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Monitoring and Modelling of Water Quality

Katarzyna Samborska, Rafal Ulanczyk and Katarzyna Korszun
*Institute for Ecology of Industrial Areas
Poland*

1. Introduction

Monitoring of water quality in the European Union is mainly regulated by the Water Framework Directive (Water Framework Directive [WFD], 2000) and other Directives, e.g.:

- Urban Waste Water Treatment Directive (Urban Waste Water Treatment Directive [UWWT], 1991),
- Drinking Water Directive (Drinking Water Directive [DWD], 1998),
- Bathing Waters Directive (Bathing Waters Directive [BWD], 1976),
- Shellfish Waters Directive (Shellfish Water Directive [SWD], 2006),
- Nitrates Directive (Nitrates Directive [ND], 1991),
- Directive on Integrated Pollution Prevention and Control (Directive on Integrated Pollution Prevention and Control [IPPC], 2008),

These Directives were established for particular water types or problems. The European legislation introduced and implemented the river basin approach to water resources management and monitoring of water quality. By means of the latter one, good water quality status should be provided. The Water Framework Directive divides the monitoring of water quality into three types: Surveillance (to establish baseline quality status and assess long term changes), Operational (to provide extra data on water bodies at risk or failing to meet the environmental objectives of the WFD) and Investigative (to determine the causes of such failure where they are unknown).

In Poland (similarly to other European countries) the European legislation on the monitoring of water quality is implemented by federal law (for example by Water Law Act) and appropriate executive regulations. These acts concern, among others: the classification of surface and groundwater regarding with its quality, the methodology and interpretation of monitoring results, requirements for the quality of potable water. Monitoring of water quality in Poland is conducted for surface water, groundwater and rainwater. The aim of the surface water monitoring is, first of all, to determine a current physico-chemical status of water and consequently to find solutions for improving it. Finally, the results enable also to design the plans for preventing water pollution. The emphasis is put on the elimination of pollutions originated from agriculture and urban areas. In addition, monitoring should provide the reliable forecasting of further changes.

The monitoring of surface water is carried out for both rivers and lakes. It is worth mentioning that Poland is involved in international systems of the surface water monitoring.

These systems are destined for monitoring of the quality of rivers which cross the boundaries of the country (transboundary monitoring). There are also systems which are addressed to the continuous observations of the surface water quality regarding to its acidification and eutrophication (ICP Waters). The monitoring of potable water needs a special type of water examinations, which should be carried out with the high accuracy of measuring and should encompass as many parameters as possible. This type of monitoring should be also coupled with modelling tools, which have to alarm the potential users in case of water quality deterioration and make the prognosis for the future usage based on different scenarios of land development.

Monitoring of groundwater quality in Poland is conducted by the Polish Hydrogeological Survey, within the basins called groundwater bodies. The monitoring is arranged in the three types: diagnostic, operational and research. Since 1991, results of examinations have been collected in the database MONBADA. Each year, the report describing the status of the groundwater quality is made on the basis of physico-chemical examinations. However, the interpretation of the chemical conditions within groundwater bodies conducted with the annual frequency might be not sufficient for the accurate evaluation of the processes responsible for the changes. Data obtained during monitoring works are available and could be used in the scientific projects though there is no possibility to work on current results on-line.

There are many modelling tools which can be fed with data derived from monitoring. Hence, measurements performed in a frame of monitoring should not be only gathered in databases and analysed sometimes several weeks or months after the sampling but rather simultaneously transformed into real signals, which can be used immediately by the management unit. Mentioned modelling tools (presented in section 7) are designed for simulation of processes occurring in atmospheric water, surface water and groundwater or for all of them together. These tools are designed for scenarios analyses or for real-time simulations. This paper presents also examples of use of coupled monitoring and modelling systems for surface and ground water (section 8).

Summarising, it can be said that creation of the real-time monitoring systems is the key issue for the water quality improvement. Moreover, coupling of real-time monitoring tools with the real-time modelling is the most suitable solution for making prognosis on the basis of monitoring results.

2. Legislation acts connected to monitoring of water quality

The Water Framework Directive (WFD) introduces a strategic legislative framework to couple the various concerns of water policy and provide a more holistic and integrated approach to water management in entire river basins (Naddeo et al., 2005). The objectives of the Water Framework Directive are to protect water of high quality (high status water), prevent potential deterioration and to restore degraded surface and groundwater to good status by 2015. The key aim of the WFD is to prepare integrated systems of water resources management functioning within hydrological catchment (river basins), hence often crossing administrative boundaries (Teodosiu et al., 2003).

Article 8 of the Water Framework Directive sets out the requirements for the monitoring of surface water status, groundwater status and protected areas:

"Monitoring programmes are required to establish a coherent and comprehensive overview of water status within each river basin district."

The programmes had to be operational at the latest by 22 December 2006, and must be in accordance with the requirements of Annex V of the WFD. Annex V indicates that monitoring information from surface water is required for, among others, (WFD, 2000b):

- The classification of status;
- Supplementing and validating risk assessment procedure (Appendix II);
- The efficient and effective design of future monitoring programmes;
- The assessment of long-term changes in natural conditions and those resulting from human impact;
- Estimating pollutant loads transferred across international boundaries or discharging into seas;
- Assessing changes in status of those bodies identified as being at risk;
- Ascertaining causes of water bodies failing to achieve environmental objectives where the reason for failure has not been identified;
- Ascertaining the magnitude and impacts of accidental pollution;
- Use in the intercalibration exercise;
- Assessing compliance with the standards and objectives of Protected Areas; and,
- Quantifying reference conditions (where they exist) for surface water bodies.

Annex V also indicates that monitoring information from groundwater is required for:

- Providing a reliable assessment of quantitative status of all groundwater bodies or groups of bodies
- Estimating the direction and rate of flow in groundwater bodies that cross Member States boundaries;
- Supplementing and validating the impact assessment procedure and use in the assessment of long term trends;
- Establishing the presence of significant upwards trends in the concentrations of pollutants;
- Assessing the reversal of such trends in the concentration of pollutants, and;
- Establishing the chemical status of all groundwater bodies or groups of bodies determined to be at risk.

The monitoring of drinking water is established by The Drinking Water Directive (DWD, 1998). The legislative act sets out quality standards for drinking water quality at the tap (microbiological, chemical and organoleptic parameters). In addition, it constitutes the general obligation of cleanliness and wholesomeness of drinking water. The Directive obliges each Member State to conduct regular monitoring of drinking water quality and as a result of that to inform all consumers about the water quality. Hence, the main aim of the Drinking Water Directive is to protect the health of the consumers in the European Union by providing them with the best quality of tap water. To achieve this goal DWD established standards for the 48 most common substances – parameters, which can be found in potable water. These microbiological and chemical substances must be examined in drinking water regularly (Hecq et al., 2006).

The Urban Wastewater Treatment Directive (UWWT, 1991) and the Integrated Pollution Prevention and Control Directive (IPPC, 1996) are mainly dealing with urban and industrial

wastewater. The UWWT Directive is related to collection, treatment and discharge of urban wastewater. It also aims to protect the environment from the negative influence of the disposal/discharge of insufficiently treated urban wastewater. The directive encompasses four activities related to wastewater management: planning, regulation, monitoring, and information and reporting. Monitoring requires ensuring (Quevauviller et al., 2006):

- appropriate monitoring capacity of parameters to be monitored;
- accurate analysis of samples by using standard methods;
- timely frequency of monitoring for: monitoring of discharges from urban wastewater treatment plants; and monitoring of waters receiving those discharges.

The Nitrates Directive's main objective is to protect water quality across Europe by eliminating the jeopardy of nitrates pollution and by agricultural practices. All Member States have to examine water with regard to nitrate concentrations and trophic state. Hence, good monitoring procedures and networks are crucial in executing the acts of the Directive. There are currently 31 000 groundwater sampling sites in the EU, and 27 000 surface water stations. There are differences between countries in the designing and using their monitoring networks. This may be due to the fact that there are no specific official guidelines and/or protocols in the European Union (Fraters et al., 2003). On the other hand, the existing (in a draft form) guidelines for monitoring under the Nitrates Directive outline the monitoring of both agriculture (nutrient balances, changes in land usage and manure storage capacity) and water quality (effects of nitrate input to surface water and groundwater).

EC Shellfish Waters Directive (SWD, 2006) aims to protect shellfish populations. Hence it specifies the way how shellfish water should be monitored throughout the year. The frequency of sampling depends on the importance of the parameter being measured. The parameters encompass physico-chemical indicators including toxic organic and metal contaminants.

In Poland, the obligatory examinations of surface water and evaluation of its quality is enclosed in "Water Law" act (Water Law Act, 2010). In turn, the operating range, procedures and criteria of the quality's evaluation might be found in several regulations concerning: habitat requirements for fishwater, extinguishing of water vulnerable for nitrates pollution, standards for drinking water derived from surface resources, classification of surface water status and types and procedures of surface water monitoring. The aim of the surface water monitoring is the establishment of basis for further activities which should improve the status of water. These actions include also the prevention from pollution, especially the elimination of the eutrophication process. The holistic assessment of the surface water condition is the main tool of water resources management within the river basins, which stand for the cardinal units in water policy.

The legal basis of groundwater monitoring constitutes two acts: "Environmental Protection" (Environmental Protection Act, 2001) and "Water Law" acts. Similarly to surface water monitoring, the detailed description of procedures and performance might be found in a set of regulations concerning: extinguishing of water vulnerable for nitrates pollution, criteria and methods of the groundwater status evaluation and forms and procedures for carrying out monitoring of surface and groundwater bodies. The monitoring actions are directed towards the creation of an information base including chemical condition of groundwater

within outlined bodies. The continuous control of groundwater quality aims at further planning of both clean-up activities and a protection from pollution, which leads to achieve good groundwater status before the date set by the European Commission.

3. Monitoring of surface water quality in Poland

The “Water Law” act introduced a division of the state area into water basins and water regions; initially, there were two main areas of water basins – the Vistula and the Oder river basins. Amendment to the Water Law act from 2005 introduced eight new water basins, which replaced the initial two (Inspectorate of Environmental Protection, 2010).

In case of examinations and evaluations of surface water quality based on monitoring, years 2010-2012 are the first period of a six-year-long project of water management within outlined water bodies. During this time, monitoring of surface water quality is performed in three types of activities: surveillance/diagnostic, operational and investigative/research. First mentioned aims to provide general assessment of water quality for each catchment and sub-catchment within the whole river basin. Information gathered during this type of research enables the determination of long-term changes in natural conditions. Second one, operational monitoring is carried out within those homogenous water bodies which, during the diagnostic phase, were described as endangered of failure to achieve the good status. This monitoring aims at evaluation of changes following the implementation of repair programmes. The last type - research monitoring - aims at observation and describing of unrecognised threats of pollution within surface water bodies.

