Thesis of Doctoral (PhD) Dissertation

APPLICABILITY EVALUATION OF WATER PROTECTION DECISION SUPPORT SYSTEMS

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RESEARCH OBJECTIVES, SCIENTIFIC HISTORY

During the past few decades the appearance of computers, especially since the 1980s personal computers have brought the possibility of a never before seen increase of the investigation and modelling of complex natural and societal phenomena. The classical objective of modelling is the description of the investigated phenomenon in mathematical form and with the use of them to explain numerically the effect of alternative strategies (scenarios).

At the beginning, the main emphasis was on the recognition of phenomena and their mathematical model development, while later on the elaboration of systems suitable for assisting decision making processes received more and more attention. Computer based models equipped with interactive user interface were usually called decision support systems (DSS). The common objective of DSSs, independently of what realization frame, methodology or technology they used was to provide correct information in time about the given subject and decision level for the decision maker. More comprehensive and increasing information needed in the decision making processes motivated more comprehensive development of DSS. Such developments became especially intensive with the general use of more and more effective and affordable personal computers.

In my dissertation I surveyed the general structure and the main elements and applications of water resources protection purpose decision making systems applicable in agro-environmental protection. I presented how water resources protection purpose decision making systems utilize the professional knowledge formulated in mathematical and verbal forms, which is useful in decision making. I demonstrated that I have worked out a number of important solution methods, which fit into many important decision making system structure elements.

The first research topic discussed in my dissertation: In the water protection purpose agro-environmental protection the cognition of solute transport processes in soils and groundwater has got an important role. From an agricultural point of view transport processes in unsaturated zone are of primary importance and, these processes are influenced by numerous complex physical, chemical and biological phenomena. In order that these potentially harmful pollution processes could be described and managed more properly, mathematical models were developed in large number, which describe various transport processes in soils. The vast majority of them deals with convective-dispersive transport in liquid phase in one- and multi-dimensional forms. Beside convective-dispersive transport, when the modelled soil is structured, models include one or more of the following processes: equilibrium or chemical-kinetic sorption, first order decay, Monod kinetic reaction, and matrix diffusion. Besides these processes, models can be applied to different initial and boundary conditions, especially when a model is based on analytical solution.

It is evident form the above that the selection and application of a transport model requires thorough theoretical and practical knowledge of numerous professional fields, such as soil physics, hydrology, geochemistry, microbiology, mathematics and computer science. Today, the selection and application of an adequate model for a case-specific problem area is getting more and more complicated because of the large number of research and management oriented available models. At the same time with the knowledge adaptable to personal computers using artificial intelligence made the development of expert system possible, which for example, make the model selection easier, taking into account solute transport processes, prevailing soil properties, applicable initial concentration distributions, and the applicable boundary conditions determined by soil and groundwater systems. *In my research one of my aims was to elaborate a rule system algorithm to describe solute transport processes in unsaturated soil zone to promote selection of models capable of describing such phenomena. In my dissertation I present an expert system (EXSOLUTE), which assists the user in the selection of deterministic solute transport model(s) for specific problem.*

The second research topic discussed in my dissertation: A significant problem of environmental protection is the pollution of surface and groundwater with nitrogen compounds (especially with nitrate). These pollutions can originate from communal, industrial and agricultural sources. The first two source-types can be identified relatively easily because of their point source character and thus these pollutions can be avoided and their effects reduced by regulations. On the other hand, pollution of agricultural origin is hard to identify, because its non-point character and related complex (partly natural, partly anthropogenic induced) processes.

In this country there are currently several hundred settlements where the water of wells used for drinking purpose does not meet public health standards, because, among others, nitrate concentration exceeds the limit. The nitrate load of near to soil surface on drinking water resources bases can essentially be attributed to three reasons: (1) the heavy use of nitrogen fertilizers in the agricultural production during the 1970s and 1980s and the loss of excess amount and infiltration into soil; (It has to be noted that due to the social-economic changes in the last two decades there was significant decrease in the use of nitrogen fertilizers and the application of advisory systems for fertilizer use helped the efficient use and in this way reducing pollution generating loss from these materials (*Sulyok, 2006; Fodor et al.; Tamás, 2008*). (2) large amount of liquid manure produced in animal husbandry and inappropriate storage and placement of dung water; (3) still underdeveloped sewerage in small settlements (though there is increasing development in this area). Tens of thousands of tons of nitrogen as loss from root zone attain to deeper soil layers, and gradually to groundwater *(OMFB, 1986; Burkart and Fehér, 1996; Ligetvári et al., 2000; Tamás, 2009). In my research one of my aims was to elaborate a model structure, which could describe nitrogen leaching from agricultural field taking into account climatic and soil conditions in the country. This model will be validated using measurement results from leaching lysimeter experiments carried out in undisturbed soil monoliths and data gained from natural condition measurements from large fields to prove the applicability of the model system in describing the solute-transport phenomena in the unsaturated soil zone.*

