UN/ECE Task Force on Monitoring & Assessment

under the Convention on the Protection and Use of Transboundary Watercourses and International Lakes (Helsinki, 1992)

Working Programme 1996/1999

Volume 3:

Application of models

ISBN 903695276X

Authors:
G.E. Arnold (RIZA)
R. Chriaštel (SHMI)
V. Novak (Inst. of Hydr. Slovak Academy of Sciences)
N.S. Ognianik (Inst. Geol. UAS)
Z. Simonffy (Techn. Univ. of Budapest)

Ministry of Transport, Public Works and Water Management
RIZA Institute for Inland Water Management and Waste Water Treatment,
The Netherlands

Slovak Hydrometeorological Institute, Bratislava,
The Slovak Republic

Institute of Hydrology Slovak Academy of Sciences, Bratislava,
The Slovak Republic

Institute of Geology of Ukraine Academy of Science,
The Ukraine

Technical University of Budapest,
Hungary

Lelystad, September 1999

Colofon

Lay-out:
Grafisch bedrijf ve&es

Cover design:
Ph. Hogeboom (Panthera BNO)
G.E. Arnold (RIZA)

Cover pictures:
KNMI
NITG-TNO
Leon Lamers, KUN
Srećko Božičević

Printed by:
Grafisch bedrijf ve&es

English corrections:
M.T. Villars (Delft Hydraulics)
I. Záborszky

Additional copies of the following 4 volumes can be ordered from RIZA, Institute for Inland Water Management and Waste Water Treatment, ECE Task Force project-secretariat, P.O. box 17, 8200 AA Lelystad, The Netherlands. Fax: +31 (0)320 249218.

- Volume 1: Inventory of transboundary groundwaters (ISBN 9036952743)
- Volume 2: Problem-oriented approach and the use of indicators (ISBN 9036952751)
- Volume 3: Application of models (ISBN 903695276X)
- Volume 4: State of the art on monitoring and assessment of groundwaters (ISBN 9036952778)

Preface

This report "Application of models" is one of the four background documents to be used for the drafting of Guidelines on monitoring and assessment of transboundary groundwaters. This report has been prepared by G.E. Arnold, R. Chriaštel, V. Novák, N.S. Ognianik and Z. Simonffy in close co-operation with P. Roncák (sub-project leader). Designated advisor for this sub-project was K. Schwaiger.

For the execution of the overall groundwater programme, a core group was established, which performed the role of guidance-committee. The core group was made up of:

G.E. Arnold	project leader groundwater programme and sub-project leader State of the Art	Institute for Inland Water Management and Waste Water Treatment (RIZA), Ministry of Transport, Public Works and Water Management, The Netherlands
Zs. Buzás	sub-project leader Inventory	Ministry of Transport, Communication and Water Management, Hungary
R.A. Bebris		Ministry of Environmental Protection and Regional Development, Latvia
J.J. Ottens	sub-project leader Indicators	RIZA, The Netherlands
P. Rončak	sub-project leader Models	Slovak Hydrometeorological Institute, Slovak Republic
R. Enderlein	secretary to the ECE Water Convention	ECE Secretariat, Switzerland
J. Chilton	advisor	British Geological Survey/UK -World Health Organisation (BGS-UK/WHO), United Kingdom
O. Tarasova	advisor	Ministry for Environmental Protection and Nuclear Safety, the Ukraine
M. Varela	advisor	Ministry of Environment, Spain

This report was discussed and accepted by the Core Group on Groundwater, established by the ECE Task Force on Monitoring and Assessment under the Convention on the Protection and Use of Transboundary Watercourses and International Lakes.

Contents

Preface		3
1.	**Introduction**	**7**
1.1	General	7
1.2	Scope and objectives	8
1.3	Project organisation	8
1.4	Outline of the report	9
2.	**Model definition and the role of mathematical models in the monitoring cycle**	**11**
2.1	General	11
2.2	Existing mathematical models in UN/ECE countries	13
3.	**Theoretical basis and nature for groundwater models**	**17**
3.1	Changes of the natural groundwater regime under technogenic impact	17
3.1.1	Groundwater resources problems	17
3.1.2	Groundwater quality	18
3.2	Mathematical modelling of groundwater flow and mass transport	18
3.2.1	Deterministic models	20
3.2.2	Stochastic models	21
3.2.3	Modelling water and solute transport in the unsaturated soils	23
3.3	Analytical and numerical approach	25
3.3.1	Aspects concerning the FDM, FEM and AEM techniques	25
3.4	Optimal location of the groundwater monitoring network	30
3.5	Scales and dimensionality	32
4.	**Input data for groundwater models**	**33**
4.1	Data for modelling the saturated zone	33
4.2	Data for modelling the unsaturated zone	35
4.3	Data for modelling water quality	36
4.4	Other data requirements	37
4.5	Use of data bases and geographical information systems in groundwater modelling	37
4.6	The role of a QA/QC system	39
5.	**Highlights**	**41**
6.	**Key points**	**43**
	Annexes	
I	Example of the use of a groundwater model in a transboundary region	47
II	Review of groundwater models	51

1. Introduction

1.1 General

The Convention on the Protection and Use of Transboundary Watercourses and International Lakes was drawn up under the auspices of the Economic Commission for Europe (ECE) and adopted in Helsinki on 17 March 1992. The Convention entered into force in October 1996 and covers, amongst others, the monitoring and assessment of transboundary waters, the assessment of the effectiveness of measures taken to prevent, control and reduce transboundary impact, the exchange of information between riparian countries and public information on the results of water and effluent sampling. Riparian Parties shall also harmonise rules for setting up and operating monitoring programmes, including measurement systems and devices, analytical techniques, data processing and evaluation procedures.

In 1994, the ECE Working Party on Water Problems established the Task Force on Monitoring and Assessment of Transboundary Waters. At its eighth session in March 1995, the Working Party agreed on a phased approach to the drafting of guidelines on monitoring and assessment of transboundary waters. This phased approach means that guidelines will be drafted for rivers, groundwater, lakes and estuaries successively. After finishing the guidelines for transboundary rivers, the Working Party requested the Task Force on Monitoring & Assessment to draw up - as a second step of its activities - draft guidelines on monitoring and assessment of transboundary groundwaters.

At the first meeting of the Parties to the Convention on the Protection and Use of Transboundary Watercourses and International Lakes in Helsinki (Finland) in July 1997, an overall workplan was agreed upon. The drafting of guidelines on monitoring and assessing transboundary groundwaters (including background documentation) was formulated as one of the activities of programme area 3 "Integrated management of water and related ecosystems". These guidelines will be considered at the second meeting of the Parties in the year 2000.

Groundwater supports various important functions. Some functions, like nature and agriculture, are directly related with the occurrence of groundwater. In other areas, like the drinking water and industrial water supply, groundwater is used as a production factor, because of its normally good and constant quality. However, a high population density, continuously growing industrialisation and intensive agriculture will have a negative effect on the quality of soil and groundwater. In recent times, the soil has become polluted more and more by private and public waste dumps, air pollution, fertilisers and use of excess manure. In shallow groundwaters, this pollution can easily be transported to locations where it may be harmful to other interests. These problems do not only occur within countries, but can also have transboundary impacts, which demand for accountable monitoring and assessment activities. Furthermore, measures should be taken to avoid these undesired developments, within, as well as between countries with joint groundwater bodies. The integral basin area approach, or ecosystem approach, which was adopted as a basic principle in the Convention is also the basis for structuring the guidelines on monitoring and assessment of transboundary groundwaters.

As with the Guidelines on Water-quality Monitoring and Assessment of Transboundary Rivers, these guidelines are brief and concise and supported by supplementary documentation. An inventory was made of monitoring and assessment practices in ECE countries, which includes an examination and evaluation of these practices. Prior to the drafting of the guidelines, additional activities have been launched to identify indicators for groundwater assessment and review the use of models. In addition, an overview of transboundary groundwaters in the ECE region was drawn up.

Co-operation has been sought with various international organisations and institutions to make best use of existing programmes and link on-going activities in the field of monitoring and assessment.

The Guidelines on Transboundary Groundwater Monitoring and Assessment are supported by a series of 4 background documents dealing with the following themes:

1. Inventory of transboundary groundwaters
2. Problem-oriented approach and the use of indicators
3. Application of models
4. State of the art on monitoring and assessment of groundwaters

The present report is the result of the activities mentioned under number 3: "Application of models".

1.2 Scope and objectives

The main purpose of this sub-project in relation with the drafting of guidelines on monitoring and assessment is to highlight the role of mathematical models in the process of monitoring and assessment of transboundary aquifers.

The main objective of this sub-project in accordance with a proposal for the drafting of guidelines on monitoring and assessment of transboundary groundwaters is:

- to make recommendations for the application of models as a tool for studying problems related to transboundary groundwaters and to incorporate such a tool in the guidelines.

Furthermore, attention in this sub-project is paid to:

- overview of existing available mathematical modelling approaches in groundwater systems
- elaborate a list of needed model variables, parameters and characteristics
- suggest appropriate problems and limits for the use and implementation of mathematical models.

1.3 Project organisation

Successful utilisation of mathematical modelling is only possible if the methodology is properly integrated with data collection, data processing and other techniques and approaches for evaluation of transboundary groundwater system characteristics.

To collect information about the existing mathematical modelling approaches in transboundary aquifers, questionnaires have been sent to the UN/ECE member states. The responses received were evaluated and summarised. The main sources of information on the mathematical modelling practices and used models were the database of the International Groundwater Modelling Centre (IGWMC), proceedings of international conferences and an extensive literature research. Furthermore, national experience and knowledge of experts working in the field of mathematical modelling from participating countries were used in this sub-project as well.

1.4 Outline of the report

The present report on the "Application of models" is focused on the overview of existing available mathematical modelling approaches in (transboundary) groundwater systems. Special attention is paid to a list of needed model variables (parameters) and characteristics for numerical models.

In Chapter 2, the definitions and the role of mathematical modelling in groundwater monitoring- and assessment cycle are presented together with brief information on the types of models applied in UN/ECE countries.

Chapter 3 contains theoretical aspects and nature of the groundwater models with special attention to the changes of the natural groundwater regime. The model application and techniques of solutions are also discussed together with general information on the limits and problems in using groundwater mathematical models with special attention to numerical modelling approaches.

In Chapter 4, the input data for groundwater models and their relation to the application of GIS is discussed. The Quality Assurance/Quality Control system is briefly presented as well.

Annex 1 contains an example of a groundwater mathematical model application in the transboundary region of the Danubian Lowland area (The Slovak Republic, Hungary). Annex 2 provides a short review of mathematical models used in the participating countries of this sub-project (The Slovak Republic, Hungary, The Netherlands and Ukraine).

The authors of this report are aware that it was not an aim to provide exhaustive information on groundwater modelling approaches. Groundwater modelling programs have been described extensively in the literature and are presented in a database compiled e.g. by the International Groundwater Modelling Centre (IGWMC). Furthermore, comprehensive and detailed reviews have been done by many authors e.g. Mercer et al. (1980), van der Heijde et al. (1988), Berkowitz (1993), etc. Models for assessing and monitoring groundwater quality have also been presented in proceedings of an International symposium at Boulder, Colorado, USA (IASH, 1995) and have been discussed during a workshop in Budapest (Hegedus, 1997).

2. Model definition and the role of mathematical models in the monitoring cycle

2.1 General

Modelling of groundwater systems refers to the construction and operation of a model where the actual aquifer behaviour is assumed. There are several definitions of models and one of them is published by van der Heijde et al. (1988) as a 'non-unique simplified description of an existing physical system'. Models are useful tools for understanding the mechanisms of groundwater systems and the process that influence their composition. They can also provide a quantitative indicator for resource evaluation where financial resources for additional field data collection are limited. This might be of great importance, especially in relation with transboundary studies. In contrast, it has to be said that a lot of data are necessary for setting up mathematical models in order to achieve satisfying results.

The model can be physical (for example, a laboratory 'sand-box' and field lysimeter), electrical analogies, 'black-box' statistical models and mathematical models, which involve both analytical and numerical techniques. In this sub-project, groundwater models are referred to as the mathematical models in which the causal relationships among various components of the system and its environment are quantified and expressed in terms of mathematics and uncertainty of information.

Thus, mathematical models might range from rather simple empirical expressions to complex multi-equation formulations. The majority of them are usually based on numerical solution techniques, which allow controlling a variety of coupled processes describing the hydrology, chemical transport, geochemistry and biochemistry of heterogeneous near-surface and deep underground. However, other types of models have been developed for simulating soil processes and deep underground processes (e.g. air and vapour transport in soils, soil mechanics, fracture propagation, stream flow and heat transport in multi-phase geothermal reservoirs). In this report, only models related strictly to soil and groundwater are taken into account.

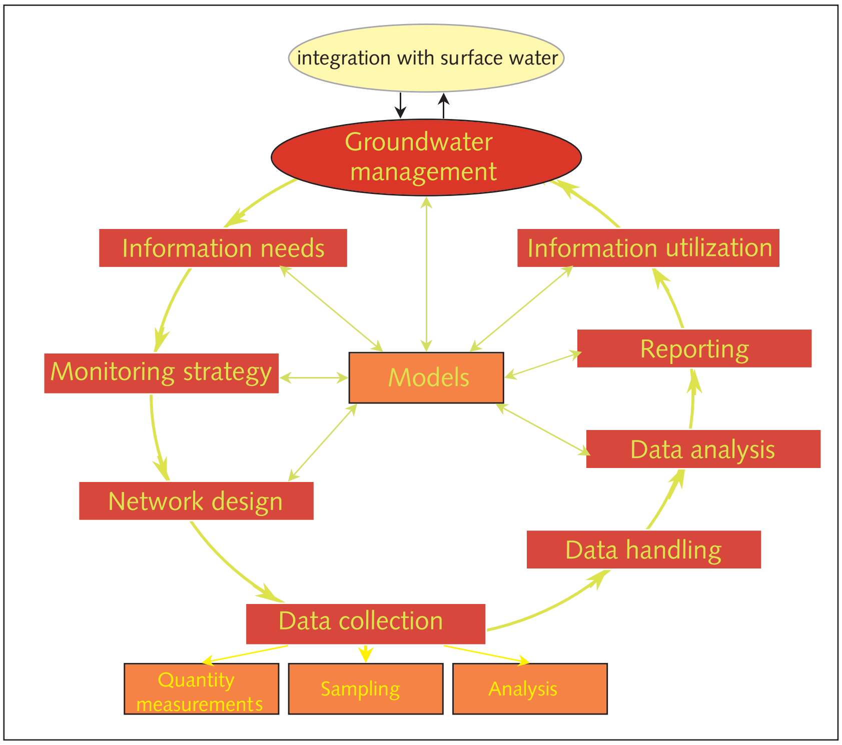
Models based on various stochastic approaches are also available. These models assume that the processes active in the system are stochastic in nature and that the variables may be described by probability distributions. Consequently, responses are characterised by statistical distributions. This report is mainly focused on groundwater models with analytical and numerical solution techniques, which are presented in the next chapter.