In case of surface water monitoring, there are ten types of sampling/monitoring points: diagnostic (MD), operational (MO), operational for water vulnerable to nitrates pollution (MORO), operational for water exposed to eutrophication (MOEU), operational for fishwater (MORY), operational for surface water abstracted for public water supply (MOPI), operational for water qualified as recreational (MORE), operational for water bodies in boundaries of which there are protected ecosystems strictly dependent on quality of water (MONA), operational related to the execution of the international agreements (MOIN), research (MB).

The range and the frequency of monitoring depend on the type of monitoring points. For the diagnostic points, the frequency of measurements is from 1 to 8 times a year for biological factors and from 1 to 12 times a year for physic-chemical parameters. For the operational monitoring points the range of measured parameters depends on the type of pressure put on the environment within water bodies. In case of units in which effluents/discharges hazardous substances, especially priority hazardous substances were observed, or in monitoring points where the amount of these substances exceeded permissible limits, the monitoring is performed annually. For other operational monitoring points the frequency of examinations is once in 3 years for fishwater and once in a year in case of surface water used for public water supply.

The key role in the monitoring system play points located in estuaries of big rivers and those flowing directly to the Baltic Sea. In these places, the frequency of sampling is not less than 12 times a year and the range of parameters being examined include heavy metals, biogenic substances and indicators describing the oxygen conditions.

Each year the evaluation of surface water status is made for water bodies which were included in the diagnostic monitoring. In year 2013, after finishing the entire diagnostic programme, the summary specification of the status within surface water bodies will be prepared. On the basis of that, using the extrapolation method, the rest of the water bodies which are not included in the diagnostic monitoring will be assessed. The scheme of evaluation of surface water status is presented on figure below (Fig. 1).

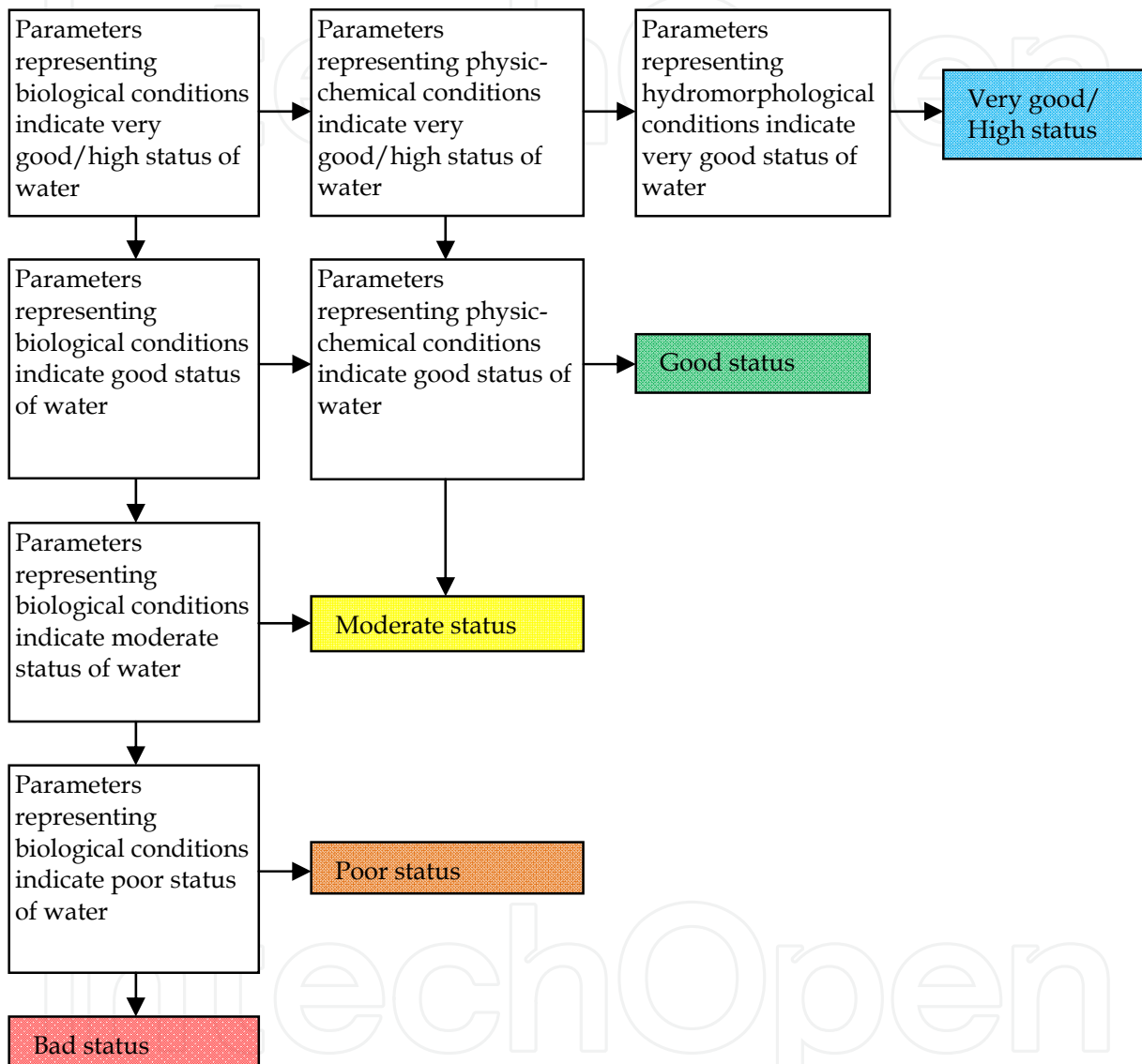


Fig. 1. Block diagram of the evaluation of surface water status, according to the Water Framework Directive (after: Loga and Sawicka, 2009)

The evaluation of the chemical status of water included in the operational monitoring depends on the type of ongoing programmes. In any case, the classification of ecological status is made on the basis of the limited number of factors depending on the potential threats of pollution and pressure put on the water environment by anthropogenic discharges. Hence, the evaluation of surface water status is fraught with uncertainties and rather informs about the success or failure in the implementation of repair programmes than about real conditions of the environment.

The State Environmental Monitoring of surface water in Poland is led by the Voivodship Inspectorates for Environmental Protection, and coordinated by the Main Inspectorate for Environmental Protection. The detailed plans of sampling campaigns, carried out in a frame of surface water monitoring, might be found in Monitoring of Environment Programmes, which are available on the website of Voivodship Inspectorate for Environmental Protection. In 2009, the number of monitoring points was 1616 and they were localised within 1328 homogeneous surface water bodies.

4. Monitoring of groundwater quality in Poland

On a national scale, the institution responsible for monitoring of groundwater is Polish Hydrogeological Survey (PSH). Their tasks are performed by the Polish Geological Institute. These tasks include (Sadurski 2005):

- performing hydrogeological measurements and observations;
- collecting and processing the data concerning groundwater condition and resources available,
- performing current analyses and assessments of hydrogeological situation;
- compiling and forwarding to the appropriate administration authorities, the forecasts of the changes in both resources and quality of groundwater, and about threats of pollution;
- compiling and forwarding to the public administration warnings about dangerous phenomena occurring in recharge zones and groundwater intakes.

Examinations of the groundwater quality are carried out within groundwater bodies defined as “determined volume of groundwater occurring within an aquifer or aquifers”. This term refers to the functioning in Polish hydrogeology term “free water occurring in the saturation zone” (Pazdro 1977).

The delineation of groundwater bodies was made taking into consideration various factors, such as circulation conditions (i.e. locations of recharge and drainage zones), administrative and hydrological boundaries (catchments, basins), lithology and stratigraphy of water-bearing rocks. Groundwater bodies are complex structures, they might consist of few water horizons.

Measurements of the ground water quality are carried out within the national observational-research network. This network was designed to evaluate the groundwater status and to determine trends in chemical changes. Monitoring actions are performed for both the qualitative and quantitative assessment of the groundwater. The latter one is embraced by diagnostic, operational and research monitoring. The density of observation points reflects the complexity of geological and hydrogeological conditions and natural and anthropogenic pressures put on the water quality. Additional attention in monitoring is paid to areas around national boundaries and to protected areas. Hence, the final location of points depends on the formulated aim of monitoring, and the network comprises of (Fig. 2):

- Hydrogeological monitoring stations;
- Points of groundwater state observations;
- Points of groundwater quality monitoring;
- Observation piezometers;
- Built-up wells.



Fig. 2. Types of monitoring points: A) Piezometer, B) Spring, C) Well. (Sources of photos: Glubiak-Witwicka et al., 2003)

Diagnostic monitoring aim is to determine anthropogenic impacts on the groundwater quality as well as the long-term trends in chemical status changes. Accordingly, the changes might be induced by natural processes and human activities. The results of this type monitoring actions help to design the further operational monitoring system. Parameters examined during the diagnostic phase of groundwater monitoring are: pH, TOC (total organic carbon), conductivity, temperature, DO (dissolved oxygen), ammonia, arsenic, nitrates, barium, boron, chloride, chromium, zinc, fluoride, phosphates, aluminium, cadmium, magnesium, manganese, copper, nickel, lead, potassium, sulphate, sodium, calcium, carbohydrates, iron, organic substances: AOX - adsorbed organochlorine compounds. The range of parameters might be extended by substances expected to be present in groundwater regarding the potential pollution sources.

Operational monitoring should provide data necessary to reach the proper level of certainty in classifying groundwater endangered by not reaching the good quality status. The second major aim is to identify upwards trends in the chemical composition which might indicate the pollution, especially human-induced. The range of measured parameters includes: temperature, conductivity, pH, DO, ammonia, nitrites, nitrates, chloride, sulphate, phosphates, bicarbonates, sodium, potassium, calcium, magnesium, manganese and iron. In addition, if some parameters measured in the diagnostic phase of monitoring, classified the groundwater status as poor or bad, they are also included into operational observations.

Research monitoring aims at extending the recognition achieved after two previous phases of monitoring. This type of researches leads to determine the reasons, sizes and influences of the accidental pollution. This monitoring might be performed for those groundwater bodies which might not achieve the good quality status by the fixed date, and which are not subjected to the operational actions (Kazimierski & Pilchowska-Kazimierska, 2006).

There are 5 classes of groundwater quality:

- I class - water of very good quality - the chemical composition results only from natural conditions and represents natural geochemical background. The measured values of parameters do not reflect any human activities,

- II class – water of good quality - values of some parameters are increased, what is caused only by natural factors. Hence, the chemical status of water is the result of geogenic processes and human impact is negligible,
- III class – water of satisfactory quality. Values of several parameters are increased mainly as a result of natural processes. However, changes in chemical composition might reflect a feeble human impact,
- IV class – water of non-satisfactory quality. Values of some parameters are significantly increased as a result of natural or human-induced processes,
- V class – water of bad quality. Chemical composition of this type of water confirms the predominant human impact.

Classes from I to III stand for good status of groundwater, whereas classes IV and V - bad status. The status of groundwater bodies is presented on the maps in a following way: area filled with green colour – good status, area filled with red colour – bad status and black points – observed trends in chemical composition of groundwater (example on Fig. 3).