The third research topic discussed in my dissertation: There is growing concern about the possible effects of climate change, which influence the environment and the economy (*Harnos, 2005; Vermes and Pálfai, 2007*). It is already more and more widely accepted that global warming would increase the average temperature in Europe with several degree °C during the next 50-80 years *(IPCC, 2008)*. Beyond this, precipitation will increase by

10%, though its spatial and temporal changes are still not properly known and their prediction is very difficult (*Láng et al., 2007; Nováky, 2007; Harnos and Csete, 2008*). Most probably winters will become wetter summers will get drier, though the intensity of summer convective rainfalls (storms, etc.) will increase. The climate change will transform natural phenomena in the environment and one of its consequences will be the modification of the salinization processes in the soils (*Várallyay, 2008*).

In Hungary more than one million hectares of saline area can be found. This accounts for 11% of the entire territory of the country and represents the highest ratio in Europe. Nearly half a million hectares is of natural origin, while the other half is potentially or secondary saline area. Because of the complexity of the salinization processes there is currently no such a mathematical model which could numerate and predict the effect of climate change on salinization scale changes of saline soil types. *In my research one of my aims was to elaborate a decision rule and parameter system and formulate an expert system to predict the direction of climate change scenario induced changes in salinization state variables of saline soil types, utilizing the knowledge accumulated in many centuries from Hungarian soil science and salinization researches and processing the findings explained verbally (in non-mathematical forms) by internationally highly recognised leading Hungarian scientists working in these fields.*

MATERIALS AND METHODS

In my dissertation the main motive, research aim and results were the elaboration of a parameter and rule system for prediction of salinization level changes in different soil types affected by climate change, and incorporating them into an expert system. As the necessary materials and methods for these works are the materials and methods of expert system development, I used the followings:

(a) I adjusted the task into a wider professional scope of work and investigated what type of water protection purpose decision support systems had been developed and how these were used in agro-environmental protection. With the review and assessment of relevant literature I summarized the main features of decision support systems relevant to field scale water management of soils.

(b) In particular I investigated those features of revealed decision support systems, whether or not they possess non-mathematical form decision making elements, and if so, what method they used.

(c) I examined whether the revealed decision support systems utilize expert system elements in their general structure.

(d) I showed the main features of expert systems and what type of problems they are used for in agro-environmental protection.

(e) I pointed out that within DSS the development of the expert system element is not a one man task. It can be done only in team work, and in this structure the knowledge engineer has a special role. The knowledge engineer is responsible for the assembling of knowledge in concern and the formulation of a knowledge base and then, on the bases of knowledge base, the elaboration and programming of the rules assuring the proper functioning of decision mechanism of the expert system.

(f) Managing the tasks of the knowledge engineer requires special professional knowledge. In my dissertation I presented my previous works which prove that prior to starting to work on the task of the main dissertation aim of developing an expert system for prediction of salinization in soils, I have done the following research:

(i) Lysimeter experiments to investigate solute transport processes in soils.

(ii) Modelling unsaturated solute transport processes in soil layers:

(ii.1) I have made scientific literature exploration for unsaturated soil solute transport model types and summarized the characteristics of both deterministic and stochastic model types, which gave the basis for establishing a model selection rule base system.

(ii.2) I have developed a rule base system for the selection of applicable models for different soil types and pollutants (*EXSOLUTE*).

(ii.3) I have worked out a model structure to simulate agricultural field scale management oriented unsaturated zone solute transport and nitrogen leaching, which is suitable for calculating, in daily time steps, the amount of nitrogen lost from manure and fertilizers applied on agricultural field, and describes leaching process into soil layers taking into account infiltration from precipitation (rain or snow) that has fallen on the field as well as water storage on the field or run-off from the field (*DISNIT2* model).

(iii) Model investigations:

(iii.1) Based on results received from water dynamics and nitrate leaching experiments in undisturbed soil monoliths carried out in laboratory condition I calculated the changes of soil water content and nitrate concentrations along the soil columns and the amount of materials leached through the bottom of the columns.

(iii.2) Determination of the infiltration rate and speed for the soils in Püspökszilágy area. Using the several decade long rain water tritium concentration time series I have done model analysis to establish dispersion coefficients for soil layers that can be found in the area. From the comparison of measured and calculated tritium concentration in the soil profile the speed of infiltrating tritium front and the time duration of reaching the first groundwater table could be determined.

(iii.2) The investigation of the Újkígyós water base area located on the South-Great Plain was carried out to determine the rate of pollution load to groundwater resources from agricultural fertilizer use.