The position of the mathematical models within the groundwater monitoring cycle is presented in Figure 2.1. The use of mathematical models in specific parts of the monitoring cycle is based on information needs and objectives of the monitoring process. The location of models in the middle of the monitoring cycle is meant for illustrative purposes and is not meant to indicate that models are the core element of monitoring.

Models can be used in what is often called the predictive mode by analysing the response of a system when existing stresses vary and when new ones are introduced. Models can assist in:

- screening alternative policies;
- designs optimising and monitoring network;
- assessing operative actions.

Figure 2.1
Monitoring cycle with model application



Models can determine impacts on the groundwater systems and also assess the risks of actions to human health and the environment.

Monitoring programme and network design

One of the most significant uses of the mathematical models is related to the design of (water-quality) monitoring programmes in groundwater systems. Most of the real cases are characterised by existing irregular networks so that the network design tends to be optimal. Technical and economical aspects generally drive the optimisation criteria. A practical strategy for the best monitoring sites should be able to:

- tailor the analytical programme and frequency of the sampling by the application of geohydrochemical analysis;
- make reductions to the monitoring programme;
- understand the process of groundwater quality deterioration and thereby selecting the right abatement strategy.

In financial terms, early investments in using geohydrological models are returned by a net lowering of the whole exploitation costs of the groundwater quality monitoring programme and consequently minimising the extent of groundwater contamination.

Data processing

Application of the model often requires extensive work regarding data pre-processing and post-processing. The advances in computer technology also allow technical planners and decision makers in transboundary groundwater management to use prediction- and simulation systems as a source of information. Nowadays, great effort is paid to build up mathematical modelling incorporated with GIS-based data exchange interfaces (for example REGIS, FEFLOW).

No universal model has been developed to solve all groundwater problems. Therefore, different types of models are appropriate for solving different types of problems.

2.2 Existing mathematical models in UN/ECE countries

In this chapter, attention is focused on the application of existing mathematical models in the ECE countries based on the returned questionnaires. Questionnaires regarding mathematical models were sent to participating countries in the UN/ECE Task Force on Monitoring and Assessment. The model questionnaire was the third part of the overall questionnaire prepared by sub-project 1 "Inventory of transboundary groundwaters". In this evaluation, the responses from the twenty returned questionnaires were used. The responses have been summarised in Table 2.1. There were seven questions in which the UN/ECE members were requested to provide information on the models used for:

1. water balance (in terms of water quantity);
2. gaining knowledge about the quantitative aspects of the unsaturated zone;
3. simulating of water flow and chemical migration in the saturated zone including river-groundwater relations;
4. assessing the impact of changes of the groundwater regime on the environment;
5. setting up/optimising monitoring networks;
6. setting up groundwater protection zones;
7. other purposes (if any, please describe type of those models).

Water balance

All responding countries stated that the mathematical models for groundwater balance are used in this part and both analytical and numerical models are applied (MODFLOW is the most frequently stated model).

Unsaturated zone

Quantitative aspects of water flow through the unsaturated zone are modelled by using both the analytical and numerical models similar to the previous item. Ten countries stated the application of such models.

Groundwater flow and chemical migration

Groundwater flow and chemical migration through the saturated zone are modelled here by using different types of models and for different spatial scales. Models simulating groundwater flow are frequently used. All responding countries stated that they use mathematical models for this aspect.

Impact of changes of the groundwater regime on the environment

In this part of the questionnaire, only ten countries responded on the use of mathematical models. However, in many cases models are only used in research activities for pilot (restricted) areas.

Table 2.1
Types of models used in groundwater system (based on Questionnaire responses of the UN/ECE members)

Country	water balance	Quantitative aspects of unsaturated zone	water flow and chemical transport of saturated zone	impact of changes of the groundwater on the environment	setting up/optimizing monitoring networks	setting up groundwater protection zones	others
Austria	*	*	*		*	*	
Bulgaria	*	*	*	*		*	
Croatia	*		*				
Czech Republic	*		*				
Finlandia	*	*	*				
Germania-Bavaria	*	*		*		*	
Germania-Baden/Wittemb.	*	*	*	*	*	*	
Germania-Brandenburg	*					*	
Germania-Rheinland/Pfalz	*	*	*			*	
Germania-Schles./Holstein	*						
Hungary	*	*	*	*		*	*1
Latvia	*		*			*	*2
Lithuania							*3
Republic of Moldova	*	*	*	*		*	
The Netherlands	*	*	*	*	*	*	
Portugal	*		*			*	
Romania	*		*	*		*	
Slovak Republic	*	*	*	*		*	
Slovenia	*		*	*	*	*	
Spain	*	*	*	*	*	*	
Ukraine	*	*	*	*	*	*	*4

*1- MINTEQ for hydrochemical processes
*2- some of different analytical models
*3- MODFLOW, MODPATH in hydrogeological researches
*4- risk assessment; nature analogy

Setting up/optimising monitoring networks

In this part, only five UN/ECE member countries stated the use of mathematical models to optimise (or the set up of) monitoring networks. Some of them were only used in pilot studies (Austria, Slovenia).

Setting up groundwater protection zones

For this task, mathematical models simulating groundwater-flows to abstraction points and the migration of pollutants in groundwater are used in fifteen responding countries.

Overall

From the responses received, it may be concluded that mathematical models are tools, which are frequently used in studying groundwater systems in UN/ECE countries. In general, mathematical models are used to simulate (or to predict) the groundwater flow and in some cases the solute and/or heat transport. Only a few countries have used mathematical models to assess the import of the groundwater regime, changes in the environment and to set up (or optimise) monitoring networks.

3. Theoretical basis and nature for groundwater models

Groundwater is a subsurface element of the hydrosphere and is part of a dynamic system, which is referred to as the hydrological cycle. A groundwater system is an aggregate of rock in which water enters and moves and which is bounded by rock that does not allow any water movement and by zones of interaction with the earth's surface and with surface water systems (Domenico, 1972).

In such a system, the water may transport solutes and biota, and interaction of both water and dissolved constituents with the solid phase often occur. Especially, in relation with transboundary aspects, knowledge of these processes is indispensable. Due to the fact that borders between riparian countries do not necessarily fit with the natural boundaries of a given aquifer, groundwater may flow from one country to another. The application of groundwater modelling may be very useful to provide a picture of the flow systems, groundwater fluxes and groundwater quality aspects.

3.1 Changes of the natural groundwater regime under technogenic impact

3.1.1 Groundwater resources problems

Human activities have significant and diverse impacts on the groundwater hydrosphere resulting in negative changes in groundwater level and quality. The changes of transboundary groundwater levels occur, due to changes of discharge and recharge induced by water abstraction, melioration activities, excavation, preparation of land plots for construction works, as well as replenishment of groundwater resources from irrigation systems, hydro-engineering activities and accumulation and discharge of surface and artificial run-off.

Artificial changes in groundwater level can result in negative impacts. An increase in groundwater level causes land deterioration, secondary salinization of soils, landslides, undermining, depressions and development of diffuse karstic processes. A decrease in groundwater level can cause extreme land desiccation, plant death, drying up wells, cessation of spring floods, land subsidence, intensification of diffuse karstic processes and an overall decrease of groundwater resources.

Reliance on groundwater for the overall drinking water supply is increasing (Shniukov et al., 1993). For many countries, groundwater is the main source of drinking water supply (Belgium, Denmark, Switzerland, Italy, Germany, France, Hungary, The Slovak Republic, etc.). That is why one of the most important tasks of planning water balance changes is the environmental justification of groundwater abstraction.

To justify a scheme of water supply, it is necessary to design and estimate the maximum allowable changes of environment. Possible quantitative and qualitative changes of the hydrological cycle in the area of formation of groundwater resources were also affected by human activities.

Therefore the importance of long-term prognoses increases and implies the development of a strategy of optimal abstraction of groundwater resources which minimises environmental impacts and considers the interaction of water resource forming dynamic human and natural factors. Nevertheless, there is not enough attention to this issue, due to insufficient studies at experimental field plots and representative basins. Mathematical modelling may assist here.

When the changes of groundwater levels and water balance cannot be acceptable, measures for minimising impact consequences are developed. In these cases, groundwater models can provide a viable, if not the only, method to predict impacts and to identify aquifer protection zones.

Changed interaction between surface water and groundwater in transboundary systems might adversely effect both the groundwater flow and quality.

3.1.2 Groundwater quality

Groundwater quality problems are defined with respect to man and environment, and are related to groundwater uses. Groundwater quality may be threatened by pollution from diffuse and point sources and by undesired effects of seepage fluxes. Activities within the recharge areas at one side of the transboundary system might degrade groundwater quality on the other side of the border. Deterioration of groundwater quality usually results from:

- infiltration of pollutants released by industrial and agricultural enterprises, waste water, depositions, surface runoff, etc. Important sources of groundwater pollution are storage facilities for pesticides, oil and oil products, chemicals, etc.;
- disturbance of hydrodynamic balance, due to drinking water abstraction and raising the level of highly mineralised groundwater that may saturate the abstracted and adjacent groundwater layers, as well as intrusion of saline marine water, polluted river water and water from accumulating ponds of liquid wastes.

Changes of groundwater quality may occur, due to an increase of water mineral content (e.g. chlorides, sulphates, calcium, magnesium, iron, fluorides, etc.) as well as from compounds of anthropogenic origin (f.e. detergents, pesticides, oil, etc.), level of groundwater, temperature and pH, smell, colour, etc.

Possible functions/uses and problems of groundwater are given in Table 2 (Uil, 1998).

3.2 Mathematical modelling of groundwater flow and mass transport

Groundwater modelling begins with a conceptual understanding of the physical problem. The next step in modelling is translating the physical system into mathematical terms. In general, the results are the familiar groundwater flow equation and transport equations. An understanding of these equations and their associated boundary and initial conditions is necessary before a modelling problem can be formulated.

Table 2
Possible functions/uses, threats and problems

Possible functions/uses		Threats	Problems
Ecological function			
Water supply	-drinking water	-land use (diffuse pollution:	-desiccation
	-agriculture	agriculture,	-desertification
	-industry	(geo) infrastructure, industry,	-acidification
		urban areas)	-excess nutrients loads
		-airborne pollution	-salinization
		-abstraction	-pollution (organic,
Storage	-waste	-point/line pollution sources	heavy metals)
	-geothermal energy	-potential pollution sources	-spreading of pollutants
Transport	-soil remediation		-public health
	-confinement of		
	pollution	-landsubsidence	
Miscellaneous	-avoid landsubsidence	-foundation problems	
	-protection of		
	foundations	-overabstraction	

Basic processes that are considered include groundwater flow, solute transport and heat transport. Groundwater flow is a process that can be modelled with or without consideration of heat and/or solute transport. Modelled by itself, it has important applications in groundwater supply and design of engineering structures such as dams, mines and excavations that interact with the groundwater system. Both solute and heat transport require simultaneous solutions which result (e.g. velocities) from a groundwater flow model.

For the evaluation of the chemical quality of groundwater two types of models may be used:

- pollutant transformation- and degradation models, where the chemical and microbiological processes are calculated independently from the movement of the pollutants;
- solute transport models simulating the displacement of the pollutants, often include transformation- and degradation processes (see box below).

Most groundwater modelling studies are conducted using either deterministic models, based on precise description of cause-and-effect or input-response relationships or stochastic models reflecting the probabilistic nature of a groundwater system.

MASS BALANCE FOR SPECIES

[Rate of change of mass in control, volume per time unit]	=	[Rate of transport of mass into and out of control, volume per time unit]	±	[Rate of transformation of mass in control, volume per time unit]
		⇓		⇓
		TRANSPORT TERM		TRANSFORMATION TERM
		-inflows -outflows		-biological reaction -chemical reaction *dissolution/precipitation* *reduction/oxidation* *radioactive degradation* -physical change *adsorption/desorption* ion-exchange

⇓

Transport Term = Dispersive Flux + Advective Flux

3.2.1 Deterministic models

Deterministic models are based on fundamental notions of mathematical physics on hydrogeological processes with synonymously defined causes and their consequences. They consider the movement (in general cases unsteady and spatial) of groundwater with solutes in pores and fissures of geological formations. Movement (mass transport) of compounds is advective and diffusive (dispersive). Advection is the transport of compound on the macro level of compounds (f.e. water and salt transport within pore solutions). Diffusion implies the transport on a molecular level due to movement of micro particles. All compounds undergo the physical and chemical transformations, which occur permanently.

Close to the ground level, there is an aeration zone composed of unsaturated geological material, which is highly aerated and contains water vapours due to the proximity of above surface level conditions.

Under the aeration zone, in the saturated zone, the groundwater (layer) is situated. Deeper, there are groundwater layers with active water exchange and impacts of human activity that are the focus of study.

Any of the above groundwater regions can be affected by external forces. Volume (mass) and surface may classify the internal forces.

The volume forces are:

- gravitation resulting from the gravitation field of the earth;
- integrated forces of internal friction resulting from liquid viscosity and roughness of solids;
- resilient forces conserving the shape and volume of physical bodies;
- balancing forces that affects the individual compounds;
- chemostatic forces affecting the micro-particle interaction, i.e. dissolved salts and water in liquid porous solution.