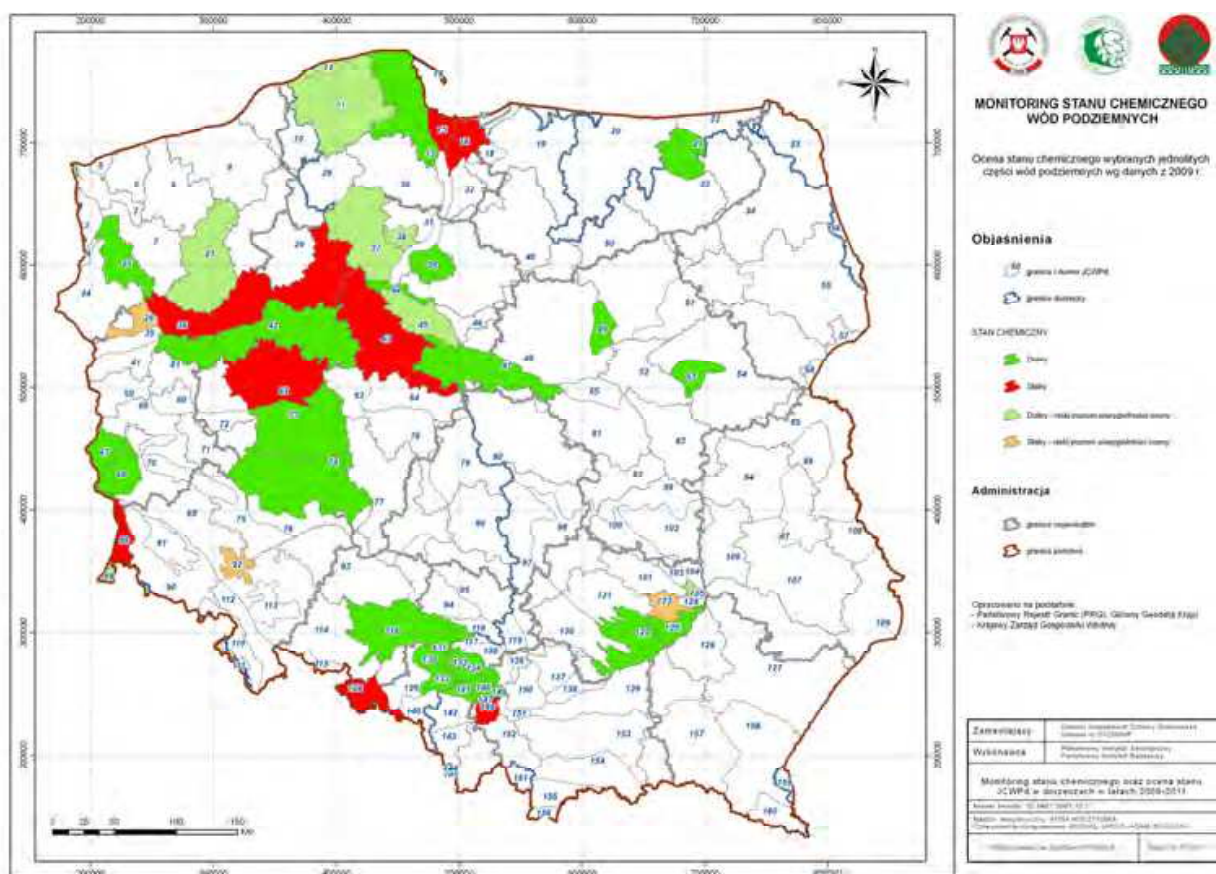


Fig. 3. The classification of groundwater status in year 2009: green colour stands for the good status of groundwater, red for bad status, light green and orange represent a high uncertainty of obtained results (source: <http://www.gios.gov.pl>)

The frequency of chemical examinations depends on both type of monitoring and type of aquifer. In case of unconfined aquifer the frequency is one time in 3 years (diagnostic monitoring) or twice a year (operational monitoring). On the other hand, in case of deeper aquifers, which are characterised by piezometric surface, the frequency is once in 6 years (diagnostic monitoring) or once a year (operational monitoring).

Results obtained during the monitoring are widespread via different publications, such as Quarterly Bulletin of Groundwater. Results are also gathered in databases, e.g.:

- SOH (Hydrogeological Observations System). This database collects information about water table level fluctuations (every Monday) and chemical condition (every year).
- MONBADA (MONitoring DataBAse) is the database of National Environmental Monitoring. It was created in 1991. In MONBADA data regarding the chemical status of groundwater and its evaluation are gathered. On the basis of collected results annual reports are prepared. These reports are published in series "Library of Environmental Monitoring" and on the National Monitoring web site (<http://www.gios.gov.pl/wodypod>).

5. Monitoring of precipitation in Poland

Qualitative monitoring of precipitation in terms of its chemical composition and occurrence of the acidic atmospheric deposition has been largely studied in different sites and locations in Central and Western Europe, North America and East Asia, during the last years (Kulshrestha et al., 2009; Li et al., 2007; Menz & Seip, 2004; Tsitouridou & Anatolaki, 2007; Wang et al., 2000).

In Poland, the National Chemistry Monitoring of Precipitation and Assessment of Pollutants Deposition were established in 1998 as a subsystem of National Environmental Monitoring. Monitoring tests in the full annual cycle were carried out for the first time in 1999. The Institute of Meteorology and Water Management in Wroclaw carried substantive supervision over implementation of these tasks. The purpose of monitoring of the precipitation chemistry and of the deposition of pollutants is to define, at a national scale, spatial and temporal decomposition of pollutants entering from the wet precipitation to the ground. National network of measurement - monitoring consists of: 25 research stations (to ensure the representativeness of precipitation chemistry measurements) and 162 rainfall stations (which characterise the average rainfall for the Poland area). At all 25 research stations the rainwater is collected continuously and analysed on a monthly basis. At the time of sampling, the amount and type of precipitation are measured. Monthly precipitation samples are analysed for the concentration of acidic compounds, nutrients and metals (including heavy metals). The monitoring includes: chlorides, sulphates, nitrites and nitrates, ammonia nitrogen, total nitrogen, total phosphorus, potassium, sodium, calcium, magnesium, zinc, copper, iron, lead, cadmium, nickel, chromium and manganese. Measurements include also pH and electrical conductivity of the precipitation. Basing on the results from all monitoring stations (25 research and 162 rainfall stations) maps of wet deposition of monitored substances are prepared.

The atmospheric precipitation collectors are characterised by a different degree of automation; the most sophisticated can record meteorological data and also some characteristics of precipitation (rate, electrolytic conductivity, pH) (Chief Inspectorate of Environmental Protection, National Chemistry Monitoring of Precipitation and Assessment of Pollutants Deposition, <http://www.gios.gov.pl/chemizm/index.html>.) The simplest collectors for total precipitation sampled for chemical analysis are glass, metal, and plastic containers. The containers are equipped with glass, steel, or polyethylene funnels. Figure 4 presents the scheme of the simplest collector (Bijman et al., 1991).

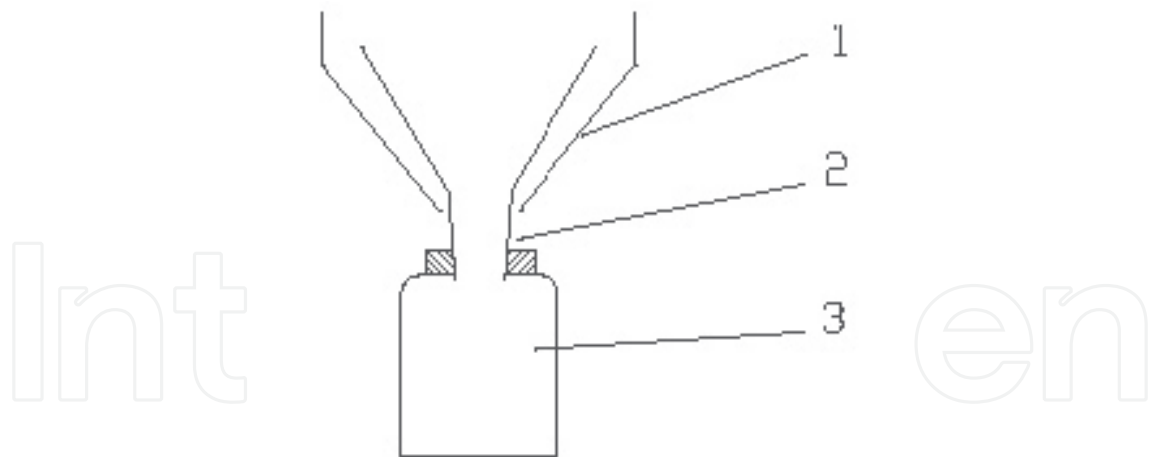


Fig. 4. Scheme of the simplest collector for total precipitation samples: 1 - outer funnel casing, 2 - funnel, 3 - bottle.

The more complicated version has an automatic cover and a humidity sensor; in this type of system dry precipitation is excluded from a sample (Fig. 5) (Ligocki et al., 1985).

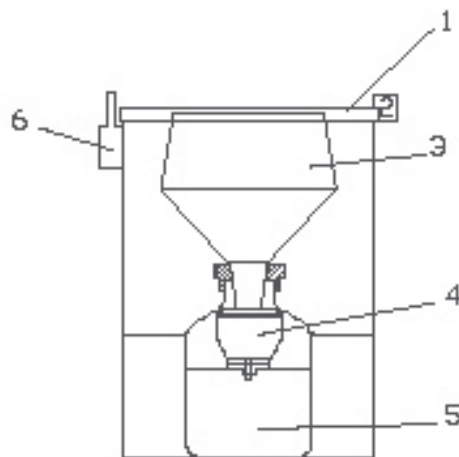


Fig. 5. Scheme of automatic collector for sampling the atmospheric precipitation: 1 - cover, 2 - electric motor, 3 - polyethylene funnel, 4 - filtration funnel, 5 - polyethylene bottle for collecting filtrate, 6 - humidity sensor.

Samplers should be placed ca. 1.5 m above the ground, in an open area, at best, overgrown with grass. The detailed conditions for collector location are given in the Polish standard (PN-ISO 5667-8), which is a translation, without any changes of the international standard ISO 5667-8:1993 (ISO, 1993).

Collection of atmospheric precipitation has to satisfy a number of conditions, especially with respect to a collection system. In compliance with recommendations of the European Monitoring Environmental Program (EMEP) the collectors for wet precipitation and total precipitation should be characterised by:

- the sampler should not be too large or bulky, because this will obstruct the air flow around the sampler; the diameter of the collector must be large enough to provide samples large enough for chemical analysis - a diameter of 20 cm is sufficient;

- collector must be made of a material, which does not alter the chemical composition of the sample, and shall give a reliable measure of the amount of precipitation on a daily basis;
- an appropriate container capacity to avoid any loss of a sample even when precipitation is very intensive.

