of refuse present in urban rivers/canals or rural reservoirs, the presence (or absence) of plant/animal species, foam and/or oil on the water's surface.

General indicators

General indicators of water quality include:

pH

The pH value of natural water varies with the geological nature of the source and presence of dissolved solids. The pH of natural waters is usually slightly acidic due to the presence of dissolved CO_2 . Extra acidity may be caused by pollution with mineral acids (acid precipitation, industry) and acid salts; pH may be determined using:

- universal indicator (rough guide value)
- narrow range pH paper
- glass electrode generates potential which varies linearly with the pH of the solution in which it is immersed

Electrical conductivity

The electrical conductivity of a water sample is a measure of its ability to carry in electrical current and varies according to its degree of mineralisation. Conductivity may be determined using a conductivity meter (units, μ S cm⁻¹; [S = Siemens]).

Temperature

The water temperature affects chemical and biological species and must be determined at the time the sample is collected.

Oxygen balance

The oxygen balance of waters provides an important guide to the level of water pollution, reflecting ability to deal with pollutant burden. Oxygen balance indicators include:

- Chemical oxygen demand (COD)
- Biological oxygen demand (BOD)
- Dissolved oxygen (DO)
- Total organic carbon (TOC)

Anions

The most commonly determined anions include chloride (salinity); nitrate (fertilisers); nitrite (evidence of bacteriological action); phosphate (fertilisers, detergents); sulphite (industrial sources); sulphite (anaerobic bacterial action) and cyanide (industrial wastes).

Cations

The most frequently encountered cations include Na^+ (salinity); Ca^{2+} and Mg^{2+} (water hardness); ammonium (bacteriological action, fertilisers, sewage) and heavy metals and metalloids such as lead, cadmium and mercury (urban runoff, dissolution of pipes, toxic waste) as well as those

that may arise from geological bedrock via aquifer water such as arsenic. Concern about heavy metals arises because of their possible toxicity to humans and animals e.g. prolonged drinking of water containing low concentrations of heavy metals may be hazardous, since the metals can be retained in the body. Techniques for the quantitative determination of heavy metals include:

- Atomic absorption spectrometry (AAS)
- Inductively-coupled plasma-source atomic emission spectroscopy (ICP-AES)
- Inductively-coupled plasma-source mass spectrometry (ICP-MS)

The toxicity of different species of metals can be significantly different, and thus for speciation studies, techniques such as anodic stripping voltammetry (ASV), sequential extractions or modelling techniques may be used.

Organic substances

Although the determination of the organic content of a water sample may be useful indicator of organic pollution, it is non-specific and includes naturally occurring organic substances from e.g. soil organic-matter in addition to the man-made contaminants (minerals oils, pesticides, detergents etc). Specific organic substances which may act as indicators of water pollution include:

- Hydrocarbons (HC)
- Polyaromatic hydrocarbons (PAH)
- Carbonyls
- Phenols
- Surfactants
- pesticides and related products (insecticides, fungicides etc)

Techniques for the quantitative determination of organics will be discussed in subsequent lectures.

Bacteriological presence

Bacteriological examination of water samples is particularly important if the water is intended to human consumption e.g. coliform bacteria (from waste effluent) may render water unsatisfactory food consumption and of an unsafe sanitary quality. Microbiological analysis of water may include examination for:

- total coliforms
- faecal coliforms
- faecal streptococci
- Salmonella
- faecal bacteriophages
- sulphite-reducing clostridia
- entero-viruses
- Ascaris eggs

Anion	Relevance	Detection method
Chloride, Cl ⁻	Chloride is one of the major anions present in water. Harmless in small quantities in drinking water, problems of salt accumulation in arid areas (irrigation, water used by livestock).	 Mohr's Titration - interference from Br', I', CN', SO₃²⁻, although these are normally present at negligible concentrations compared to Cl⁻ Colorimetry (automated ferricyanide method) Ion selective electrodes Ion chromatography
Nitrate, NO ₃ -	A naturally occurring ion, found in most waters. Increased concentrations may arise as a result of the use of nitrogenous fertilisers.	 Colorimetry Ion chromatography Ion selective electrodes Cadmium reduction method
Nitrite, NO ₂ -	It may occur as a result of the decomposition of proteinaceous matter. When correlated with ammonia and nitrite concentrations may indicate organic pollution.	• Colorimetry (Nessleriser or Griess-Ilosvaydiazaotisation method)
Phosphate, PO ₄ ³⁻	It is relatively immobile in all but sandy soils and thus natural levels tend to be low. However, it may enter the water supply through domestic effluent (detergent, human and animal sewage). High levels of phosphate can encourage excessive growth of algae, especially earth N levels are high.	ColorimetryIon chromatography
Sulphite, SO ₃ ²⁻	It can occur in industrial effluent.	• Titrimetry
Sulphate, SO ₄ ³⁻	It occurs naturally in many waters, although high concentrations may be derived by leaching from oxidised pyrite waste and deposits.	• Titrimetry
Cyanide, CN ⁻	It occurs chiefly as a result of pollution by cyanide effluent.	Colorimetry (Nessleriser)

Table 2.8.1 Relevance of anions in monitoring pollution levels and detection methods

Reporting

Reporting is an important part of monitoring activities since it is the basis for assessment of data and possible decision making. To allow proper usage of environmental analytical data, it is essential that the procedures used, as well as all relevant additional information, are reported properly. The minimum information to be provided are descriptions of sampling strategy, method of sampling, sample properties, handling between sampling and analysis (including e.g., storage conditions. pre-treatment, homogenisation, sub-sampling), and the analytical methodology (including calculation and validation procedures). A detailed discussion of aspects of reporting is covered in an IUPAC project (Egli et al. 2003).

Monitoring activities in many countries are usually dependant the environmental on compartments (e.g. air, water and soil). This compartmentalisation also relates to environmental regulations (e.g. European Water Framework Directive or German Soil Protection Law) where some are based on global agreements but many are regional, national or local. Furthermore it is often the case that different organizations are responsible for monitoring in these individual compartments. Thus important connections and relationships in pollutant behaviour across these compartments can be overlooked

Impact

Each monitoring study has to be evaluated for its benefits and implications of possible findings

prior to starting the study. This include as full assessment of socio-ethical considerations. It is important to assess possible outcomes and their consequences before starting the monitoring. Considering all the aspects outlined above prior to starting the study will be important in order to obtain robust data from a monitoring of water quality and pollutant levels.

Integrated Water Cycle Management in Kazakhstan

IB No. 7535

Signed for publishing 01.10.14. Format 60x84 1/8. Offset paper. Digital printing. Volume 25,41 printer's sheet. Edition: 100. Order No.1824. Publishing house "Qazag university" Al-Farabi Kazakh National University, 71 Al-Farabi, 050040, Almaty Printed in the printing office of the "Qazag university" publishing house

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