The surface forces are the following:

- forces that affect the solution because of atmospheric pressure;
- menisci forces resulting from the boundary surface curving between liquid and solid bodies;
- sorption forces and surface tension between surfaces of different liquids;
- forces of biological nature, impacts from micro-organisms in plant roots, etc.

The external forces are responsible for the impact from the surrounding geological material, more exactly from solid, liquid and gaseous compounds. They occur at boundaries of the studied space or boundary conditions.

The natural boundary conditions, including hydraulic pressure, concentrations and flux are the first order boundary conditions. Conditions including the velocities and flows, among them velocity when a boundary is impermeable, are second order boundary conditions. Parameters that depend upon hydraulic forces, flows or concentrations are third order boundary conditions. These aspects are described in more detail in Chapter 4.

In a state of rest, the only forces that exist are the gravitation force in the saturated zone with clean free water and soft geological material, and external forces affecting the volume of geological material due to atmospheric pressure, geological material weight, and hydraulic pressure of above groundwater column. If the sum of all these forces is zero, the compounds are in the state of rest or steady movement.

This brief description on the status of solutes of geological material shows how complicated the geological processes are. However, studying the definite territories, in a majority of cases we deal with temporal and spatial effects of a certain set of natural or designed conditions. These allow the study to be conducted with accuracy, sufficient for the practical application of obtained results. Integrated equations of mass transport consisting of equations of mass balance, laws of movement and laws of unsteady thermodynamics are verified and presented in many publications (Cherny, 1963; Lukner and Shestakov, 1976, 1986; Ognianik et al., 1985; etc.).

Integrated equations of mass transport are based on assumptions of a representative elementary volume, such as:

- geometrical homogeneity and averaged properties of porous geological material;
- known forces affecting the liquid;
- known properties of liquid itself and velocities of its flow during the time periods, etc.

These assumptions allow us to perform the approximations of dissipation. The problem is to find out if the errors of these approximations will satisfy the practical objectives of mass transport. These problems can be solved through the laboratory- and field experiments and by using models that are more complicated. For example, in multi-layer aquifers it is possible to apply a transport model for each layer and transport through the slightly permeable layers. In some cases, the density convection has to be considered. This would require the simultaneous solution of tasks of mass transport and filtration and will depend upon the density distribution of liquid related to migrant concentrations.

In subsurface (soil and subsoil) zones, thermal diffusion may occur, due to significant fluctuations of temperature that will create mass transport due to a temperature gradient. In electric fields, the mass transport may occur under influence of gradient of electric voltage. The micro-organism diffusion may be accompanied by chemotaxic transport that is presented by movement of micro-organisms towards the plots with higher concentrations of essential components or nutrients. The specific features of transport of non-mixing liquids (such as oil and oil products) may require different approaches when simultaneous movement of non-mixing liquids, gas and water in saturated and unsaturated media should be considered.

In most cases, all enumerated cases of mass transport are of local importance and should be considered when their velocities are comparable with dispersion, convection, and mass transport. Besides, many of the above mentioned problems need special theoretical and experimental justifications.

3.2.2 Stochastic models

Stochastic models of hydrological processes may be classified as follows:

1. deterministic boundary tasks of filtration (mass transport) and, on the whole, probabilistic solution of the problem;

2. deterministic mathematical description of the process (differential equations and boundary conditions), probabilistic description of medium properties in the studied area with randomised and statistic distributions;
3. statistic boundary conditions (hydrological regime of boundary water bodies and watercourses, hydrophysical and hydrochemical conditions at the soil surface, etc.) providing that deterministic mathematical description of the process itself is within the area;
4. probabilistic and probability statistical models.

The first group of models may be computed by Monte-Carlo techniques.

The second and third group of models are typical for the majority of models for real fields of geofiltration. This is due to the exact value of their parameters within their probable variability that simulate, with a certain probability, the potential functions and velocities of mass transport. If data are available, the simulation models are applied; the influence of some parameters on the process is estimated and acceptable errors are established. They serve as a base for planning and implementation of explorations and experimental investigations for the creation of a model of appropriate probability.

The fourth group of models is known as "black box" and probability-statistical models. Sometimes, it is helpful to treat a pollution event as a "black box". With regard to the entrance and exit of pollution, the water layer is considered as the ‘black box. The mechanism inside the "black box" is unknown. The effect of the "black box" is examined by the incoming and outgoing functions of pollution. This method can be applied on a large scale, when pollution of the studied area is multi-component, but can be integrated in one image.

Application of probability and statistical methods do not establish functional relationships but rather correlation between fluctuation of potential function (level, migrant concentrations) and one or few factors of the regime.

These methods are applied when there are long term observation data for the subject of prognosis or subject analogy and the position of potential functions may be extrapolated. Usually, by this method, the average annual concentrations of migrants, water levels of the current year or number of following years, or certain date or period are calculated. The paired and multiple correlated relations, regression models and harmonic analysis are usually applied and they are well described in existing publications (Kisle, 1972; Zaltzberg, 1976; Devis, 1977, etc.).

The cybernetic method of mathematical modelling, namely the method of group assemblage of augments (Ivakhnenko, 1975), should be mentioned as well. This method is based on the principle of heuristic self-organisation. By this, principle mathematical models of optimal complexity correspond with the minimum of some criterion named the ‘selection criterion’. In some tasks, the criteria of regularity and non-displacement of models is used as selection criteria. For others, a criteria of variable balance is used.

The volume of complete application decreases with algorithms of multi-raw selection. The study of the subject will last until a complete list of observed variables is chosen (the medium of tasks solution) and the universal selection criterion are indicated for the model of optimal complexity. All available experimental data are divided into two sets, the so-called 'learning' and 'verifying' sequences. With these sets, the searching and assessment of a model of optimal complexity is verified.

The following five basic tasks should be solved:
1. choice of selection criteria;
2. choice of model medium or the list of possible variables, the so-called system of elements of given complex subjects;
3. choice of the basic function and its complexity;
4. calculation of coefficients of the basic function (task of adaption) of optimal complexity obtained from the solution of the third task;
5. prognoses and automatic management of subject. The equation laws, describing the studied process, are applied as basic functions.

If choosing a physical law for modelling is difficult, the other approach, the so-called induction, is applied. The structure of the model of optimal complexity is selected by testing many models (more often regressions) with corresponding selection criteria.

3.2.3 Modelling water and solute transport in the unsaturated soils

The importance of the unsaturated zone as an integral part of the hydrological cycle has long been understood. The zone plays an inextricable role in infiltration, soil water storage, evaporation, plant water extraction, groundwater recharge, runoff and soil erosion. The soil-water regime as a basic condition for plant growth depends on soil properties and can be quantitatively assessed by mathematical modelling. Recently, studies of the unsaturated zone are increasingly motivated by concerns about soil and groundwater pollution from industrial, municipal and agricultural sources (Van Genuchten, 1991). Experiments and field measurements are basic sources of data for studying such processes and mathematical model design and verification. However, for routine purposes measurements are expensive and time consuming. Therefore, mathematical models as tools for quantification of soil water and solute transport are preferred.

Soil is generally known to be a heterogeneous media and transport of water is performed through different types of pores, distributed in soil.

A variety of mathematical models are available to predict groundwater flows and solute transport between land surface and the groundwater table.

The most popular models continue to be the models based on the Richards´ equation for unsaturated, homogeneous soil. This deterministic description of water and solute movement in the unsaturated soil is based on the Darcy flux equation as well as on the continuity equation. Solute movement is characterised by the convection-dispersion equation, (Kutilek, Nielsen, 1992). Models based on Richards'-type equations can estimate root extraction patterns by a sink term, which is added to the basic equation. Initial conditions should be expressed as soil water content or soil water potential distribution in the soil profile at the beginning of the processes. Upper and lower boundary conditions are usually given by meteorological characteristic and by flux intensity and soil water potential courses, respectively (Van Dam et al., 1997; De Leeuw and Arnold, 1996).

Practically, all applied models are numerical, because the Richards´ equation is non-linear and cannot be solved analytically. This non-linearity is given by the non-linear dependence of unsaturated soil hydraulic conductivity as depending on soil water potential. The difference in soil hydraulic conductivities between relatively dry soil (wilting point) and saturated soil is usually several orders of magnitude. Recent progress in computer design allows the Richards´ equation to be easily and quickly solved as a part of a mathematical model.

The most advanced models of this kind are developed in a way to make their operation easy. This can be done by using a windows interface, as it is used in the models based on the HYDRUS series (Simunek et al., 1997).

During the last several years, the usefulness of the classical models (based on Richards' equation) for predicting actual field-scale water and solute transport is increasingly being questioned. Problems mainly caused by preferential flow through soil macropores should lead to the development of a new type of models, or to include preferential flow into classical models. Another group of problems includes: temporal and spatial variability in the soil hydraulic properties and non-equilibrium processes affecting chemical transport (Van Genuchten, 1994).

A number of different deterministic and stochastic models have been proposed to deal with field-scale heterogeneities, and in some cases these can be used for management purposes. The main problem is how to quantitatively describe preferential pathways - usually macropores - in such a way as to be able to include them into mathematical models. This problem remains unsolved until now. The core of the problem i.e. randomly distributed preferential ways and their spatial and time variability, leads to rather pessimistic conclusions relating to their quantification and modelling.

Many models with regularly distributed preferential pathways (cracks, root holes, integrated pores, etc.) have been presented (Van Genuchten, 1994, Slawinski et al., 1996), but macropores representation is far from reality. It seems to be more promising using relatively, big representative volumes of soils in which the influence of preferential ways on water and solute transport is implicitly involved (Novak, Simunek et al., 1997).

Soil heterogeneity at various spatial scales remains a frustrating problem when designing mathematical models of water and solutes in the unsaturated zone. Nevertheless, existing models as tools for quantification of water and solute transport processes are effective and they are used worldwide.

Mathematical models of water and solute transport in soil unsaturated zones are - as any other mathematical models – a simplified representation of reality. They describe quantitatively only some features of real processes. The main limitations of their use are the following:

- Models describe transport of water, heat and chemicals in homogeneous soils. Non-homogeneity of soils can be described in terms of well-defined boundaries between homogeneous areas or soil layers. Mathematical models can describe transport of liquids in vertically layered soils, but soil layers must be homogeneous themselves. Alternatively, models can describe vertical transport of water and chemicals in horizontally non-homogeneous soils, but elementary areas should be homogeneous and well defined.
- The role of plants in water, energy and solute transport is simplified in models. The plant canopy is characterised by a leaf area index, canopy height, canopy resistance and some other simple parameters. Therefore, models can describe some features of the quantitative role of plants in

the system, but not the mechanisms of the processes.
- There are problems related to soil characteristic assessment. Methods of estimation are time consuming and expensive. During the last decade, effort has been made to indirect methods of soil physical property estimation. So-called pedotransfer functions have been developed; herewith it is possible to estimate soil water characteristics through easily assessed soil characteristics.

3.3 Analytical and numerical approach

The governing equations for groundwater systems are usually solved either analytically or numerically. Analytical models contain analytical solution of the field equations, continuously in space and time. In numerical models, a discrete solution is obtained in both the space and time domains by using numerical approximations of the governing partial differential equation.

Various numerical solution techniques are used in groundwater models. They include Finite-Difference Methods, integral Finite-Difference Methods, Galerkin and variable Finite-Element Methods, Collation Methods, Boundary-Element Methods, Particle Mass Tracking Methods (e.g. Random Walk), and Methods of Characteristics.

Among the most used approaches in groundwater modelling, three techniques can be distinguished:
- the Finite Difference Method (FDM),
- the Finite Element Method (FEM) and
- the Analytical Element Method (AEM).

All techniques have their own advantages and disadvantages with respect to availability, costs, user friendliness, applicability, and required knowledge of the user, all of which may vary on both sides of a national border.

3.3.1 Aspects concerning the FDM, FEM and AEM techniques

The Finite Difference Method is based on quadrangular grids that apply over the vertical. The aquifer system is discretisised into a mesh of points termed 'nodes', forming rows, columns and layers (Figure 3.1). Conceptually, the nodes represent prisms of porous material, termed cells, in which the hydraulic properties are constant, so that any value associated with a node applies to or is distributed over the extent of a cell.

For defining the configuration of cells with respect to the location of nodes, two conventions exist: the 'block centred' and the 'point-centred' formulations. Both systems start by dividing the aquifer with two sets of parallel lines, which are perpendicular to each other (Figure 3.2). In the block-centred formulation, the blocks formed by the sets of parallel lines are the cells; the nodes are at the centre of the cells. In the point-centred formulation, the nodes are at the intersection points of the sets of parallel lines, and cells are drawn around the nodes with faces halfway between nodes. In both cases, spacing of nodes should be in such a way that the hydraulic properties of the system are, in fact, uniform over the extent of a cell.

Although MODFLOW can accept both formulations, only the block-centred formulation is included in the general version. The basic finite-difference equation for a three-dimensional groundwater flow with constant density follows from the application of the continuity equation per cell, i.e. the sum of all flows into and out of the cell must be equal to the rate of change in storage within the cell.