6. Water quality modelling

Mathematical model is described in different ways. The encyclopaedia of life support system described a model as an approximate description of a class of real-world objects and phenomena expressed by mathematical symbolisms (Agoshkov, 2002). Concise Oxford Dictionary (1990) described a model as a simplified form of a system that assists calculations and predictions of a condition of a system in a given situation. The United States Environmental Protection Agency USEPA (EPA, 2009) described water quality models as tools for simulating the movement of precipitation and pollutants from the ground surface through pipe and channel networks, storage treatment units and finally to receiving waters (Kannel et al., 2011).

Model predictions might be used in addition to or instead of monitoring data for several reasons:

- Modelling might be feasible in some situations where monitoring is not.
- Integrated monitoring and modelling systems could provide better information than one or the other alone for the same total cost.
- For example, regression analyses that correlate pollutant concentration with some more easily measurable factor (such as streamflow) could be used to extend monitoring data. Models can also be used in a Bayesian framework to determine preliminary probability distributions of impairment that can help direct monitoring efforts and reduce the quantity of monitoring data needed for making decisions.
- Modelling can be used to assess (predict) future water quality situations resulting from different management strategies. For example, assessing the improvement in water quality after a new wastewater treatment plant is built, or the effect of increased industrial growth and effluent discharges (UNESCO, 2005).

Water quality modelling for decision-making occurs at a disciplinary divide between science and management. Workers in science and management operate in fields that traditionally have different objectives, priorities and expectations. These differences can create barriers to the effective use of scientific models by watershed managers (McNamara, 2004).

Water quality models include both mathematical expressions and expert scientific judgement. They include process-based (mechanistic) models and data-based (statistical) models. The models should be characterised by following features:

- link management options to meaningful response variables (such as pollutant sources and water quality standard parameters),
- incorporate the entire chain from stressors to responses,
- be consistent with scientific theory,
- have reported the uncertainty,

- compatible with the quantity and quality of available data (The use of complex mechanistic models for water quality prediction in situations with little useful water quality data does not compensate for that lack of data. Model complexity can give the impression of credibility, but this is usually misleading).

It is often preferable to begin with simple models and then, over time, add additional complexity as justified by the collection and analysis of additional data. This strategy makes efficient use of resources. It targets the effort toward information and models that will reduce the uncertainty as the analysis proceeds (UNESCO, 2005).

Water quality models can be applied to many different types of water system, including atmospheric water, groundwater, wetlands, streams, rivers, lakes, reservoirs, estuaries, coastal waters and oceans.

The fact that most, if not all, water quality models cannot accurately predict what actually happens does not detract from their value. Even relatively simple models can help managers understand the real world prototype and estimate at least the relative, if not actual, change in water quality associated with given changes in the inputs resulting from management policies or practices (UNESCO, 2005).

7. Tools for water quality modelling – Examples and purposes of use

Models simulating water quality are used for three main purposes:

- Planning remediation of degraded areas or protection of water resources, soils, health and ecosystems.
In this case models calculate results of different scenarios. This type of models answers “what if” question and finds the solution which is best according to a specified objective and satisfying physical, technical, legal and other constraints (Wagner, 1992).
Groundwater quality models can analyse possibilities for removing a plume of polluted water or control its flow away from wells, streams, lakes. For such purpose models can simulate scenarios including: inserting curtain walls, removing polluted soil, in situ (bio)chemical remediation or installing pumping/recharge wells (Wagner, 1992). For surface waters this type of models is used for development of long-time management scenarios for river basins or lakes and for assessment of the results of planned land use changes and investments (Kardaetz et al., 2008; Thebault & Qotbi, 1999; Yoshimura et al., 2009). Models of this type for atmospheric water quality are used widely to predict the impact of pollutants emissions on the eutrophication and acidification processes. For all types of water (including water distribution networks and wastewater collecting systems) models can be used also for planning better and cost-effective monitoring and controlling systems.
- Simulating ongoing processes using real-time modelling systems. Real-time refers to a state where data referring to a system is analysed and updated at the rate at which it is received (i.e. at the rate at which the system operates). Real-time modelling (also referred to as online modelling) refers to the process of employing numerical models to make predictions about current or near future system states and outputs based on newly received (and forecasted) data. Real-time modelling is employed in a range of environmental fields, including meteorology, hydrology, and in urban water systems (UWS), typically for one of the following purposes (Hutton et al., 2010):

- To provide warnings of future events,
- To inform management of future system states and potential anomalies,
- To explore a range of possible control strategies such that the control solution that optimises some function is implemented (typically a system property such as: combined sewer overflows discharge, operational cost, surface water intakes management or groundwater in-situ remediation processes).
- Analysing past events. This type of models is used for example when there is a need for information about:
 - Influence of historical human activities or natural processes (as climate changes) on the present water quality status (Olsson et al., 2009).
 - Trends in long-term processes occurring in the water environment (e.g. eutrophication) (Heiskary & Swain, 2002).

Surface water quality models include processes to simulate (Deltares, undated; Hipsey et al., 2009):

- dissolved oxygen, organic matter (detritus),
- inorganic and organic nutrients (nitrogen, phosphorus, silicon),
- chlorophyll, phytoplankton species, microphytobenthos species, macrophyte species, vegetation species, zooplankton, zoobenthos species, fish species and other higher biology,
- carbon dioxide, methane,
- sulphates, sulphides,
- organic micropollutants (including European Water Framework Directive priority pollutants),
- heavy metals, iron,
- bacterial contaminants,
- salinity, chlorides,
- suspended sediment,
- dissolved conservative substances,
- pH, pe, light regime, temperature.

Groundwater quality models can simulate among others:

- Groundwater ages,
- Species transport,
- Propagation of mineral dissolution and precipitation fronts,
- Mineral buffering during acid mine drainage,
- Cation exchange,
- NAPL dissolution,
- BTEX degradation and corresponding geochemical changes,
- Temperature-dependent pyrite oxidation during deep well injections,
- Natural attenuation of ammoniacal liquor: Phenol degradation, nitrification and ion exchange of ammonium,
- Seawater intrusion and mixing,
- Fixed-pressure gas-phase equilibria,
- Isotope mole balance,
- any kinetically controlled reactions.

Atmospheric water quality models are usually parts of tools simulating air quality. In those models atmospheric water quality is simulated mostly as an element of

- aerosols formation,
- wet deposition.

In following tables are presented examples of modelling tools used for simulation of:

- atmospheric water quality (Table 1),
- surface water quality (Table 2),
- ground water quality (Table 3),
- surface-groundwater quality (Table 4).

Model name	Short description	Availability/ Producer	Source
FRAME (Fine Resolution Atmospheric Multi-pollutant Exchange)	FRAME is a Lagrangian atmospheric transport model with high spatial (5x5km) and horizontal resolution (33 layers). Model can be used to assess the long-term annual mean deposition of reduced and oxidised nitrogen and sulphur. FRAME was developed initially to focus in particular on transport and deposition of reduced nitrogen and was named the Fine Resolution AMmonia Exchange model. Recent developments in the treatment of sulphur and oxidised nitrogen mean that it may now be considered as a robust multi-chemical species tool.	http://www.frame.ceh.ac.uk/ / Center for Ecology & Hydrology	(Anthony et al., 2003)
RAQM (regional air quality model)	RAQM is a three-dimensional Eulerian model, which is constructed on a spherical and terrain-following coordinate system. A mass conservation equation in model includes a series of physical and chemical processes (advection, diffusion, multiphase chemistry, dry deposition, cloud mixing and wet scavenging). The continuity equation is solved by a time-splitting technique, which allows different time steps to be used for various processes for computational efficiency and for easy incorporating or updating of new modules. RAQM, which includes 37 species and 91 reactions employs a modified QSSA (quasi-steady-state assumptions) technique with a predictor-corrector algorithm to solve the chemical equations.		(Han, 2006; Han et al, 2006)

<p>REM-CALGRID (Regional Eulerian Model - California Grid Model)</p>	<p>REM-CALGRID (RCG) is a chemical transport model development designed to fulfil the requirements of the ambient air quality framework directive 96/62/EC of the European Commission. It is an Eulerian grid model of medium complexity that can be used on the regional and the urban scale for short-term and long-term simulations of oxidant and aerosol formation.</p> <p>Intended field of application is the modelling of pollutants (photo-oxidants, aerosols) on different scales from Europe-wide domains down to urban domains.</p>	<p>http://www.geo.fu-berlin.de/met/ag/trumpf/RCC/index.html / Freie Universität Berlin</p>	<p>(Stern, 2009)</p>
<p>RAINS (Regional Air Pollution Information and Simulation)</p>	<p>The Regional Air Pollution Information and Simulation (RAINS) model developed by the International Institute for Applied Systems Analysis (IIASA) combines information on economic and energy development, emission control potentials and costs, atmospheric dispersion characteristics and environmental sensitivities towards air pollution. The model addresses threats to human health posed by fine particulates and ground-level ozone as well as risk of ecosystems damage from acidification, excess nitrogen deposition (eutrophication) and exposure to elevated ambient levels of ozone. These air pollution related problems are considered in a multi-pollutant context quantifying the contributions of sulphur dioxide (SO₂), nitrogen oxides (NO_x), ammonia (NH₃), non-methane volatile organic compounds (VOC), and primary emissions of fine (PM_{2.5}) and coarse (PM₁₀-PM_{2.5}) particles. The RAINS model also includes estimates of emissions of relevant greenhouse gases such as carbon dioxide (CO₂) and nitrous oxide (N₂O). Work is progressing to include methane (CH₄) as another direct greenhouse gas as well as carbon monoxide (CO) and black carbon (BC) into the model framework.</p>	<p>http://www.iiasa.ac.at/rains/documentation.html?sb=11 / International Institute for Applied Systems Analysis</p>	<p>(Amann et al., 2004)</p>

Table 1. Models for simulation of atmospheric water quality

Model name	Short description	Availability / Producer	Source
SPARROW - SPATIALLY REFERENCED REGRESSIONS ON WATERSHED ATTRIBUTES	<p>SPARROW (SPATIALLY REFERENCED REGRESSIONS ON WATERSHED ATTRIBUTES) is a watershed modeling technique for relating water-quality measurements made at a network of monitoring stations to attributes of the watersheds containing the stations. The core of the model consists of a nonlinear regression equation, describing the non-conservative transport of contaminants from point and diffuse sources. The model predicts contaminant flux, concentration, and yield in streams and has been used to evaluate alternative hypotheses about the important contaminant sources and watershed properties that control transport over large spatial scales.</p>	<p>http://water.usgs.gov/nawqa/sparrow/sparrow-mod.html / US Geological Survey (free)</p>	<p>(Shwarz et al., 2006)</p>
SMS (SURFACE WATER MODELING SYSTEM)	<p>The Surface Water Modeling System (SMS) is environment for one-, two-, and three-dimensional hydrodynamic modelling. A pre- and post-processor for surface water modelling and design, SMS includes 2D finite element, 2D finite difference, 3D finite element modelling tools. Supported models include RMA2, RMA4, ADCIRC, CGWAVE, STWAVE, BOUSS2D, CMS Flow, and CMS Wave models. An interface has also been developed for facilitating the use of the FHWA commissioned analysis package FESWMS. The TUFLOW numerical model with flood analysis, wave analysis, and hurricane analysis is supported. SMS also includes a generic model interface, which can be used to support models which have not been officially incorporated into the system.</p> <p>Primary applications of the models include calculation of water surface elevations and flow velocities for shallow water flow problems, for both steady-state or dynamic conditions. Additional applications include the modelling of contaminant migration, salinity intrusion, sediment transport (scour and deposition), wave energy dispersion, wave properties (directions, magnitudes and amplitudes) and others.</p>	<p>http://www.aquaveo.com/sms/ / AQUAVEO (commercially available)</p>	<p>(AQUAVEO, 2011)</p>