(g) The scope of the research works listed in par (i), (ii) and (iii) gave a good background knowledge for the elaboration of the dissertation's main aim, namely to establish a parameter system and related rule base and organise them into an expert system to predict the changes of salinization level in different soil types exposed to climate change. Naturally, it has to be emphasized that I had to summarize the knowledge of a long time experienced, outstandingly knowledgeable researchers' team as knowledge engineer of the expert system in question.

SUMMARY OF RESULTS

Expert system to select solute transport models

EXSOLUTE groups models into different classes by using the following separators:

1. *Number of ions* considered in the model. Models may be separated into single-ion transport models, and multi-ion or multi-component transport models. A relatively simple multi-ion transport model involves the transport of radionuclides which form a consecutive first-order nuclear decay chain.
2. *Geometry of the model.* Transport models may be classified in terms of (a) the dimensionality of the problem, (b) the type of coordinate system to be used (e.g., Cartesian, radial, cylindrical), and (c) the domain of each coordinate axis (finite, semi-infinite, or infinite).
3. *Transport processes.* This separator considers all terms in the governing partial differential equation for solute transport, such as those accounting for (a) convective transport with flowing water, (b) diffusion or hydrodynamic dispersion, (c) sorption or exchange, (d) vapour phase transport, (e) volatilization, (f) production, (g) degradation, (h) matrix (or intra-aggregate) diffusion in fractured rock or macroporous field soils, (i) filtration, and (j) sources or sinks of solutes in the system.
   EXSOLUTE considers both convective-dispersive transport, as well as solute diffusion in the absence of convective transport. Sorption and exchange are further separated in linear and nonlinear processes (e.g., Freundlich or Langmuir type adsorption-desorption), and in equilibrium and time-dependent (chemical-kinetic) processes. The simplest formulation for non-equilibrium sorption is that of first-order kinetics, often denoted as the one-site sorption model. We also included two-site non-equilibrium sorption models which assume that sorption sites in a soil can be divided into two fractions, with each fraction having its own unique equilibrium or kinetic adsorption characteristics. Theoretically, any combination of linear, nonlinear, equilibrium, and kinetic sorption or exchange processes may be invoked for a given transport model.
   The expert system currently considers only zero-order production. On the other hand, degradation may be modelled as a first- or higher-order process, or by using Monod kinetics. Finally, depending upon the dimensionality of the

model, different types of sources or sinks can be included, including point, line, rectangular, parallelepiped, and cylindrical sources or sinks.

4. *Soil properties.* From an application point of view, proper spatial characterization of the soil or aquifer properties is one of the most critical steps. My expert system uses two major categories. One separator pertains to the presence of layered versus non-layered (or uniform) soils. These two types of soil may require different mathematical solution techniques. Similarly, different transport models may be needed when the soil profile is not homogeneous but structured or aggregated, or when the groundwater system is fractured. Different geometries of the aggregates (or matrix blocks) may be assumed, including spherical or solid cylindrical geometries. We also considered structured soils containing rectangular voids or hollow cylindrical macropores. In addition, the expert system provides the possibility of including mobile-immobile (two-region) type models. In essence, these models assume that the geometry of the aggregates is unknown or irrelevant, and that diffusion exchange between the mobile (inter-aggregate) and immobile (intra-aggregate) liquid regions can be approximated by means of a quasi-empirical first-order mass transfer equation.
5. *Type of initial condition.* The initial condition can be constant, or may involve a step, pulse, rectangular, parallelepiped, spherical, exponential or some arbitrary function over the domain.
6. *Type of boundary condition*. Three types of boundary conditions are considered: (a) first- or concentration-type boundary conditions, also known as Dirichlet conditions, (b) second-type boundary conditions, essentially those assuming constant concentration gradients, and (3) third- or flux-type (or Cauchy-type) boundary conditions. The first- and third-type conditions can specify constant, step, pulse, exponential or arbitrarily-defined time-dependent functions for the concentration in those boundary conditions.
7. *Type of mathematical solution*. Both analytical and numerical solutions may be employed. At present, most transport models in *EXSOLUTE* are based on analytical solutions. Numerical techniques are normally needed for nonlinear sorption, non-uniform (layered) soil profiles, and arbitrary-defined initial or boundary conditions.