Figure 3.1
A discretised hypothetical aquifer system

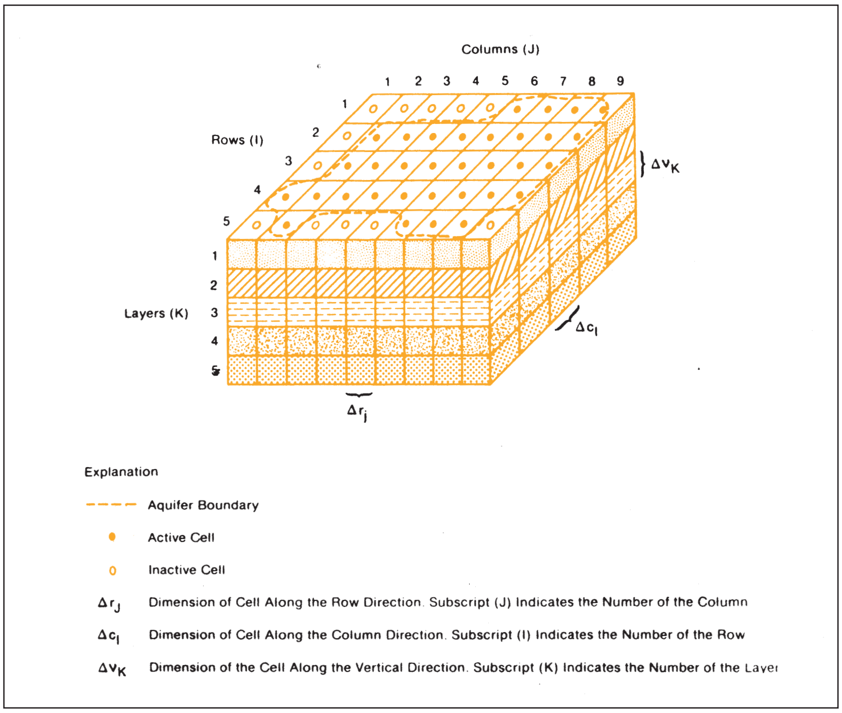
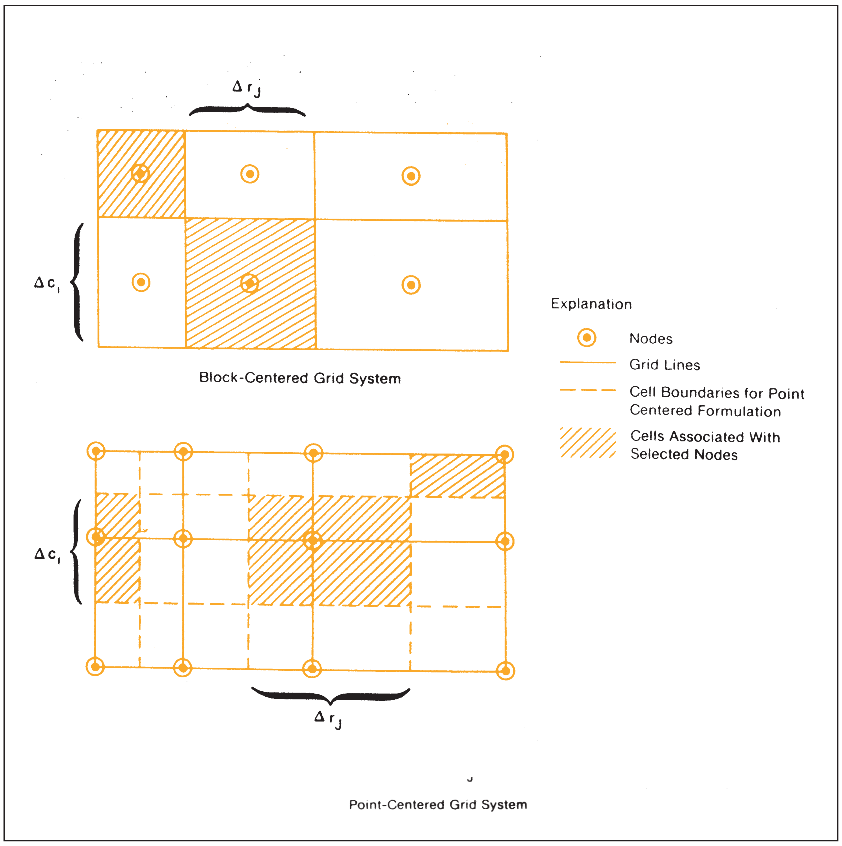


Figure 3.2
Grids showing the difference between block-centered and point-centered grids



The Finite Element Method is generally based on triangular grids but can also be based on quadrangular grids. The areas of the elements can vary by gradually changing the node spacing. In MICRO-FEM confined, semi-confined, phreatic, stratified and leaky multiple-aquifer systems can be simulated (Figure 3.3). (Hemker, 1997)

The finite element method solves the differential equation for semi-three-dimensional groundwater flow per element, using a minimisation of a certain error all over the model In general, finite element grids are more flexible than finite difference grids for simulation of special boundaries such as river courses. The major application aspects are not much different from that of finite difference methods.

The Analytical Element Method is based on analytic solutions of the differential equation describing groundwater flows (De Lange, 1991). A model is constructed by combining different types of analytic elements, which are based on the principle of superposition. Examples of analytic elements are the well, the line-sink, the area-sink and the inhomogeneity (Figure 3.4). Each type of analytic element can simulate different types of geohydrological features (abstraction wells, rivers, polders, infiltration areas, aquifer inhomogeneities, leakage layers between aquifers etc.). Actually, modelling with analytic elements is the modelling of geohydrological features rather than generating parameter values of elements in a mesh, like in FDM and FEM.

Analytical elements apply in infinite aquifers. Therefore, a model of analytic elements is not bounded as a model based on finite element or finite difference modelling techniques. The boundary of a model of an analytic element is actually a surrounding zone that also consists of analytic elements generating the effects of the outside world on the actual modelling domain (the domain of interest). Interchanging elements of the surrounding zone and those of the connected model carry out connection of models.

Each element is defined and can be changed individually. A model may consist of just a few elements in case only little is known of the subsoil. The more knowledge comes in, the more elements may be defined in the model. When dealing with large-scale models, the first step is to build a coarse model that approximates the main geohydrological features in the domain of interest. By doing this, attention can be paid as to how these main geohydrological features act upon the groundwater flow. In this step the surrounding zone may also be adapted, e.g. to model the leakage between aquifers using area-sinks (Figure 3.5). In the next steps, parts of the domain of interest can be refined while using this coarse model for the remaining area (Figure 3.6). This enables one to build a large model while diminishing the computation effort needed and to focus on a limited amount of modelling problems at one time. Eventually, the complete domain of interest can be covered in the refined way. After that, any part of the model can be refined, and the process can be repeated (also density problems like saltwater intrusion can be included).

Schematisation

The Finite Difference Method and the Finite Element Method are grid-based (quadrangular or triangular respectively). Because of the shape of the elements, the FDM with quadrangles has less flexibility in schematisation than FEM with triangles. The Analytic Element Method is the most flexible with respect to schematisation. Any form or size of the element is possible relating to the area of interest.

Figure 3.3
Examples of finite element grid generation (meandering ribvers and sheet piling or excavations) (Hemker, 1997)

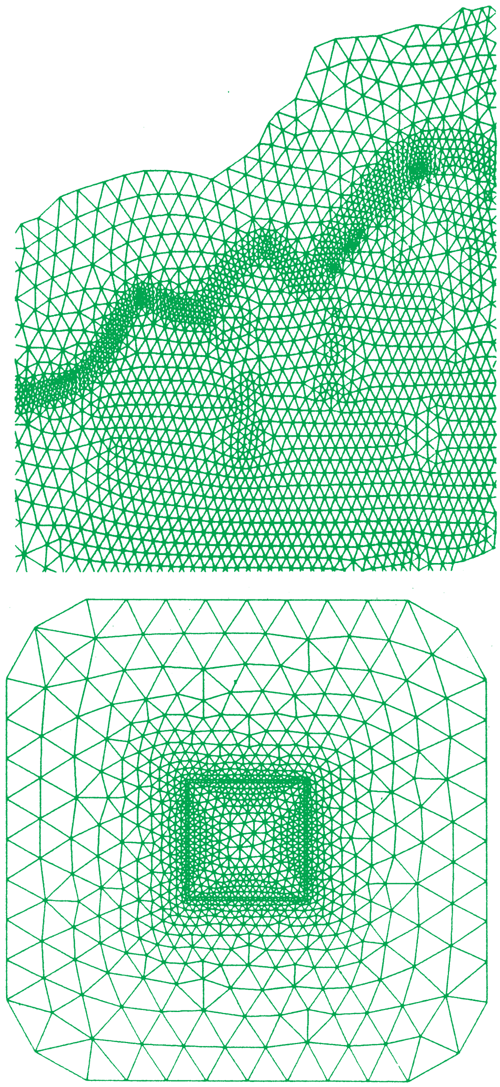
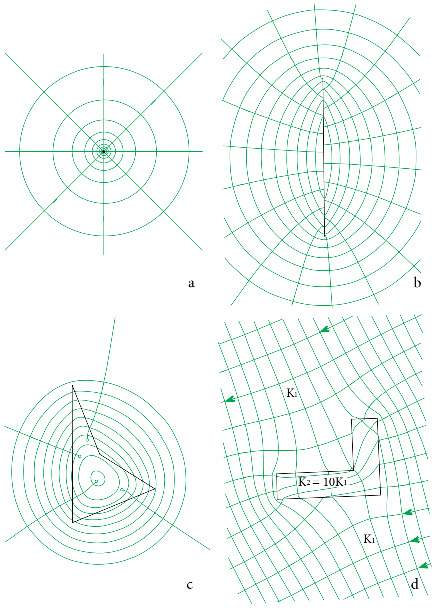


Figure 3.4
Examples of analytic elements:
a) well, b) line-sink, c) area-sink
d) inhomogeneity



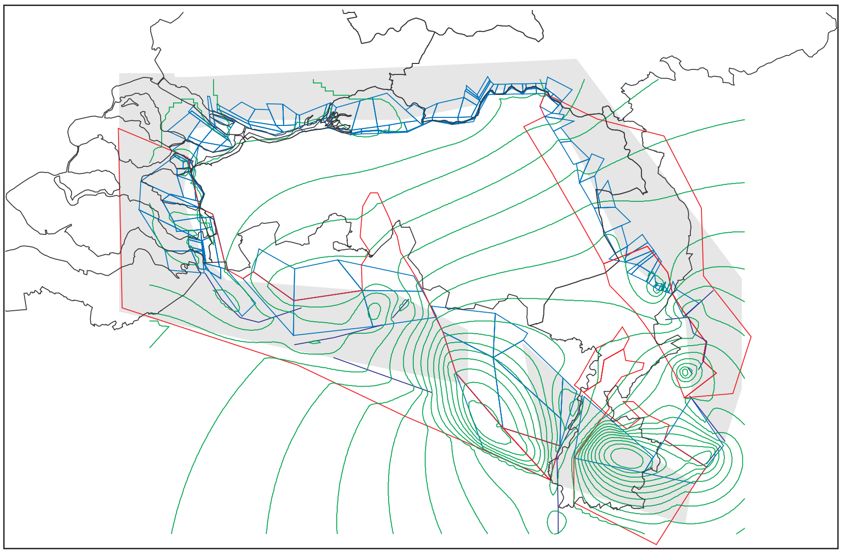
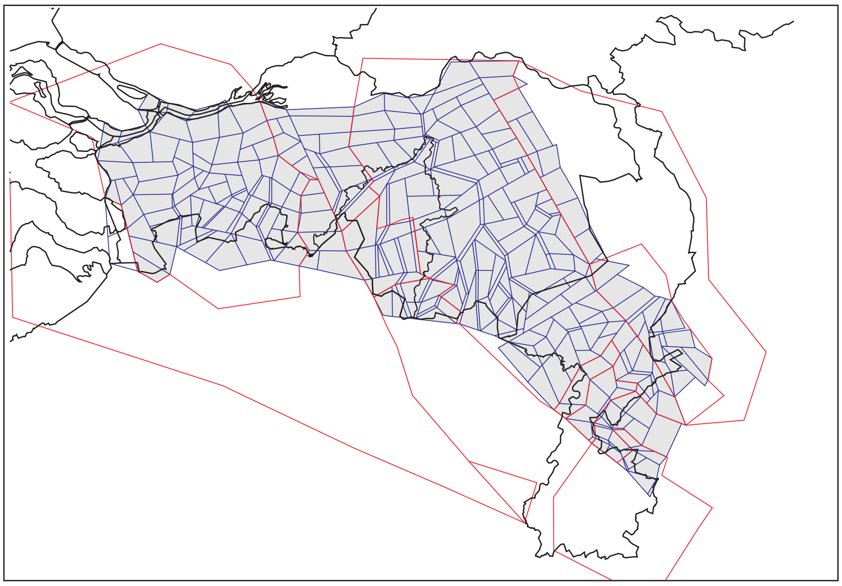


Figure 3.5
Surrounding zone of the supra regional NAGROM submodel of (the province of) Brabant, The Netherlands



.
Figure 3.6
Partly refined model of the supra-regional NAGROM submodel of (the province of) Brabant, The Netherlands

Accuracy

With respect to accuracy, it can be said that the AEM exactly calculates the water balance, i.e. the hydraulic head coincides with the flow pattern. For the FDM and FEM where this is not always the case, the accuracy largely depends on the iteration criteria. With the use of post processors, this problem can be corrected.

Data (input and output)

When using the Finite Difference Method or the Finite Element Method, many data are needed because all cells need to be filled. With the help of modern GIS-based pre-processors, this problem can be solved easily. Input data for aquifers are common values such as transmissivities, aquitard resistances, abstraction rates, groundwater recharges, surface water levels, etc. The most common output data are groundwater levels,

Note:
Figures 3.5 and 3.6 are examples of NAGROM, a NAtional GROundwater Model, based on the analytic element method. NAGROM is developed as one of the instruments for integrated water management in The Netherlands.

fluxes, velocities and changes in these parameters due to stress put into the model.

For the Analytical Element Method, input data are not different from the other techniques when using wells, area-sinks or inhomogeneity polygons. When using some other types of elements, such as line-elements e.g. for sheet-pile walls, or when modelling anisotropy, less common parameters such as the resistance to flow (sheet-pile wall, anisotropy), total discharge or a head distribution along the line (seepage faces) need to be specified. Output of this method is similar to that of the other methods, except that at any inside elements the head and flux distribution is also fully determined by analytical functions.

Graphical User Interfaces (GUI) and Geographical Information Systems (GIS)

When using these types of models a GUI or GIS is a good and often indispensable tool in elaborating the generally large quantity of input and output data and in presenting the results. This is especially true in case of FDM and FEM, where the parameter allocation for a large number of nodal points or cells is practically impossible in a traditional way (through filling input files manually).