<p>QUAL2K (River and Stream Water Quality Model)</p>	<p>QUAL2K (or Q2K) is a river and stream water quality model that is intended to represent a modernised version of the QUAL2E (or Q2E) model. Q2K is similar to Q2E in the following respects:</p> <ul style="list-style-type: none"> • The channel is well-mixed vertically and laterally. • The system can consist of a mainstem river with branched tributaries. • Non-uniform, steady flow is simulated. • The heat budget and temperature are simulated as a function of meteorology on a diel time scale. • All water quality variables are simulated on a diel time scale. • Point and non-point loads and withdrawals are simulated. <p>The QUAL2K model simulate among others:</p> <ul style="list-style-type: none"> • slowly oxidizing form of BOD (slow CBOD) and a rapidly oxidizing form (fast CBOD). • Sediment-water fluxes of dissolved oxygen and nutrients as a function of settling particulate organic matter, reactions within the sediments, and the concentrations of soluble forms in the overlying waters. • attached bottom algae with variable stoichiometry. • light extinction as a function of algae, detritus and inorganic solids. • alkalinity and total inorganic carbon. • generic pathogen as a function of temperature, light, and settling. • hydraulics of weirs as well as the effect of weirs and waterfalls on gas transfer. 	<p>http://www.epa.gov/athens/wwqtsc/html/qual2k.html / Environmental Protection Agency (free)</p>	<p>(Chapra et al., 2007)</p>
<p>SWAT (Soil and Water Assessment Tool)</p>	<p>SWAT predicts the effect of management decisions on water, sediment, nutrient and pesticide yields with reasonable accuracy on large, ungaged river basins. Model includes:</p> <ul style="list-style-type: none"> • elements of water balance: surface runoff, return flow, percolation, ET, transmission losses, pond and reservoir storage, crop growth and irrigation, groundwater flow, reach routing, water transfer, • nutrient and pesticide loading, • nutrients, pesticide, bacteria, conservative metals and sediment transport routing, • simulation of water quality parameters: algae, CBOD, dissolved oxygen, • plant growth cycle, • set of land management practices (e.g. planting, harvesting, tillage, fertiliser/pesticide application, street cleaning) 	<p>http://swatmodel.tamu.edu/ / Texas A&M University (free)</p>	<p>(Neitsch et al., 2004, Neitsch et al., 2005)</p>

<p>HSPF (Hydrological Simulation Program-Fortran)</p>	<p>HSPF simulates for extended periods of time the hydrologic, and associated water quality, processes on pervious and impervious land surfaces and in streams and well-mixed impoundments. HSPF uses continuous rainfall and other meteorological records to compute streamflow hydrographs and pollutographs. HSPF simulates interception soil moisture, surface runoff, interflow, base flow, snowpack depth and water content, snowmelt, evapotranspiration, ground-water recharge, dissolved oxygen, biochemical oxygen demand (BOD), temperature, pesticides, conservatives, fecal coliforms, sediment detachment and transport, sediment routing by particle size, channel routing, reservoir routing, constituent routing, pH, ammonia, nitrite-nitrate, organic nitrogen, orthophosphate, organic phosphorus, phytoplankton, and zooplankton. Program can simulate one or many pervious or impervious unit areas discharging to one or many river reaches or reservoirs.</p>	<p>http://water.usgs.gov/software/HSPF/ / US Geological Survey (free)</p>	<p>(Bicknell et al., 1997)</p>
<p>CAEDYM (Computational Aquatic Ecosystem Dynamics Model)</p>	<p>The Computational Aquatic Ecosystem Dynamics Model (CAEDYM) is an aquatic ecological model that may be run independently or coupled with hydrodynamic models DYRESM or ELCOM. CAEDYM consists of a series of mathematical equations representing the major biogeochemical processes influencing water quality. At its most basic, CAEDYM is a set of library subroutines that contain process descriptions for primary production, secondary production, nutrient and metal cycling, and oxygen dynamics and the movement of sediment.</p>	<p>http://www.cwr.uwa.edu.au/software1/models1.php?mdid=3/ Center for Water Research (commercially available)</p>	<p>(Hipsey et al., 2009; Hipsey, 2009)</p>

WASP (Water Quality Analysis Simulation Program)	<p>WASP is a generalised framework for modelling contaminant fate and transport in surface waters. Its flexible, compartmental approach allows it to address problems in one, two, or three dimensions. It is designed to allow easy substitution of user-written routines into the program structure. WASP has been used to answer questions regarding biochemical oxygen demand, dissolved oxygen dynamics, nutrients and eutrophication, bacterial contamination, and organic chemical and heavy metal contamination. The current WASP (v 7.41 - 2011) software package includes the scientific modules TOXI, EUTRO, and DYNHYD. TOXI models the transport and transformation of chemicals, EUTRO simulates dissolved oxygen and eutrophication processes, and DYNHYD is a hydrodynamic model used for prediction water flow and volume.</p>	<p>http://www.epa.gov/athens/wwqtsc/html/wasp.html / Environmental Protection Agency (free)</p>	<p>(EPA, 2006)</p>
AQUATOX	<p>AQUATOX is a simulation model for aquatic systems. AQUATOX predicts the fate of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates, and aquatic plants. This model is a valuable tool for ecologists, biologists, water quality modellers, and anyone involved in performing ecological risk assessments for aquatic ecosystems.</p>	<p>http://water.epa.gov/scitech/datait/models/aquatox/index.cfm / Environmental Protection Agency (free)</p>	<p>(Park, Clough, 2009)</p>

Table 2. Models for simulation of surface water quality

Model name	Short description	Availability / Producer	Source
biomoc - A multispecies solute-transport model with biodegradation	BIOMOC is a two-dimensional model that can simulate the transport and biotransformation of multiple reacting solutes. The program is general and flexible, allowing for any combination of biodegradation processes. A number of expressions for biological transformation rates have been included as options in the code. These include single, multiple, and minimum Monod kinetics and competitive, noncompetitive, and Haldane inhibition. The kinetic parameters can be formulated to simulate zero-order or first-order approximations of biodegradation rates. The growth and decay of several microbial populations performing the transformations is also accounted for. The microbial growth can be disabled, limited by biomass inhibition, or limited by the availability of a specified nutrient.	http://water.usgs.gov/software/BIOMOC/ / US Geological Survey (free)	(Essaid, Bekins, 1997)
PHREEQC - Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations	PHREEQC version 2 is a computer program written in the C programming language that is designed to perform a wide variety of low-temperature aqueous geochemical calculations. PHREEQC is based on an ion-association aqueous model and has capabilities for (1) speciation and saturation-index calculations; (2) batch-reaction and one-dimensional (1D) transport calculations involving reversible reactions, which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibria, and irreversible reactions, which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes; and (3) inverse modeling, which finds sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainty limits.	http://www.brr.cr.usgs.gov/projects/GWC_coupled/phreeqc/ / US Geological Survey (free)	(Parkhurst, Appelo, 1999)

<p>PHAST - A Computer Program for Simulating Groundwater Flow, Solute Transport, and Multicomponent Geochemical Reactions</p>	<p>The computer program PHAST (<i>PH</i> REEQC A nd <i>H</i> <i>ST</i> 3D) simulates multicomponent, reactive solute transport in three-dimensional saturated groundwater flow systems. PHAST is a versatile groundwater flow and solute-transport simulator with capabilities to model a wide range of equilibrium and kinetic geochemical reactions. The flow and transport calculations are based on a modified version of HST3D that is restricted to constant fluid density and constant temperature. The geochemical reactions are simulated with the geochemical model PHREEQC, which is embedded in PHAST. Major enhancements in PHAST Version 2 allow spatial data to be defined in a combination of map and grid coordinate systems, independent of a specific model grid (without node-by-node input). At run time, aquifer properties are interpolated from the spatial data to the model grid; regridding requires only redefinition of the grid without modification of the spatial data.</p>	<p>http://www.brr.cr.usgs.gov/projects/GWC_coupled/phast/ / US Geological Survey (free)</p>	<p>(Parkhurst et al., 2010)</p>
<p>HST3D - Heat and Solute Transport in Three-Dimensional Ground-Water Flow Systems</p>	<p>The Heat- and Solute-Transport Program (HST3D) simulates ground-water flow and associated heat and solute transport in three dimensions. Over the years since the release of Versions 1.0 through 1.4, various additions, modifications, and corrections have been made to the original simulator. Major changes included in Version 2 are (1) a revised data-input file with all spatial information described by coordinate location; (2) a new iterative solver for the matrix equations based on a generalised conjugate-gradient method; (3) an evapotranspiration boundary condition; (4) a division of the simulator output into many files; (5) a new set of output files designed for use by post-processing programs for graphical visualization and for flow totalization; (6) a pre-processor for evaluating dimensioning requirements; and (7) a post-processor for totalizing boundary flow rates and cumulative amounts. The post-processing program for graphical visualization must be supplied by the user. Version 2 of the simulator has been verified using five test problems selected from the published literature. One involves heat transport, four involve solute transport, and all have variable-density fluids.</p>	<p>http://www.brr.cr.usgs.gov/projects/GW_Solute/hst/ / US Geological Survey (free)</p>	<p>(Kenneth, Kipp, 1997)</p>

SUTRA (Saturated-Unsaturated Transport)	<p>SUTRA (Saturated-Unsaturated Transport) is a computer program that simulates fluid movement and the transport of either energy or dissolved substances in a subsurface environment. The original version of SUTRA was released in 1984. The version SUTRA 2.2 (2010) is an upgrade that adds to the previous version the ability to specify time-dependent sources and boundary conditions (without programming) and to output information pertaining to source and boundary condition nodes in a convenient format. The code employs a 2D or 3D finite-element and finite-difference method to approximate the governing equations that describe the two interdependent processes that are simulated:</p> <ol style="list-style-type: none"> 1) Fluid-density-dependent saturated or unsaturated ground-water flow; and either 2) (a) transport of a solute in the ground water, in which the solute may be subject to: equilibrium adsorption on the porous matrix, and both first-order and zero-order production or decay; or (b) transport of thermal energy in the ground water and solid matrix of the aquifer. 	<p>http://water.usgs.gov/nrp/gwsoftware/sutra/sutra.html / US Geological Survey (Free)</p>	<p>(Voss, Provost, 2010)</p>
GMS - Groundwater Modeling System	<p>GMS provides tools for every phase of a groundwater simulation including site characterization, model development, calibration, post-processing, and visualization. GMS supports both finite-difference and finite-element models in 2D and 3D including MODFLOW 2000, MODPATH, MT3DMS/RT3D, SEAM3D, ART3D, UTCHEM, FEMWATER, PEST, UCODE, MODAEM and SEEP2D. GMS can be used for simulation of:</p> <ul style="list-style-type: none"> • Solute Transport <ul style="list-style-type: none"> • Simple analytical transport modelling with ART3D • Simple 3D transport with MT3D, MODPATH, or FEMWATER • Reactive 3D transport with RT3D or SEAM3D • Multi-phase reactive transport with UTCHEM • Unsaturated Zone Flow and Transport <ul style="list-style-type: none"> • Fully 3D unsaturated/saturated flow and transport modeling with FEMWATER or UTCHEM 	<p>http://www.aquaveo.com/gms/ / AQUAVEO (commercially available)</p>	<p>(AQUAVEO, 2011b)</p>

PMWIN (Processing MODFLOW)	<p>Processing MODFLOW (PMWIN) is a integrated groundwater modeling system including:</p> <ul style="list-style-type: none"> • 3D finite-difference groundwater model MODFLOW. Supports multiple versions, including MODFLOW-96, MODFLOW-2000, and MODFLOW-2005. MODFLOW-88, MODFLOW-96, and MODFLOW 2000. • Solute transport models MT3DMS (v5.2), MT3D, RT3D (v2.5), and MT3D99. • Multicomponent reactive transport model PHT3D (v2.0) that incorporates MT3DMS (v5.2) for the simulation of three-dimensional advective-dispersive multi-component transport and the geochemical model PHREEQC-2 (v2.14) for the quantification of reactive processes. • Variable-density groundwater flow and multi-species solute and heat transport model SEAWAT (v4.0) . • Nonlinear parameter estimation package PEST (v12.0). Supports advanced features such as regularization, truncated singular value decomposition (SVD), and powerful SVD-Assisted Parameter Estimation. • Particle-tracking Model PMPATH which uses a semi-analytical particle-tracking scheme similar to MODPATH to calculate the groundwater paths and travel times. Through the interactive graphical modelling environment of PMPATH, the user can place particles and perform particle tracking with just a few mouse clicks. 	http://www.pmwin.net/pmwin5.htm / Wen-Hsing Chiang (free)	(Chiang, Kinzelbach, 2001)
MARS (Multiphase Areal Remediation Simulator)	<p>MARS (Multiphase Areal Remediation Simulator) can be used to model recovery and migration of light nonaqueous phase liquids in unconfined heterogeneous, anisotropic aquifers. MARS writes input flow files for the BIOF&T model which simulates multispecies dissolved phase transport in heterogeneous, anisotropic, fractured media, or unfractured granular porous media. It models flow of water and light nonaqueous phase liquid (LNAPL) and aqueous phase transport of up to five species in ground water with multiple pumping and/or injection wells. MARS is a finite-element model that allows accurate representation of highly-irregular material and physical boundaries in a heterogeneous and anisotropic media.</p>	http://www.scisoftware.com/environmental_software/product_info.php?products_id=46 / (commercially available)	(SSG, 2011)

VisualMODFLOW	<p>VisualMODFLOW simulate groundwater and surface water interactions, and changes to groundwater chemistry. This modelling system includes:</p> <ul style="list-style-type: none"> • MODFLOW-2000, 2005 the standard for 3D groundwater flow • SEAWAT v.4, for 3D variable-density groundwater and heat flow • MODPATH, the standard package for particle tracking • MT3DMS, the multi-species contaminant transport engine • PHT3D, multi-component geochemical reactive transport • MT3D991, for multi-species reactive transport • RT3D, for reactive transport simulations • Zone Budget, for sub-regional water budget calculations • LAK Package, for surface water/groundwater interactions • Multi-Note Well (MNW) package for well simulations • ETS1 Package, for evapotranspiration modeling • WinPEST, automated calibration and predictive analysis • VMOD 3D-Explorer, 3D visualization and animations • SAMG Solver1, for convergence of complex models • GMG, the USGS Geometric Multi-Grid solver • MGO, for pumping well optimization 	http://www.swstechnology.com/groundwater-software/groundwater-modeling/ Schlumberger (commercially available)	(Schlumberger, 2010)
BIOF&T (Biodegradation, Flow and Transport)	<p>BIOF&T models biodegradation, flow and transport in the saturated and unsaturated zones in two or three dimensions in heterogeneous, anisotropic porous media or fractured media. Model simulates convection, dispersion, diffusion, adsorption, desorption, and microbial processes based on oxygen-limited, anaerobic, first-order, or Monod-type biodegradation kinetics as well as anaerobic or first-order sequential degradation involving multiple daughter species.</p>	http://www.scisoftware.com/environmental_software/product_info.php?products_id=33/ (commercially available)	(SSG, 2011)

HYDROGEOCHEM	<p>HYDROGEOCHEM is a numerical model of fluid flow, thermal transport, hydrologic transport, and biogeochemical kinetic/equilibrium reactions in saturated/unsaturated media. It iteratively solves three-dimensional fluid flow, heat transfer, and reactive biogeochemical transport equations. The Richards equation is solved for fluid flow, the thermal transport equation is solved for heat transfer, and the advection-dispersion- reactive transport equations are solved for all mobile component equations and kinetic-variable equations.</p> <p>HYDROGEOCHEM is designed for generic applications to reactive transport problems controlled by both kinetic and equilibrium reactions in subsurface media.</p>	http://www.scisoftware.com/environmental_software/product_info.php?products_id=44 / (commercially available)	(ORNL, 2004)
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Table 3. Models for simulation of groundwater quality

Model name	Short description	Availability / Producer	Source
WATEQ4F	<p>WATEQ4F is a chemical speciation code for natural waters. It uses field measurements of temperature, pH, Eh, dissolved oxygen and alkalinity, and the chemical analysis of a water sample as input and calculates the distribution of aqueous species, ion activities, and mineral saturation indices that indicate the tendency of a water to dissolve or precipitate a set of minerals. The model assumes homogeneous aqueous phase equilibria, except for redox species. Equilibrium with respect to mineral solubilities is not assumed. The program results are used primarily to examine the tendency of a water to reach mineral solubility equilibria as a constraint on interpreting the chemistry of natural waters.</p>	http://www.brr.cr.usgs.gov/projects/GWC_chemtherm/software.htm / US Geological Survey (free)	(Ball, Nordstrom, 2001)

MODHMS	<p>MODHMS is a physically based, spatially distributed, integrated surface/subsurface modeling framework hydrologic system. MODHMS extends MODFLOW-SURFACT subsurface modeling code to include overland and channel flow and transport. Model addresses complex water resources management issues including:</p> <ul style="list-style-type: none"> • Integrated water resource assessment • Groundwater availability & safe-yield analysis • Conjunctive surface water-groundwater use • Stream flow restoration • Flood prediction and mitigation • Agricultural irrigation management • Cleanup of industrial contaminants • Watershed-scale analysis of point source and nonpoint source pollution • Fluvial hydraulic analysis 	http://www.hglsoftware.com/Modhms.cfm/ HGL (commercially available)	(HGL, 2006)
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Table 4. Models for simulation of surface and groundwater quality

8. Examples of use of integrated systems for water quality monitoring and modelling

In this section two examples of integrated real-time monitoring and modelling systems are presented. Both systems are up-to-date (are being still developed under ongoing projects). Both are also aimed at providing managers with additional information about the environment, information needed for efficient operation. First of mentioned systems is the system for feedback-driven in-situ remediation developed in the UPSOIL project (Sustainable Soil Upgrading by Developing Cost effective, Biogeochemical Remediation Approaches) (UPSOIL, 2011). The second is system developed in the ZiZOZap project, aimed at supporting the management and protection of dammed reservoir (ZiZOZap, 2011).

Monitoring-modelling system for in-situ chemical oxidation

One of the UPSOIL project test sites (used here as an example) was located in an industrial area at the port in Belgium. Until 2001 a warehouse for non-hazardous (no soil polluting) goods was located on this site. Since 2002 the storage of hazardous products (acetone, isopropyl alcohol, methyl ethyl ketone, vinyl acetate, acrylates, ethyl acetate, fatty acids, acetic acid) was started on the site. Contaminants present at the site included: heavy metals, mineral oil, polycyclic aromatic hydrocarbons, volatile organic compounds, benzene, toluene, xylene, extractable organic halogen, oils and grasses, trichloroethylene and total organic carbon.

The remediation process was based on the optimal interaction between the injected remedial agents and the target contaminants. The first version of the injection system (MIP-IN) was a combination of the commercially available Geoprobe MIP system for in-situ detection of volatile contaminants and a system for in situ injection of remediation liquids into the soil. The system, for 12 months was under iterative “modification - evaluation” process, incorporating suggestions and technical requirements defined by the stakeholders involved within project. The whole “contaminant detection - injection cycle” encompasses the following scheme:

- Volatile contaminants enter the MIP device and are detected over 0.3 m vertical soil column.
- App. 25 samples from each 0.3 m depth interval are transported by the carrier gas to the field Gas Chromatograph (GC) which is giving a very high data resolution of the contaminant spreading.
- The field GC signal from the 0.3 m interval and correlating depth interval is shown on the interface. The MIP signal response is logged automatically.
- When contamination is detected the operator has to define a balanced volume of solution to be injected at the corresponding 0.3 m interval. The volume to be injected is entered on the laptop and the program automatically gives a signal to inject this volume when the injection part of the probe is at the same depth as the corresponding MIP signal.
- Under pressure the injection pump delivers at a defined flow rate the volume of solution defined for a given depth interval. Pressure, flow rate and injected volume are logged automatically.
- The solution is entering the soil under pressure where it is spread due to the geological settings.

Real-time monitoring system used in this test site included 14 monitoring wells, which were equipped with sensors logging values of pH, redox, temperature and conductivity with 15-minutes intervals (Fig. 6). This system was established before the injections. It operated for four months after the injection and during the field work it was a complement to the measurements done with the gas chromatograph coupled with a system for in-situ injection.