Availability and applicability

The Finite Difference Method (FDM) and the Finite Element Method (FEM) are both examples of the grid-based modelling technique. A well-known and frequently used application of the Finite Difference Method is the MODFLOW-model (MODular three-dimensional finite-difference groundwater FLOW model, McDonald and Harbaugh, 1984). MICRO-FEM (Finite-Element Computer Program for Multiple-Aquifer Steady-State and Transient Groundwater Flow Modelling, Hemker, 1997) is an example of the Finite Element Method. An example of the Analytical Element Method is MLAEM (Multi-Layer Analytic Element Model).

Both MODFLOW and MICROFEM are well documented and rather cheap (US$ 1000). The price of MLAEM varies with the complexity of the model (US $750 - US$12,000). Both MODFLOW and MICRO-FEM consist of a user-friendly set of programs for the different stages (pre-processing, calculation, post-processing, graphical interpretation and plotting. Depending on all the program module needs, the price can increase to $1500 – 2000 $). MLAEM is also embedded in a Graphical User Interface and may by used in combination with all kinds of generally available pre- and post-processing software, such as Surfer, Arc-Info, Arc-View, Excel etc.

3.4 Optimal location of the groundwater monitoring network

A practical strategy should be able to determine where and how often sampling is needed taking into account the cost of such a task. Several methodologies for monitoring network design and sampling optimisation are reported in literature (ASCE Task Committee, 1990; Andricevic and Foula-Georgiou, 1991; Storck et al. 1995; and Passarella, 1997, etc.).

In the Ukraine for example, the concept of **P**ermanently **O**perating **H**ydrological **M**odels (POHM) for large territories has been developed by the Institute of Geological Sciences of National Academy of Sciences of Ukraine to meet the needs for optimisation of monitoring networks. According to their scientific findings, transboundary territories may be classified according to the type of groundwaters (recharge, transportation and discharge aquifer vulnerability, existing hydrodynamic and hydrochemical conditions). This allows to identify the most intensive relationships of groundwater for two neighbouring territories and possible pollutant migration towards one or other direction. POHM's are created to control and to forecast the water regime in such territories and to develop the preventive managerial measures to avoid the adverse impacts from human activities.

The field hydrological studies and planning of regime control measurements by creating a preliminary model based on the available hydrogeological information are necessary steps in the creation of the POHMs.

The monitoring network of the groundwater regime, planned with a preliminary model and optimised by POHM, is in reality the optimal groundwater monitoring network. POHM's were created for some territories in the Ukraine, which are characterised by an active regime of groundwaters, namely, the Lower Dniepro left bank and the Crimea plains. The specific feature of these models is the active interaction of sea and groundwaters that, to some extent, match the transboundary aspects.

Loaiciga (1989) couples geostatistics with statistical parameter estimation and field information with the models. Minimisation of the statistical parameter estimation (variance) is not necessarily a realistic ultimate goal in sampling design, as desirable as it would be. Christacos and Killiam (1993) optimise certain objective functions emerging from the physical regulatory and monetary considerations of site specific clean up processes. James and Gorelick (1994) find the optimal number and the best location for a sequence of observation wells that minimise the expected costs. The criterion of the optimisation solution are usually either a comparison of model and nature functions with permissible errors or a minimisation of expenditures for abstraction, including modelling and remediation of groundwaters.

Bogardi et al. (1983) combined geostatistic and multi-criteria approaches to design the basic monitoring network with spatially correlated and anisotropic variables. The methodology also is applicable when existing monitoring networks should be improved. These approaches consider mapping costs, priority of different variables, different geostatistic properties of variables, assessment of accuracy or error of criteria for different variables.

The problem of where to place monitoring wells is also compounded by the uncertainty that is characteristic for groundwater problems. The main sources of uncertainty which influence the design of a monitoring well network are the hydrogeological uncertainty associated with groundwater flow and contaminant transport and the uncertainty about the exact location of the contaminant sources. In many cases, the objectives typically considered when determining the performance of a monitoring well network are conflicting. These objectives are usually as follows:
- to minimise the number of monitoring wells in the network;
- to maximise the probability of the well network detecting a contaminant and
- to minimise the extent of contamination after the first detection by the well network.

The conflicting nature of these matters precludes the existence of one optimal solution and forces the water manager to consider a number of non-inferior networks (Storck et al., 1985). To cope with these aspects, groundwater flow models, including solute and/or heat transport models are usually combined with an optimisation model.

3.5 Scales and dimensionality

The definition of spatial and temporal scales is one of the important aspects in the application of models. Among others, the selection of scales depends on the nature of the system modelled, and the chosen solution techniques.

Spatial scales in transboundary aquifers range from several meters to hundreds of kilometres for the assessment and management of regional groundwater systems. In general, human-induced influences on groundwater systems affect local and intermediate scales, while large, regional scale phenomena are of natural origin. Some human-induced changes are also on a regional scale, such as for example irrigation groundwater withdrawal, application of fertilisers and pesticides, acidification of groundwaters and urbanisation impacts.

Temporal scales are also important for groundwater modelling. Two major categories may be distinguished for temporal scales. They are:
- steady state or average state and
- time varying or transient state.

Periodic fluctuations on a diurnal or seasonal scale are frequent in hydrogeology. Some processes exhibit a strong temporal effect immediately after their initiation but become stable after a while, moving to a steady state. The steady state is also assumed when the analysis period is so short that temporal effects are not noticeable.

Local simulations such as chemical spills have short-term effects for weeks or months. Mid-term scales can be related to agricultural use, de-watering of mining sites and local pollution problems. Long-term effects are relevant in regional water resource developments, hazardous waste displacement and regional non-point pollution by highly toxic, non-degradable chemicals and radionuclides. Generally, temporal scales are directly dependent on the extent of polluted areas, geology, hydrological and biogeochemical processes. Dimensions in the time domain range from hundreds or thousands of years in risk analysis for long-term isolation of radioactive waste, to seasonal, monthly, weekly, daily and hourly scales for field systems.

In terms of spatial orientation, models may be capable of simulating systems in one, two, or three dimensions (from local to regional aquifers). Another distinction for models is the way of handling parameters, i.e. whether the parameter distribution is lumped or distributed. Lumped parameter models assume that a system may be defined with a single value for the primary system variables. In distributed-parameter models, the system variables reflect detailed understanding of the physical relationships in the system.

4. Input data for groundwater models

The input data for a groundwater model include natural and artificial stress and parameters as well as the dimensions and physico-chemical properties of all aquifers considered in the model. It must be kept in mind that a finer level of detail of the numerical approximation (solution) greatly increases the data requirements. Some data requirements for groundwater modelling are presented in sections below.

4.1 Data for modelling the saturated zone

Three-dimensional or quasi three-dimensional models including only the saturated zone are acceptable for the calculation of piezometric heads if the recharge and the discharge at the groundwater level can be determined as independent parameters or by a given -not necessarily linear- function of the calculated head.

Geometric characteristics

Data needed include:

- topography (digitised contour lines map);
- surface of separated layers (digitised contour lines map) (hydrogeologic cross-sections, if a three-dimensional interpolator is available for the determination of the above surfaces);
- rivers, channels, drains, lakes, reservoirs (digitised map).

Hydrogeologic characteristics

Data are needed for each model-layer. Two modelling approaches for defining layers are:
(1) model-layers are fit to the real hydrogeological strata or
(2) model layers are the results of the vertical discretisation of the modelled space considering only geometric aspects; this approach is rare.
For each layer data are needed on the boundary of homogeneous sub-areas (preferably in digitised maps) and the following parameters for each homogeneous block:

- horizontal hydraulic conductivity;
- horizontal and vertical anisotropy (in case of a three-dimensional approach);
- horizontal anisotropy of the aquifer and leakage coefficient or resistance of the aquitard (in case of a quasi three-dimensional, multilayer approach);
- storage coefficient (transient problem in confined system);
- specific yield (transient problem in unconfined system);
- density vs. temperature function;
- viscosity vs. temperature function.

Note:
Determination of model-layers and allocation of hydraulic parameters can be efficiently assisted by sophisticated three-dimensional graphical tools, destined for the set-up of the three-dimensional hydrogeological structure of modelled space, based on data from boreholes and/or hydrogeological cross-sections).

Data on boundary and initial conditions

- at given head boundaries: time series of the measured groundwater heads (averages in case of steady state problems). Linear approximation is accepted for points in between;
- at given flux boundaries: time series of the fluxes (averages in case of steady state problems);
- initial groundwater levels for each model layer (digitised contour lines map).

Data on surface waters

For each homogeneous section (characterised by the same geometric and hydraulic parameters), the following are needed:

- width of the river bed;
- elevation of river bottom at the beginning of each section and at the end of the last section;
- leakage coefficient or resistance of the river bed;
- surface water levels (continuously or at least at the beginning of each layer and at the end of the last homogeneous section) for the period to be modelled; averages can be used in case of steady state problems and time series in case of transient problems;
- discharge at the starting section and the roughness-coefficient of the river bed for each homogeneous river section (if - according to the conceptual model - the surface water level is influenced by the flux at the river bottom and the surface water level is calculated in "real-time" as a function of the discharge and the flux through the river bottom).

Data on subsurface drains

For each homogeneous section:

- elevation of the top and the bottom of the drains at the beginning of each section and at the end of the last homogeneous section;
- conductance of the drains (quotient of the conductivity and the resistance of the filter).

Open drains are handled as surface waters. In case of a dense open drainage-system, lumping of canals by irrigated conductance is also possible.

Recharge/discharge

Boundaries of homogeneous areas (homogeneity can be defined by precipitation, irrigation, potential evapotranspiration, land use, vegetation, and/or soil type from the surface to the groundwater level, and should be indicated on a digitised map, preferably under GIS) and the following parameters for each homogeneous area are the:

- long-term average of the recharge in areas where the groundwater level is so deep that there is no evapotranspiration from groundwater;
- recharge/discharge characteristic function i.e. parameters of the function describing the long term average flux at the groundwater level as a function of the average groundwater level (in case of steady-state problems);
- time series of the flux at the groundwater level for the investigated period (in case of transient problem).

Groundwater abstraction or injection

- location of abstraction or injection point;
- elevation or depth of screens, or at least the identification and depths of the exploited aquifer;
- rate of pumping or injection (time series in case of transient problems).

Observed data

- location of observation points (co-ordinates and elevation of the surface level);
- elevation or depth of the screen;
- piezometric levels;
- water quality data (useful for the calibration of the flow model).

Remarks on the data requirements for modelling the saturated zone

Maps should be in the same co-ordinate system and the co-ordinates of any specified locations as well.

Usually, the lack of direct knowledge of parameters can be replaced by indirect information on the characteristics of the system:

- hydraulic parameters can be replaced by the types of media grain size distribution curves, or results of pumping tests;
- instead of roughness-coefficient or resistance of river bed, information on the state of the river bed is also very useful;
- conductance of drains can be replaced also by technical data of the construction;
- parameters of the recharge/discharge characteristic curve can be estimated by direct parameter estimation based on precipitation (irrigation), potential evapotranspiration, land use, vegetation and soil profile information, or by calibration, or by separate unsaturated flow modelling (the data requirement for the modelling of unsaturated zones will be discussed in the next chapter);
- in case of large numbers of surface waters, integrated conductance (integral of the quotient of a wetted river bed surface and river bed resistance) and an average surface water level can replace them.

4.2 Data for modelling the unsaturated zone

In case of a steady-state problem, the recharge/discharge characteristic curve can be determined for a given "soil column-vegetation-meteorological situation" complex by one-dimensional unsaturated model with a series of different "fixed head" lower boundary conditions representing different average groundwater levels.

In case of a transient problem, if the head-dependent function of the flux at the groundwater levels is not known or the soil moisture content is also to be modelled, the unsaturated model must be coupled with the saturated model.

Geometric characteristics

- depths of different soil types between the ground surface and the expected lowest groundwater level;
- soil types of each layer.

Soil-physics and seepage parameters

For each separate soil layer:

- hydraulic conductivity of the saturated soil;
- porosity;
- residual water content;
- parameters of pF-curve (in case of van Genuchten's formula, two parameters are needed);
- parameters of the relationship between unsaturated hydraulic conductivity and suction (water content) (in case of Van Genuchten's formula + one parameter).

Meteorological characteristics and data on boundary and initial conditions

- time-series of potential evapotranspiration (or the sum of the potential and actual evapotranspiration if the Morton's complementary concept is applied);
- time-series of the infiltration at the ground surface (precipitation-interception-surface runoff-evaporation from temporarily stored water at the ground surface);
- time series of given potential at the ground surface;
- given head boundary conditions at the bottom of the soil column: time series of the ground water level;
- given flux boundary conditions at the bottom of the soil column: time series of the deep percolation;
- initial water content (or suction).

Data on vegetation

- time series of the interception capacity
- vertical distribution of the root zone (and its changes in time if relevant)
- parameters of the stress-function describing the decrease of the actual evapotranspiration as a function of the decreasing soil moisture (in case of Van Genuchten function, this requires 2 parameters).

Observed data

For soil type or soil profile:

- hydraulic conductivity and pF-curve, measured in laboratory;
- in situ soil moisture time series;
- time series of shallow groundwater levels.

Remarks on the data requirements for modelling of the unsaturated zone

Soil-physics parameters, seepage parameters and parameters of the pF-curve and the unsaturated hydraulic conductivity function can be estimated according to the soil types, based on parameters of similar soils.

4.3 Data for modelling water quality

Additional data necessary for flow modelling are described in the paragraphs below.

Soil-physics parameters

- bulk density of the solid phase

Transport parameters

- molecular diffusion coefficient;
- longitudinal and transversal dispersivity;
- type and parameters of the sorption isotherm.

Transformation parameters

For each chemical component:

- parameters of zero and first order degradation in the liquid phase;
- parameters of zero and first order degradation in the adsorbed phase;
- types and thermodynamic parameters of the (bio)chemical processes to be considered.

Boundary and initial conditions

For each chemical component:

- type and location of the pollution source;
- in case of given flux boundary conditions: time series of the rate of pollution;
- in case of given concentration boundary conditions: time series of the concentration;
- at flow boundaries: concentration (time series) of the inflow to the model area (including surface water quality);
- initial conditions: spatial distribution of the concentration (in contour line map).