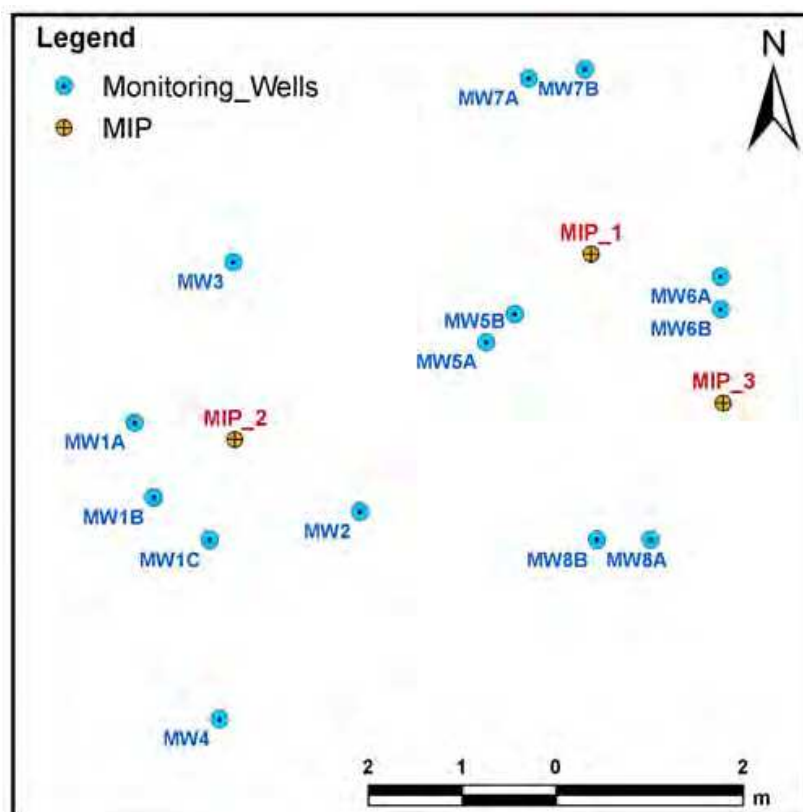


Fig. 6. Location of the 3 MIP-IN injection points and 14 monitoring points

Apart from real-time monitoring system, six sampling campaigns were done and key physical and chemical parameters were measured in each monitoring well. Samples were taken 17 weeks before injection (campaign T0b), 1 week before injection (T0a), 1 week after injection (T1), 3 weeks after injection (T2), 8 weeks after injection (T3) and 16 weeks after injection (T4).

During this remediation test a mathematical transport model was developed to enable optimal designing of the injection process as well as the re-arranging the whole procedure after the first step of the remediation (e.g. add new wells, change the volume of oxidants). Within the UPSOIL project relatively simple and operational software was developed for preliminary site specific design and further optimisation of the injection. In addition, during and after the injection field work this software serves additionally as a tool gathering all the field data including the real-time logged parameters (like pH, temperature, oxidation-reduction potential, conductivity) and the chemical data measured periodically during the sampling campaigns. The model consists of the Excel-Python module for calculations of physical parameters of the injection, and PhreeqC based module for hydro-geochemical simulations. The outcome of the first part of the model (physical module) includes:

- suggested radius of influence (ROI),
- total bulk treatment volume,
- total volume of reactant to be delivered,
- maximum volume of oxidant required at each injection interval,
- duration of injected oxidant effectiveness,
- effective velocity of the groundwater,
- injection time to reach the suggested ROI,
- suggested number of injection wells in the treatment area,
- suggested injection depth intervals to be used,
- suggested concentration of oxidant to be used (at averaged amounts of pollutants + natural demand).

The physical module of the model can be used to define the optimal injection strategy before moving into the field. Later, during the injection field work additional site specific data can be gradually inserted into the model in order to observe the soil absorption capacity (actual volume of liquid that can be injected at a given depth interval at a reasonable flow and with no “surface break through”) and radius of influence at a given injection volume and flow/pressure rate.

In combination with the physical module (Excel-Python application) a 1D transport and chemical reactions module was elaborated for the oxidation processes (permanganate as an oxidant) using the PhreeqC code. This model requires input data including: parameters of the liquid to be injected, the baseline geochemistry (situation before injection) and the concentrations levels and type of contamination in the soil. The objective of the transport and chemical model is to simulate the chemical response to the injection and predict when (if required) it would be optimal to carry out next injection campaign. The prediction is gradually more solid when field monitoring data after injection are put into the model. Thanks to the continuously updated database of the developed tool it is possible to get actual comparisons of results derived from loggers, chemical monitoring and numerical modelling.

During the field works, at 3 points (Fig. 6) 435 kg NaMnO₄ in 5.2 m³ of water was injected at a depth between 2 and 7 m below ground level. Successful reaching of targeted interval by oxidant was observed via:

- visual detection of the purple colour in monitoring wells,
- significant decrease of the oxidation-reduction potential
- increase in electric conductivity.

Results of the remediation are shown also as an example of benzene concentrations before and after the injections (Fig. 7).

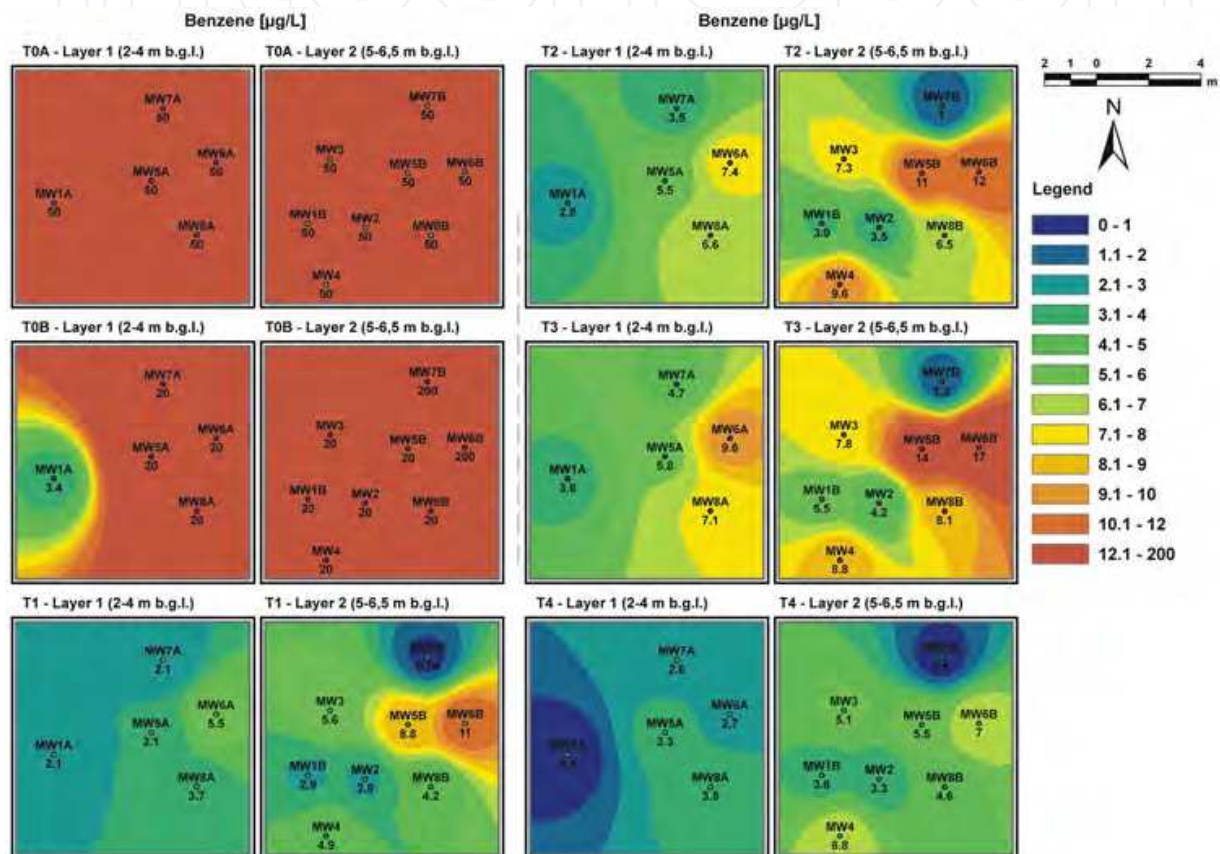


Fig. 7. Concentration distribution map for benzene and six sampling campaigns

Monitoring-modelling system for the dam reservoir management and protection

The ZiZOZap project is a part of the efforts to develop numerical multidimensional models of water reservoirs, which are undertaken in leading world countries. These models facilitate management of reservoir for their ability to predict the effects of the decisions undertaken. The purpose is to enhance the environmental safety and public health of local population exploiting water resources. The object of the project study, Goczałkowice Water Reservoir, is a crucial water resource for 3,5 millions of inhabitants of Upper Silesia region (southern Poland). The Reservoir is also a unique natural area - a habitat for number of valuable species of birds, mammals, fish, small invertebrates and plants. Accommodation of environmental values and human needs in the area of The Reservoir is one of major tasks of the project.

The model which will be obtained as a result of the project will support the process of decision making and management of the Reservoir. Moreover, the model after necessary adaptations should be applicable for other water reservoirs (IPIS, 2011).

For the case study reservoir a monitoring and analyses of various environmental elements are carried out by interdisciplinary groups of experts. Data on hydrological, hydrogeological and physico-chemical conditions of water and bottom sediments as well as parameterised ecological and hygienic indicators referring to fauna, flora and the natural environment around the reservoir are collected in integrated databases. Project partners try to identify the key issues related to optimal management of the dam reservoir and build an information system together with a database. Based on the obtained research results and water management scenarios a numeric model of the reservoir is being developed. This will allow continuous assessment of the quality and functional state of the reservoir as well as stimulation and forecast of its changes. It is expected that in practice the system of reservoir models will enable to predict qualitative and quantitative changes in water resources which will affect water treatment and minimisation of costs, as well as forecasting water fertility and changes in the reservoir or the surrounding ecosystems (IETU, 2010).

As a part of created modelling system, a model for reservoir hydrodynamics and ecosystems was developed using ELCOM and CAEDYM software. ELCOM (Estuary, Lake and Coastal Ocean Model) is a three-dimensional hydrodynamics model for lakes and reservoirs, and is used to predict the variation of water temperature and salinity in space and time. The model forms the three-dimensional hydrodynamics driver to the CAEDYM water quality model (Hodges & Dallimore, 2009). The CAEDYM (Computational Aquatic Ecosystem Dynamics Model) is an aquatic ecological model that consists of a series of mathematical equations representing the major biogeochemical processes influencing water quality. At its most basic, CAEDYM is a set of library subroutines that contain process descriptions for primary production, secondary production, nutrient and metal cycling, and oxygen dynamics and the movement of sediment (Hipsey et al., 2009; Hipsey, 2009). Variables simulated by CAEDYM model include: light, inorganic particles, sediments and resuspension, dissolved oxygen, carbon, nitrogen, phosphorus and silica, phytoplankton dynamics, bacteria, zooplankton, higher biology, pathogens and microbial indicator organisms, geochemistry and metals, sediment diagenesis (Hipsey et al., 2009).