Observed data

- location of the observation well;
- time series of measured concentrations;
- parameters of sorption isotherms measured in the laboratory;
- parameters of biochemical processes measured in the laboratory.

Remarks on the data requirements for modelling water quality

Exact knowledge of parameters of the transport and chemical processes can be replaced by sensitivity analyses, considering the possible range of the given parameters.

4.4 Other data requirements

- economic and logistic information of water supply;
- legal and administrative rules;
- environmental factors;
- planned changes in water management.

4.5 Use of data bases and geographical information systems in groundwater modelling

Considering the large variability and the quick development of groundwater models a new, more sophisticated model can often replace a previously applied model. Additionally, the reconsideration of the conceptual model and the regeneration of the mesh may need a new allocation of the parameters. Therefore, it is important that model data (information) are stored independently from a given model, with a preference for GIS-based databases. Considerable development in the field of user-friendly GIS and data base servers makes the set-up and the modification of models easier and more time-effective.

In vector based geographical information systems, data can be stored in the form of:

- points (data of wells, characteristics of point-source pollution, data from observation sites, digitised maps, etc.);
- lines (location of rivers, conduits);
- polygons (boundaries of homogeneous areas from a soil type, land use, hydrological and hydrogeological point of view).

The parameters in the models can also be classified in three groups:

- parameters related to a specific location (water abstraction or source/sinks terms);
- parameters related to lines (water levels of rivers, width, depth, resistance of the river bed, source of pollution from water courses or from conduits);

- spatially distributed parameters (ground surface, surface of geological features, hydrological and hydrogeological parameters like precipitation, evapotranspiration, groundwater levels or hydraulic conductivity, storage coefficients, concentration of chemicals, etc…).

In numerical models, the space is discretised by nodal points or by homogeneous cells. In general, the allocation of the parameters means the determination of the corresponding value for selected nodal points or cells (specified by their co-ordinates) based on the available information. If the point-form parameter is given by point-form data, the task is simple: to find the closest nodal point. Parameters corresponding with a line can be constant or changing along the line. In the first case, the problem can be solved by finding the closest nodal points near the line and allocating the constant value. In the second case, available data are usually stored in point-form information and an interpolator is needed to automatically determine the value of the parameter for inner nodal points.

In case of spatially distributed parameters, maps of homogeneous areas (polygons), point-form observations, and digitised maps (many point-form data) are usually the basis of the parameter allocation. If the parameters change by homogeneous sub-areas (for example soil parameters and hydraulic conductivity are in this group), nodal points located inside the polygons must be selected or a spatial average must be calculated for cells. In case of parameters of continuous functions of space, a two- or three-dimensional interpolator is necessary.

In case of new software, simple programming of a new interface between stored data and software input files usually needs to be carried out. Recently developed software packages (GMS, TRIWACO for Windows, FEFLOW, etc.) already have direct connection to GIS and databases.

Time series stored in databases allow the modeller to easily determine the following parameters, according to the conceptual model:
- the averages of a selected period;
- approximation of the time series by stress periods with constant values;
- approximation of the time series by stress periods with linear changes.

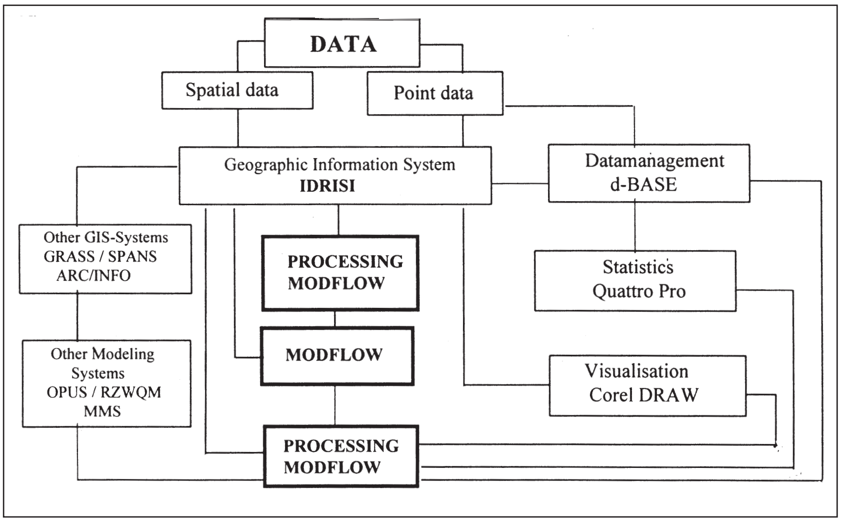


Figure 4.1
Scheme of the data flow and the linkage between GIS, model and the geohydrological database
(Flügel and Michl, 1996)

Databases and GIS are also very helpful during the evaluation of flow systems by comparative analysis of the available maps on hydrological and hydrogeological information and any other information like soils, vegetation and land use etc. This technique can considerably improve the reliability of the conceptual model. As an example of the linkage between different software tools, the schematic presentation (Figure 4.1) from the case study in the area near Bonn, Germany is used (Flügel and Michl, 1996).

4.6 The role of a QA/QC system

Quality assurance (QA) in groundwater modelling is a very important component and should be applied to all phases of the modelling process. Taylor (1985) has defined the role of QA in groundwater modelling as the procedural and operational framework put in place by the organisation managing the modelling study, to assure technically and scientifically adequate execution of all project tasks included in the study and to assure that all modelling based analysis is verifiable and defensible.

A major element of QA is Quality Control (QC) which refers to the procedures that ensure the quality of the final products. These procedures include the use of appropriate methodology, adequate validation and proper usage of the selected methods and models.

QA in model application studies should consist of using appropriate data, data analysis procedures, modelling methodology and technology, administrative procedures, and auditing. It should address such issues as (Van der Heijde, 1988):
- formulation of information needs;
- study description and objectives;
- modelling approach;
- conceptualisation of system and processes, including hydrogeological framework, boundary conditions, stresses and controls;
- detailed description of assumptions and simplifications;
- data acquisition and interpretation;
- protocols for parameter estimation and model calibration;
- the role of sensitivity analysis;
- presentation and documentation of results and answers;
- evaluation of how closely the modelling results address the questions raised by management.

QA for model application should include a complete record, keeping track of each step of the modelling process.

5. Key points

Successful utilisation of mathematical modelling is only possible if the methodology is properly integrated with data collection, data processing, and other techniques and approaches for evaluation of transboundary groundwater system characteristics.

Mathematical models can also be used in gathering the first information and as useful tools for understanding the mechanisms of transboundary groundwater systems. Furthermore, models can assist in:
- screening alternative policies;
- optimising engineering designs (including monitoring network);
- assessing operative actions in order to determine their impacts on groundwater systems and also on the risk of these actions to human health and the environment.

There are benefits from using mathematical models for the optimal setting up of groundwater monitoring and assessment to avoid mistakes and oversights during the routine monitoring program.

Regarding the connection of monitoring and modelling for transboundary groundwater systems, the following conclusions and recommendations can be made:

1. The efficient integrated modelling of transboundary areas should be preceded by a large scale regional groundwater flow analysis. In this stage of the work, emphasis is given to the analysis of the available information and to the establishment of the conceptual (or identification) model. This task requires a rather simplified modelling approach with the focus on the regional scale and should be carried out in close co-operation with the involved countries.

   Models described in Chapter 3 and in Annex 2 should be considered as examples. Other models satisfying the requirements for this modelling phase can also be used. Selection of the model is the first common task of the project. During the selection, the following recommendations should be considered:
   - well defined, well documented and validated models should be applied;
   - the analytical element approach seems to be suitable for this regional scale work (flexibility in schematisation and conceptualisation), but it is rather new and until now, there is not so much experience with this type of modelling. Models based on FDM and FEM are already frequently used in many countries and are widely accepted. Several types of software, consisting of well documented, user-friendly programs are available on the market. With respect to user-friendliness, the degree of difficulty and the cost aspects, the Finite Difference and Finite Element models are probably most advantageous.

2. Using the commonly established calibrated regional model, a preliminary analysis can be made to check the quantitative and qualitative impact of the existing and planned activities on the

transboundary groundwater system. Those activities, which can influence the groundwater in the neighbouring country, are of special interest.

3. In the next phase, the regional model should be refined in the sub-areas of special interest and areas where (additional) necessary information is available. The monitoring network should be designed, based on this more detailed model. This work can be carried out in co-operation with or by individual countries. The essential thing is that the concept of the regional model must be accepted.

   The regular evaluation of the quantitative and qualitative characteristics provided by the monitoring network can lead to the modification of the model. The data of the transboundary monitoring network must be available to all countries involved.

   In case of separate modelling activities by the countries involved, they can independently decide on the applied model (software). It should be emphasised that when modelling a transboundary area, the standardisation of data and data accessibility (including interfaces to databases and to GIS) is equally (or more) important than the standardisation of the software. If the conceptual model and the basic data are reliable, the results should be comparable even if the applied software is not the same.

   In this type of co-operation, regular exchange of information is necessary to ensure the homogeneity of the modelling concept. This can be done during regular meetings used for the common evaluation of the situation and for the preparation of decisions.

6. References

- Andrevic, R., Foula-Georgiu, E., 1991. A Transfer Function Approach to Sampling Network Design for Groundwater Contamination. Water Resources Research., 27 (10), pages 2759-2769.

- ASCE Task Committee on Geostatical Techniques in Geohydrology of the Groundwater Hydrology 1990. Review of Geostatics in Geohydrology. II: J. of Hydraulic Engineering. v. 116 (5). pages 633-658.

- Berkowitz, B., 1993. Groundwater Modelling. WMO/TD-No. 540, Technical reports in hydrology and water resources No. 38. WMO, Geneva, Switzerland.

- Bogardi, S., Bardossy, Douckstain, L., 1985. Multi-criteria on network design using geostatistics. Water Resources Research, 2, pages 199-208.

- Cherny, I.A., 1963. Groundwater hydrology. Gostoptechizdat, page 396 (in Russian).

- Christakos, G., Killam, B. R., 1993. Sampling Design for Classifying Contaminant Level Using Annealing Search Algorithms. Water Resources Research, 29 (12), pages 4063-4076.

- Dam, J.C. et al., 1997. Theory of SWAP version 2.0. Simulation of water flow, solute transport and plant growth in the Soil-Water-Atmosphere-Plant environment. Department Water Resources, Wageningen Agricultural University (Report 71). DLO Winand Staring Centre, Wageningen (Technical Document 45). The Netherlands.

- Devis, D., 1977. Statistic and analysis of geological data. Mir, 1977, page 572 (in Russian).

- Domenico, P., 1972. Concepts and Models in Groundwater Hydrology. McGrawhill, New York,

- Flügel, W.A., Michl, C., 1996. Using MODFLOW/MODPATH combined with GIS analysis for groundwater modelling in the alluvial aquifer. In: Models for assessing and monitoring groundwater quality. IAHS publication No. 227.

- Frid, Z., 1981. Pollution of Groundwater. Nedra, 1981, page 304 (in Russian).

- Genuchten, M.Th. van, 1991. Recent progress in modelling water flow and chemical transport in the unsaturated zone. In: Hydrological interaction between atmosphere, soil and vegetation. IAHS Press. Inst. Of Hydrology, Wallingford, IAHS Publication No. 204, pages 169-183.

- Genuchten, M.Th. van, 1994. New issues and challenges in soil physics research. Trans. 15th World Congr. of Soil Sciences, Acapulco, Mexico, vol.1: Inaugural and state of art conference, 5-27.

- Heijde, P.K.M. van der, El-Kadi, A.I., Wiliams S.A.,1988. Groundwater Modelling: An Overview and Status Report, CR-812603, GWS, Indianopolis, Indiana 42208, USA

- Hemker, 1997. Finite-Element Computer Program for Multiple-Aquifer Steady-State and Transient Groundwater Flow Modelling. Amsterdam, The Netherlands.

- Hudák, P.P., Loaiciga, H.A., 1993. An optimatisation method for network design in multi-layered groundwater flows systems. Water Resources Research 8, pages 2835-2845.

- Ivakhnenko, A.G., 1975. Longtime prediction and proceedings of complex systems. Technika, page. 312 (in Russian).

- James, B.R., Gorelick, S.M., 1994. When enough is enough: The worth of monitoring data in aquifer remediation design. Water Resources Research 12, pages 3499-3513.

- Kajol, C., 1972. Analysis of time series and hydrological data. Gidrometeoizdat, page 138 (in Russian).

- Knopman, D.S., Voss, C.T., 1989. Multi-objective sampling design for parameter estimation and model discrimination in groundwater solute transport. Water Resources Research 10, pages 2245-2258.

- Konoplancev, A.A., Semionov, S.M., 1979. Investigation, prediction and mapping of groundwater regime. Nedra, page 192 (in Russian).

- Kovalevski, V.S., 1974. Fundamentals of prediction natural regime of the groundwater table . Strojizdat, page 204 (in Russian).

- Kutilek, M., Nielsen, D.R., 1994. Soil hydrology. Cremlingen-Destedt, Catena Verlag.

- Lange, W.J. de, 1991. A groundwater model of The Netherlands. National Institute for Inland Water Management and Waste Water Treatment (RIZA), Note nr. 90.066. The Netherlands.

- Leeuw, A.M. de, Arnold, G.E., 1996. Sustainable use of water with the aid of MOZART. In: Proceedings Workshop on crop-water-environment models. Sustainabilty of irrigated agriculture. 16th International congress on irrigation and drainage. Caïro, Egypt, September 1996.

- Loaiciga, H. A., 1989. An Optimisation Approach for Groundwater Quality Monitoring Network Design. Water Resources Research 25 (8), pages 1771-1782.

- Lukner, L., 1986. Modelling of groundwater migration. Nedra, 1986, page 208 (in Russian).

- Mercer, J.W., Faust. R.C.,1980. Groundwater Modelling: An Overview. Groundwater 18, 2, pages 108-115.

- McDonald, M.G., Harbaugh, W., 1984. MODular three-dimensional finite-difference groundwater FLOW model. U.S. Department of the Interior, U.S. Geological Survey, National Center. Reston, Virginia.

- McKinney, D.C., Loucks, D.P., 1992. Network design for prediction groundwater contamination. Water Resources Research 1, pages 133-147.

- Mayer, P.D., Brill, E.D., 1988. A method for location wells in a groundwater monitoring network under conditions of uncertainty. Water Resources Research 8, pages 1277-1282.

- Novak, V., Simunek, J., 1997. Mathematical submodel of the infiltration of water into cracked soil. In: Proceedings 5th Poster Day Transport of Water, Chemicals and Energy in the soil - plant - atmosphere system. Inst. of Hydrology SAS, Bratislava, 82-84.

- Ognianik, N.S., Rudakov, V.K., 1985. Protection of groundwater in technogenetic development condition. Kiev:Vyšca škola, page 221 (in Russian).

- Ognianik, N.S., Paramonova, N.K., 1977. Arguments for point mapping at aproximation of parameter with demand error. Geol. journal, 1-2, pages 159-164 (in Russian).

- Project PHARE/EC/WAT/1, 1995. Bratislava, Danubian Lowland-Groundwater Model.

- Romanenko, V.D., Oksiuk, O.P., Zukinskij, V.H., Stolberg, F.V., 1990. Ecological evaluation of the influence on hydrotechnical buildings on water objects. Naukova dumka (in Russian).

- Simunek, J., Huang, K., Sejna, M., Genuchten, M.Th. van, Majercak, J., Novak, V., Sutor, J., 1997. The HYDRUS -ET software package for simulating the one-dimensional movement of water, heat and multiple solutes in variable-saturated media. Version 1.1. Institute of Hydrology SAS, Bratislava, page 184.

- Slawinski, C., Sobczuk, H., Walczak, R.T., 1996. Submodel of bypass flow in cracking soils. Part 1-Theory. Int. Agrophysics, 10, pages 189-195.

- Shniukov, E.F., et al., 1993. Economical geology of the Ukraine. Kiev: Naukova Dumka, page 407 (in Russian).

- Stoepker, K.E., Visser, A., Lange, W.J. de, 1989. Groundwater modelling of the Kempian Plateau and the Meuse Valley, note 89.149X. Institue for Inland Water Management and Waste Water Treat-ment, Lelystad.

- Storck, P., Valocchi, A. J., Eheart, J. W., 1995. Optimal location of monitoring wells for detection of groundwater contamination in three-dimensional heterogeneous aquifers. In: Models for assessing and monitoring groundwater quality. IAHS publication No.227.

- Strack, 1989. Multi-Layer Analytic Element Model.

- Taylor, J.K., 1985. What is Quality Assurance? In: Quality Assurance for Environmental Measurements, pages 5-11, ASTM Technical Publication 867, American Society for testing and Materials, Philidelphia, Pennsylvania.

- Uil, H., Geer, F.C. van, Gehrels, J.C., Kloosterman, F.H., 1998. UN/ECE Taskforce on Monitoring and Assessment, working programme 1996-1999. Volume 4: State of the Art on monitoring and assessment of transboundary groundwaters. NITG-TNO, 1999

- UN/ECE, TFMA, 1996. Guidelines on water quality monitoring and assessment of transboundary rivers. RIZA report No. 96.034.

- Vurro, M., Passarella, G., 1997. Methodologies for planning monitoring networks with special regard to regional variability. In: Workshop proceedings "Groundwater depletion in basin regions", Budapest, Hungary.

- Witmer, C.H.M., 1989. Integral watermanagement at regional level, an environmental study of the Gooi and the Vechtstreek, Ph.D. thesis. University of Utrecht, The Netherlands.

- Yeh, W.W.G., 1986. Review of parameter identification procedures in groundwater hydrology: The inverse problem, Water Resources Research, Volume 22, 2, pages 98-108.

- Zaltzberg, E.A., 1976. Statistical methods predictions of natural regime of the groundwater table. Nedra, page 99 (in Russian).

ANNEX I Example of the use of a groundwater model in a transboundary region

The Danubian Lowland between Bratislava and Komárno is an inland delta formed in the past by river sediments from the Danube. This alluvial aquifer receives infiltration water from the Danube in the upper parts of the area and discharges it into the Danube and the drainage channels in the downstream parts. The aquifer, including the Danube creates a transboundary region between the Slovak Republic and Hungary and is an important water resource.

Construction of the hydraulic structures in connection with the hydropower plant at Gabcíkovo has significantly altered the hydrological regime in the region and on the floodplain. To increase knowledge of the changing hydrologic regime and to provide a comprehensive technical/scientific based management tool for decision making process in the Slovak Republic, an integrated mathematical modelling system describing flows, water quality processes, sediment transport/erosion in the river, floodplain, reservoir and groundwater system has been developed. This integrated system has been defined within the PHARE programme agreed upon between the Commission of European Communities and the Government of the Slovak Republic (PHARE/EC/WAT/1). (Below, both the quantitative and qualitative aspects of the Regional Groundwater Modelling are presented.

A.1 Regional groundwater modelling

The main objectives of the regional groundwater modelling activities were:

- to provide reliable boundary conditions for local scale models;
- to study the impacts of the damming of the Danube on hydrological regime within Zitny Ostrov, in particular on groundwater levels and dynamics, as well as selected groundwater quality parameters.

A.1.1 Mathematical modelling system

The scientific/technical core of the groundwater modelling is created by an integration of DHI´s modelling systems MIKE SHE and MIKE 11. MIKE SHE is a deterministic, fully distributed and physically based modelling system for describing the major flow processes of the entire land phase of the hydrological cycle. This system solves the partial differential equations for the processes of overland and channel flow, and unsaturated and saturated subsurface flow. The flow equations are solved numerically using finite difference methods. MIKE 11 is a comprehensive, one-dimensional modelling system for the simulation of flows, sediment transport and water quality in rivers, irrigating systems and other water bodies. The hydrodynamic module of MIKE 11 is based on the complete partial differential equations of open channel flow (Saint Venant). This module forms the basis for morphological and water quality studies by means of add-on modules.

For groundwater quality purposes, the biogeochemical processes associated with infiltration of the Danube River water have been included in the modelling subsystem. The MIKE SHE family of models, the MIKE SHE AD model (DHI, 1993) and the GEOCHEMISTRY and BIO-DEGRADATION models have been used to develop models.

The aim of unsaturated zone and agricultural modelling activities was to evaluate the changes in agricultural potential and irrigation requirement and to evaluate the changes in the risk of nitrate as a function of different management strategies of the Gabcíkovo dam. The applied modelling system was DAISY, a one-dimensional single column model for simulation of crop production, soil water dynamics and nitrate dynamics at various agricultural management practices. The processes considered include transformation and transport processes in flowing water, heat, carbon and nitrogen.

A.1.2 Input data and parameters

The model input comprises information on physical and geometrical properties of the model area. The main input data are very briefly described below:

Surface Topography was digitised from topographical maps (Scale 1:10,000 and 1: 25,000).

The River System data comprised location of river branches, and river cross-sections as well as the measurement of flow, water levels and water quality **parameters** for model calibration and validation.

Climatological data comprised time-series of precipitation, potential evapotranspiration and temperature.

Vegetation in MIKE SHE is described in terms of leaf area index and root depth.

Groundwater Abstractions are included as time series of abstracted water at relevant locations.

Soil Physical Properties used in the unsaturated zone calculations are described in terms of soil water retention curves and saturated hydraulic conductivities. The applied data are the same as in the DAISY simulations.

Geology and hydrogeology are included in the model in terms of hydraulic conductivities, specific yield and storage coefficients in different soil horizons (geological layers).

Water quality is included as time series of selected water quality variables and **parameters** (partition and coefficient, etc.) which describe sorption, **degradation** and geochemical processes within aquifer and surface water systems.

Multi-screen wells are installed in the upstream region of the Danubian Lowland just south of Bratislava, in a cross section that is 7.5 km long parallel to the general groundwater flow direction. The distance between wells increases with the distance from the Danube River. In this system of wells, both qualitative and quantitative measurements are currently being made.

A.2 Areas of model application

Groundwater recharge
Groundwater recharge is calculated through the MIKE SHE/MIKE 11 coupling.

Groundwater flow and chemical migration in the saturated zone
The degradation/geochemistry transport model with focus on the saturated zone has modelled specific geochemical processes.

Groundwater/Surface water model for floodplain
The coupled MIKE SHE/MIKE 11 model was used for the ecological modelling to calculate various scenarios.

Monitoring network optimisation
Outcomes from the MIKE SHE/MIKE 11 model were used to set up and to optimise both groundwater and surface water monitoring networks. For groundwater, monitoring the area of direct influence of the Gabcíkovo Dam was distinguished. For surface water, critical sites were selected based on both eutrophication and sedimentation processes.

Assistance for decision making process
Results of the modelling effort have been used to define and create technical measures to mitigate potential negative effects on the environment (both surface water and groundwater).

ANNEX II Review of groundwater models

THE SLOVAK REPUBLIC

1. Name of the model
BEFLOW
Doc. Ing. Kovarik, CSc.
Katedra geotechniky
Stavebná fakulta V_D Zilina, The Slovak Republic

2. Objectives
- steady, partially unsteady flow
- one and two-dimensional groundwater flow in various hydrogeologic conditions
- analysis of technical measures in groundwater flow (wells, hydrodynamic barriers, underground walls, etc.)

3. Description of model structure
- numerical model
- method of solution-boundary element method
- input data: piezometric head or flux on the boundary, interval boundary conditions, hydrogeologic parameters

Used on local and regional level.

1. Name of the model
ANSYS 5.0.-5.2
Swanson Analysis System, Inc.
P.O.Box 65, Johnson Road, Huston, USA

2. Objectives
- steady, unsteady, transient flow
- one, two, and three-dimensional modelling of groundwater flow in various hydrogeologic media
- one, two, and three-dimensional modelling of pollution transport in groundwater flow

3. Description of model structure
- numerical model
- finite element method
- boundary conditions
  - piezometric head
  - free water table
  - flux
  - hydrogeological parameters
  - thickness of the aquifer
  - permeability (filtration coefficient)

Used on local and regional level

1. Name of the model
PLTMG

2. Objectives
- steady and unsteady groundwater flow
- two-dimensional modelling of groundwater flow; by special modification, the model can be used to solve the time dependent two-dimensional groundwater flow and pollution problems

3. Description of model structure
- numerical model
- finite element method
- boundary condition
  - piezometric head on the boundary
  - groundwater effluent or groundwater discharge
  - point source or line source of pollution
  - dispersion
  - chemical reaction

Used on local and regional level

1. Name of the model
SEFTRANS
A Simple and Efficient two-dimensional groundwater flow and transport model
Oxford Geotechnica International
Oxford - Durban, UK

2. Objectives
- two-dimensional modelling of groundwater flow in various hydrogeologic media and modelling of pollution transport in groundwater flow
- steady and unsteady free surface flow and flow with confined groundwater level

3. Description of model structure
- numerical model
- finite element method
- boundary conditions
  - free watertable
  - dispersivity
  - saturation
  - hydrogeologic parameters
  - thickness of the aquifer
  - permeability (filtration coefficient)

Used on local and regional level.

1. Name of the model
MODYW (Model of Dynamics of Water) = (INKANS+SKOKY)
Ing. Karol Kosorin, DrSc.
Institute of Hydrology SAS
Racianska 75, P.O.BOX 94
830 08 Bratislava, Slovakia

2. Objectives
- unsteady and steady three-dimensional groundwater flow in real, layered geology,
- INKANS for (large) domains below free water surface coupled with
- SKOKY for confined domains and interaction with hydraulic and other structure
- described effects:
  - full (detail) interaction with surface water
  - bottom siltation
  - preferential ways
  - boiling
  - leakage and other effect of gaps in basin and reservoir walls

3. Description of model structure
- numerical model
- INKANS: transformation into boundary problem for free boundary, three-dimensional velocity field obtained, space and time integrating by means of the mean value method and the predictor-corrector method (explicit algorithm)
- SKOKY: smooth function for velocity and hydraulic head distribution in computational elements, velocity jump conditions along interfaces between elements (implicit algorithm)

Used on local and regional level, respecting simultaneously interaction with surface waters and hydraulic structures.

HUNGARY

1. Name of the model and authors
HYDRUS/MINTEQA2 (HYTEQ)
HYDRUS is a one-dimensional flow and transport model, developed by HydroGeologic Inc., USA
MINTQA2 is geochemical box model, developed by Environmental Research Laboratory, USA
HYTEQ is the coupled version of HYDRUS and MINTEQA2 merged by HydroGeologic, USA

2. Objectives
Determination of recharge/discharge characteristic in case specific soil column.
Evaluation of vulnerability of shallow aquifers.
Modelling of leaching of pollutant into groundwater.
The geochemical module has been applied for the analysis of redox conditions.

3. Description of model structure
HYDRUS

The one-dimensional model solves the Richards equation for flow by finite element discretisation with fully implicit scheme in time. Root zone, stress function and hysterisis are included in the model. The model uses the Genuchten formulas for pF-function and unsaturated hydraulic conductivity. Considered transport processes: advective transport, dispersion, adsorption, desintegration.

A pre-and post-processor has been developed for HYDRUS at VITUKI (Water Resources Research Centre, Hungary).

MINTEQA2

Geochemical equilibrium box model, based on the solution (Newton-Raphson iteration technique) of thermodynamic equations of selected processes. A database for thermodynamic characteristics is included. PREODEFA2 is a pre-processor in order to help the user in the selection of involved species and in the preparation of datafiles.

HYTEQ

The coupled version of HYDRUS and MINTEQ2 is used to simulate multi-component chemical transport in a variably saturated soil column.

4. Applicability in transboundary regions
For analysis of specific water quality problems. Results can be incorporated into regional transport models. Easy to modify source code is available.