Within the ZiZozap project the integrated ELCOM-CAEDYM model was coupled with mentioned above databases, which are used for storing the periodically collected and real-time measured data. Monitoring database includes among others:

- Real-time measured parameters: inflow (main river, pumping stations), outflows, water intake, water conductivity, pH, water temperature (at 1m depth intervals), dissolved oxygen, chlorides, nitrates, chlorophyll, redox potential, turbidity, air temperature, wind speed and direction, air humidity, air pressure, precipitation, solar radiation.
- Periodic measurements: complex water chemistry, physical parameters, pathogens and microbial composition, plankton, benthic organisms.

Sample output from the ELCOM model (water velocity at different weather and inflow conditions) is presented on Figure 8. Example of output from the CAEDYM model (dissolved oxygen, temperature) is shown on the Figure 9.

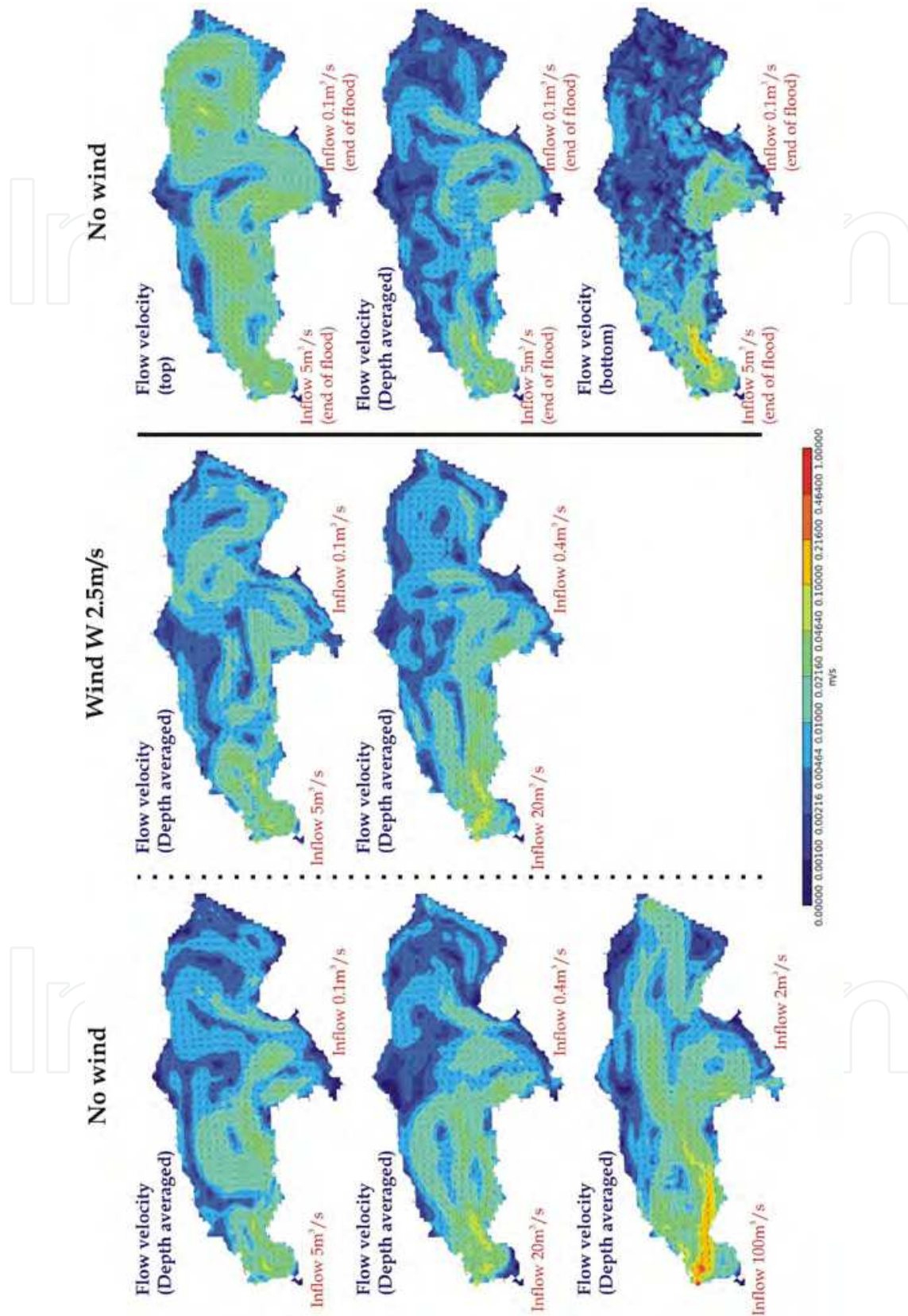


Fig. 8. Sample output from the ELCOM model for Goczałkowice Reservoir (velocities distribution)

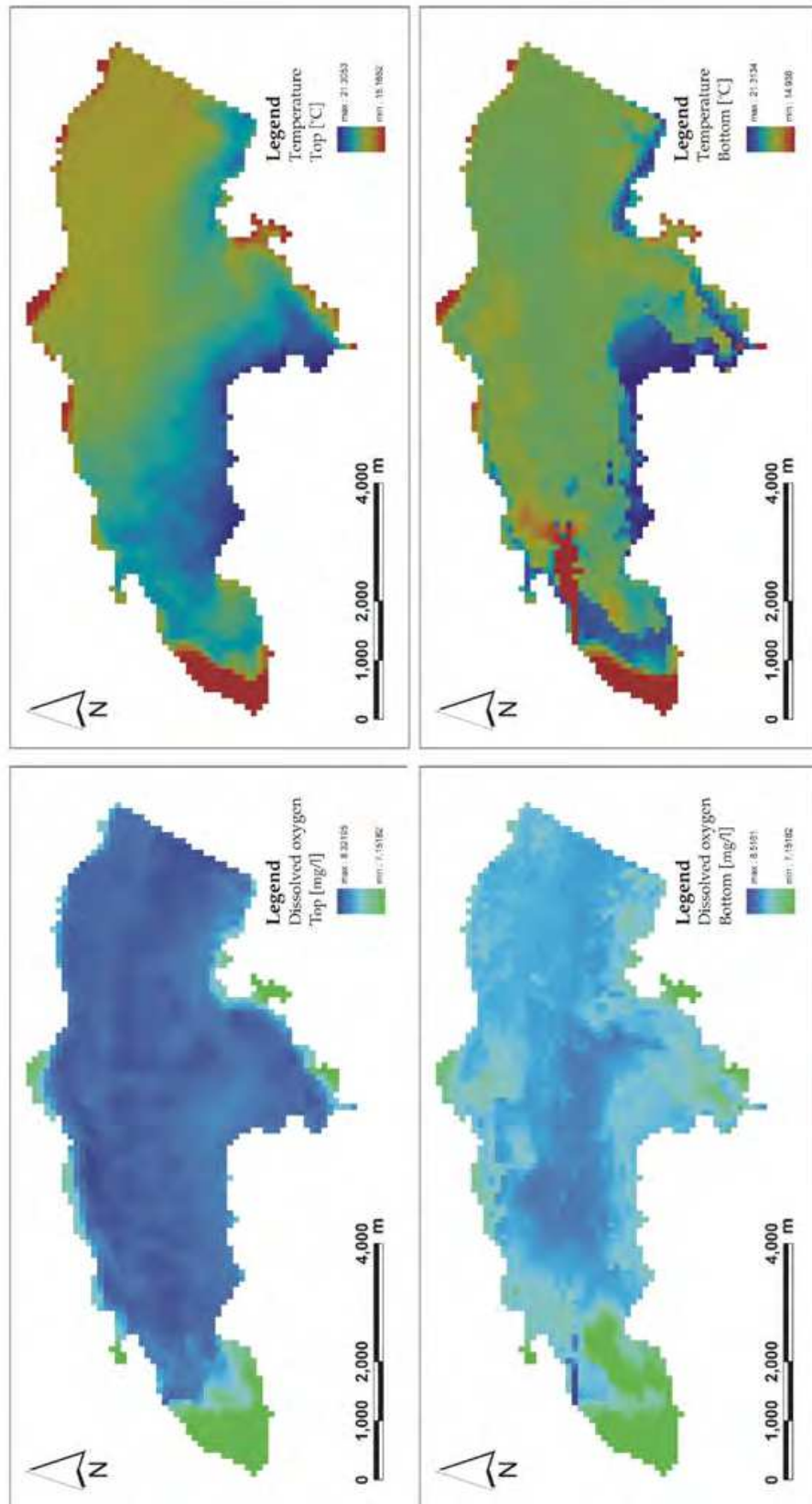


Fig. 9. Sample output from the CAEDYM model for Goczalkowice Reservoir (dissolved oxygen, temperature)

9. Conclusions

General conclusions of this chapter are as follow:

- Monitoring of the water quality (for atmospheric water, surface water and groundwater) should be designed in a way:
 - Ensuring spatial and temporal comparisons of the results - It is possible only if the monitoring is integrated in time and space, and if the structure of the monitoring system is uniform in all monitoring points.
 - Addressing local and regional problems.
- Results of the monitoring should be stored in a form allowing their immediate use (e.g. as online databases).
- If there are no resources or technical/environmental possibilities for monitoring of needed water quality parameters, appropriate models should be used. Models can be coupled for this purpose with monitoring systems including simple parameters, directly related to the water quality.
- Each short and long-term activities potentially affecting the water quality should be preceded by detailed analyses of different scenarios and their impacts. For such tasks a set of widely used modelling tools is easily available.

10. References

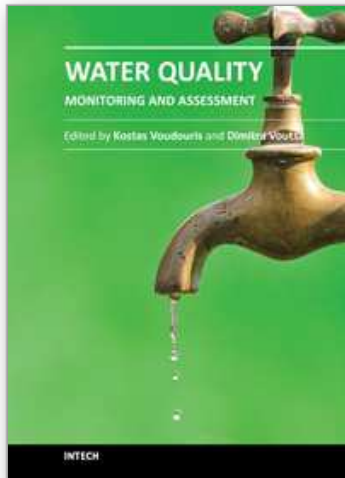
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Water Quality Monitoring and Assessment

Edited by Dr. Voudouris

ISBN 978-953-51-0486-5

Hard cover, 602 pages

Publisher InTech

Published online 05, April, 2012

Published in print edition April, 2012

The book attempts to covers the main fields of water quality issues presenting case studies in various countries concerning the physicochemical characteristics of surface and groundwaters and possible pollution sources as well as methods and tools for the evaluation of water quality status. This book is divided into two sections: Statistical Analysis of Water Quality Data;Water Quality Monitoring Studies.

How to reference

In order to correctly reference this scholarly work, feel free to copy and paste the following:

Katarzyna Samborska, Rafal Ulanczyk and Katarzyna Korszun (2012). Monitoring and Modelling of Water Quality, Water Quality Monitoring and Assessment, Dr. Voudouris (Ed.), ISBN: 978-953-51-0486-5, InTech, Available from: <http://www.intechopen.com/books/water-quality-monitoring-and-assessment/monitoring-and-modelling-of-water-quality>

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51000 Rijeka, Croatia
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