1. Name of the model and authors
TRIWACO/TRACE/FLUZO/SORWACO
Developed by IWACO Bv., The Netherlands

2. Objectives
Description of regional groundwater problems (national groundwater flow model including transboundary area from Romania, Ukraine, Serbia and Croatia; Danube-Tisza ridge; Maros alluvial cone; Transdanubian karstic mountain).
Determination of protective areas of waterworks.

3. Description of model structure
TRIWACO/LFUZO

A quasi three-dimensional triangular finite element model for saturated flow, with numerical solution with conjugate gradient method.
Determination of flux at groundwater level by one-dimensional unsaturated flow model (simplified water balance model used as explicit module).
TRIWACO includes several modules for pre and post-processing, grid generator, graphical editor for parameter allocation, visualisation of parameters and calculated heads, and macros for ARC/INFO connection.

TRACE

Particle tracking module for calculation and presentation of path lines in both backward and forward direction with marker in path lines as given travel times, in plan and cross-sectional view.
3D interpolation procedure for determination of components of velocity vectors at a given point, using the results of the flow calculation.

SORWACO

Calculation of transport along path lines (determined by TRACE). Considered processes: advective transport, adsorption, groundwater level, chemical reactions

4. Applicability in transboundary regions
Advantages: numerous facilities for data preparation, easy exchange of data in standard ARC/INFO or transformable form, flexibility in grid generation, integrated modelling of unsaturated and saturated flow in case of transient problems, relatively low price.
Shortcomings: not real 3D model, 3D transport module is missing, difficult modification.

1. Name of the model and authors
MODFLOW/PMPATH/MT3D - PMWIN

MODEFLOW is 3D groundwater flow model, originally developed by the U.S., Geological Survey
PMPATH is a particle tracking module form the developer of PMWIN
MT3D is a transport module developed by Papadopulos & Associates Inc.,
PMWIN is a pre-and postprocessor for the above models developed by Chiang and Kinzelbach

2. Objectives
regional groundwater problems (Danube-Tisza ridge, Maros alluvial cone, Danube lowland at Szigetkˆz and Zitny ostrov).
Determination of protective areas of waterworks
Groundwater pollution problems

3. Description of model structure
PMWIN

pre-processor: edition	model geometry, grid generation, graphical for parameter allocation (plus interpolator for scattered points, geostatistical module),
parameter optimisation:	data preparation for PEST
run:	MODFLOW, PMPATH, MT3D
post-processor:	contour lines of piezometric heads and concentration, velocity vectors, path lines, water budget

MODFLOW

3D block-centred finite difference groundwater flow model for saturated zone only, numerical solution with preconditioned conjugate gradient method.

PMPATH

Particle tracking module for calculation and presentation of path lines in both backward and forward direction with marker in path lines at given travel times, maps of contour lines of piezometric heads and velocity vectors as additional information, in plan and cross-sectional view,
3D interpolation procedure for determination of components of velocity vectors at a given point using the results of the modelling; retardation caused by adsorption is included via modification of the velocity

MT3D

3D transport model, using the results of the separate MODFLOW calculation.
Considered processes: advective transport, dispersion, adsorption, degradation.
Applied methodologies: method of characteristics (MOC) and its modified versions (MMOC, TIMOC), explicit finite difference transport model.

4. Applicability in transboundary region
Advantages: numerous facilities for data preparation, easy exchange of data in standard form, extended worldwide experience, continuous development, source code is available, relatively low price.
Shortcomings: surface runoff and unsaturated flow are not included, hence in case of transient problems, MODFLOW cannot be applied if the flux at the groundwater table depends on the calculated head and the function is not known in advance.

THE NETHERLANDS

1. Name of the model
NAGROM / MLAEM (modeling technique)
Dr. W.J. de Lange
Institute for Inland Water Management and Waste Water Treatment
P.O. Box 17, 8200 AA Lelystad
mail w.dlange@riza.rws.minvenw.nl

2. Objectives NAGROM
- model include data describing the entire country of The Netherlands
- analysis of water management scenarios at national and regional scale (changes in surface water systems, in groundwater abstraction strategy)
- analysis of technical measures in groundwater flow (wells, dredging, sheet-pile walls, etc.) at regional and local scale

Objective MLAEM
- modeling technique used in NAGROM
- steady and (partially) transient flow
- superposition of analytic solutions for Dupuit-Forchheimer flow
- semi-three dimensional groundwater flow in multi-aquifer systems
- account for three-dimensional continuous density variation

3. Description of model structure
NAGROM model
- 9 connectable models
- model exists of different types of analytic elements (point-sinks for wells, curved or straight line-sinks for canals or brooks, line-dipoles for inhomogeneities and resistance walls, areal-elements with variational strength for infiltration, lakes, polders, leakage between aquifers, etc.)
- model can be transformed in transient by using areal elements for computation of storage using finite differenc elike appoach

MLAEM code:
- hybrid code of advanced analytical solutions and numerical solution techniques
- input data: piezometric head or flux or linear relation between head and flux on the boundary, transient boundary conditions, hydrogeologic parameters adapted to parameters of analytic elements

Used on national, regional and local level.

1. Name of the model
MOZART
Ir. G.E. Arnold
Institute for Inland Water Management and Waste Water Treatment
P.O. Box 17, 8200 AA Lelystad
mail g.arnold@riza.rws.minvenw.nl

2. Objectives MOZART
- the model include data describing the entire country of The Netherlands
- analysis of water management scenarios at national and regional scale (changes in climatological conditions, land use, surface water systems, in shallow groundwater abstraction strategy)
- analysis of technical measures in groundwater flow at regional and local scale

3. Description of model structure- vertical one-dimensional and horizontal two-dimensional water balance model
- soil physical processes, relation surface water-groundwater, seepage/infiltration
- timestep: fixed (10 days) and variable
- input data: meteo, land use, crops, crop rotation, surface water, soil (physicsl), geohydrology, irrigation
- output data: groundwater levels, discharges, crop yields, reduction in crop yields (by drought, salinity or wet circumstances)

Used on national and regional level

THE UKRAINE

1. Name of the model
Skalsky A. S., Kubko Yu. I.: Permanently existing model of zone of forced migration exposed to Chernobyl accident. Institute of Geological Sciences of the National Academy of Sciences of Ukraine, Kyiv, 1992.

2. Objective

- design of the radioactive and hydrogeological monitoring networks, evaluation of water protection measures and forecasting of radionuclide distribution in groundwater.

3. Description of model structure

The model is based on the hydrographical network as the initial conditions of I and III Types and the existing water sampling network as initial condition of II type. The computation of the model is performed with the computer and software GWFS of Russian-Sweden firm „Geosoft-EastLink", based on a finite differential approximation of differential equations of partial derivates with chess iteration algorithm of Chebyshev.

A radionuclide migration was computed for the aeration zone and the soil aquifer along the ribbons of flow with application of analytical relationships considering the convection and dispersion.

Applicability in transboundary regions

Advantages: the model is applied to territories of the Republic of Belarus and Ukraine with the most favourable ecological conditions; it simulates the top aquifers, that are used in economy; it may be used to solve other filtration tasks, as well as mass transport; the model is applied and constantly improved with new data obtained from studied territories.

Disadvantages: The simulation of radionuclide migration and other pollutants needs some improvement.

1. Name of the model

Shestopalov V. M., Zhuk S. G., Sukhorebry A. A.: Model of Dnipro Artesian Basin. Institute of Geological Sciences of National Academy of Sciences of Ukraine, Kyiv, 1989.

2. Objective

- a study of regional relationships of formation and assessment of groundwater resources within the zone of intensive water exchange of Dnipro artesian basin.

The groundwater resources and additional resources for water supply of settlement were estimated with unified hydrogeological model; the main relationships of water exchange of upper hydrodynamic zone of Dnipro artesian basin were found.

3. Description of model structure

The model covers about 200,000 square km, 30,000 of which are located in the Russian federation and 6,400 in the Republic of Belarus.

In the model 5 aquifers and 4 regional separating layers are considered.

The finite-differential approximation of plane flows of aquifers was used in the model; for individual layers the one-dimensional vertical filtration was assumed.
The model was designed for static conditions. Infiltration (natural and technogenic) and parameters of inflow were determined through the solution of reverse tasks. The model computation was done by computer

and software MIR-3, developed by the Dnipropetrovsk Branch of Institute of Mineral Resources. The system of linear finite-differential equations was solved with the iteration method of Guass-Seidel.

Applicability in transboundary regions
Advantages: the model covers the wide territory of three countries (Ukraine, Russian Federation and Belorus) with intensive technogenic pollution including radionuclide pollution from the Chernobyl accident; the model includes aquifers that are the sources of drinking water for many settlements including such large cities as Kyiv, Kharkov, Poltava, Sumy; generalising the vast amount of field hydrological data. The porous solutions of slightly permeable formations under natural and disturbed water exchange were studied; after some adaptions, the model can be used as a solution of other tasks of geofiltration.

Disadvantages: the model of mass transport needs further development.

1. Name of the model
Shestopalov V. M., Rybin V. F., Lysychenko G. V.: Simulation of Volyn-Podilia Artesian Basin. Institute of Geological Sciences of National Academy of Sciences of Ukraine, Kyiv, 1977.

2. Objective
- assessment of perspective resources of groundwater of Volyn-Podol Artesian Basin.

3. Description of model structure
Models of three components of an artesian basin: (I-Ternopol, II-Rivne and III-Khmelnytsky) were created.

All three models were developed for electronic-analogy net integrator BUCE-70 by Libman/s scheme; the model includes the whole hydrographic network and drinking water intakes as the boundary of III and II types. The models are verified through the solution of reverse tasks with simulation of water intake operations. The interactions with river water were monitored by measurements of hydrometric posts.

Applicability in transboundary regions
The advantages: the models cover the large territories of Western Ukraine between the border of Belarus and the river Dnister, and almost up to the borders of Moldova and Romania. The models are developed for the most abundant groundwater layers and water layers for drinking water intake.
Some or all of the model data may be used for development of models for transboundary regions (Ukraine, Belorus, Poland, Slovak Republic, Hungary, Romania, Moldova).
The drawbacks: the models were developed for electronic-analogy equipment and are currently not being used; the models of water transport were not developed.

1. Name of the model
Briks A. L., Ognianyk M. C.: The complex of models for water intakes in the middle part of the Siversky Donets river basin. Institute of Geological Sciences of National Academy of Sciences of Ukraine, Kyiv, 1983 - 1985.

2. Objective
- reassessment of groundwater resources for disturbed natural water regime impacted by technogenic factors.

3. Description of the model structure
The models were created for the water intake nodes: I - Lysychansk-Rubizhne; II - Idaro-Derkulske.

Applicability in transboundary regions
The major drawback: the transport of pollutants from multiply sources of pollution was not included in the models (accumulating ponds for industrial wastes, waste treatment facilities, etc.).

The models are located near the borders of the Russian Federation. If necessary, the data of these models may be used, and some parts of these models may be applied after some amendments in transboundary regions.

1. Name of the model
Paramonova N.K.: The permanently operating mathematical model of the rivers Dnipro and Molochna confluence. The research Institute „UkrVodProekt", the State Committee of Water Management, Kyiv, 1976-1990.

2. Objective
- investigation of irrigation system impact on groundwater; possible raising of water level; measures on remediation and prevention of negative impact.

3. Description the model structure
The model covers the territory of 25,000 square Km and is situated at the northern slope of Black Sea depression within the boundaries of alluvial terrains of the river Dnipro, Askania and Tokmak loess plains. The model is developed for electronic analogy nets of the Libman´s scheme, verified by solutions of reverse tasks. During the application, the model was improved; more detailed fragments were created and solved with application of filtration equations of finite-differential approximation.

Applicability in transboundary regions
The main drawback: the model of mass transport was not developed. Presently, this model is not applied, though all data for its restoration exist. It was used and may be used as a solution for the protection of the Black and Azov Seas.

1. Name of the model
Zildebrandt M.M., Kubko Yu.I., Ognianyk M.S., Romanenko O.A., Sutnikov A.B., Skalsky A.C.: The complex of models of the northern wing of the Black Sea depression between the rivers Dnister and Southern Bug. Institute of Geological Sciences of the National Academy of Sciences of Ukraine, Research Institute „HydroVodProekt" of the State Committee of Water Management of Ukraine, Kyiv, 1979-1982.

2. Objective
- prognoses of hydrogeological and melioration changes under impact of irrigation systems and hydroengineering constructions for designing the Danube-Dnister canal.

3. Description of model structure
The southern boundary of models follow the coastline of the Black Sea, the northern boundary follows the zone of influence of the future canal and irrigation systems.
The finite-differential approximation was used. The calculation was performed with the electronic-analogy nets by the Libman´s scheme and integrator BUSE-70. The two first fragments were duplicated by digital models with solution of finite-differential equations by the integrated method for the BESM. There are some territories with more detailed consideration of filtration and salt transport (near canal zones, estuaries water surface, the city Odessa).

Applicability in transboundary regions
The advantages: include more than 400 km of the border with the Republic of Moldova.

The drawbacks: currently this model is not applied; the model for ?? regional mass transport is not developed.
The data of this model or its parts may be applied for transboundary issues.

1. Name of the model
Havlovsky S.A., Ognianyk M.S.: Model of lowland Crimea and left bank of the Lower Dniper. Institute of Geological Sciences of the National Academy of Sciences, Kyiv, Ukraine, 1987.

2. Objective
- development of the strategy of rational use of the groundwater resources and its protection from the depletion, mineralization and pollution.

3. Description of model structure
The model is developed for the territories within the Black Sea depression, and includes its northern and southern slopes.

The finite-differential approximation with 4 km is applied. The internal boundaries are given as waterbodies, rivers, large canals, Syvash bay, drinking water intakes, the system of artificial recharge of groundwater. The model is verified by solution of the reverse tasks and epignostic modeling, calculations were performed on the electronic-analogy nets by Libman/s scheme.

Applicability in transboundary regions
The advantages: modeling the flow confluences, formed between the river Dniper, the river Molochna and Crimea Peninsula.

The drawbacks: the regional model of mass transport is not developed; the model is currently not being used.

The model data and the model fragments may be used if needed.