As shown schematically in Figure 1, *EXSOLUTE* consists of three parts: (i) a knowledge base for the model selection process, (ii) a database of information for all available models, and (iii) run-type versions of the executable codes. The user specifies for each model a set of characteristics in the knowledge base. The system represents knowledge on (1) how to select a given model in response to a series of user requirements, (2) how to substitute one type of model by another model if no model fits all user requirements, and (3) how to determine a confidence level for those models which do not completely fit the user requirements, but still can be used with some restrictions. The inference engine governs the sequence of questions when it interrogates the rules in response to answers by the user. *EXSOLUTE* carries out the following functions: (a) From question to question, the expert system calculates a confidence value for each model available in the system; (b) If the newly calculated confidence level of a model falls below the user specified threshold value, *EXSOLUTE* drops that model from further consideration; (c) When one or more models are found which meet the user requirements, the expert system reports those models to an external manager program; (d) When only a few models are available in the database, it may be possible that no model will meet all imposed user requirements.

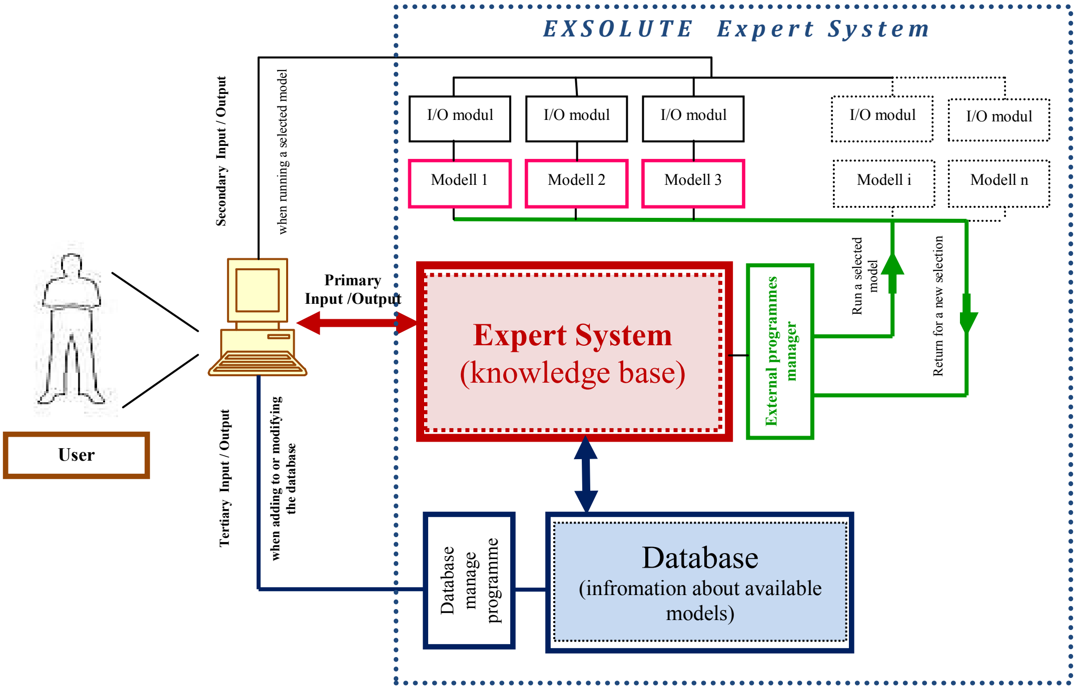

Figure 1. Schematic of EXSOLUTE expert system

One-dimensional solute transport model to calculate nitrate movement in unsaturated soil layers (DISNIT2)

In nature, nitrogen takes part in a complicated dynamics, one of the decisive phases of which happens in the soil (primarily within the root zone). At the same time, the so-called vadose zone between the root zone and groundwater table can not be disregarded, because this zone plays a significant role in water dynamics and solute-transport. Nitrogen transformation in soil consists of complex physical, chemical and biological processes. The *physical processes* incorporate (1) getting nitrogen in to soil from dry fall-out from air, by precipitation, irrigation water, with manure and/or fertilizer; (2) transport of different nitrogen forms within soil profile; (3) gaseous phase nitrogen leaving the soil. The *chemical processes* mean (1) transformation between different nitrogen forms; (2) adsorption in soil matrix or desorption of nitrogen forms. Biological *processes* primarily include plant nitrogen uptake as well as micro-organisms induced nitrogen transformation activity.

The system, which was developed within the frame of an OTKA financed research programme, calculates the water and nitrogen dynamics from the soil surface to groundwater table in daily time step. The model describes water movement and solute transport in vadose and saturated soil zones by Richards' equations, and convection-dispersion equation complemented with one source term, respectively.

The major assumption of water flow equation is that (1) flow of the fluid phase is one-dimensional and isothermal and Darcy's law is valid; (2) the effect of the air phase as well as interaction of solid and liquid phase on water flow is negligible; (3) soil is considered as porous matrix and effects of cracks and macropores are neglected.

Assumptions in the solute transport equation include that (1) convection-dispersion transport is one-dimensional; (2) liquid phase properties are independent of concentration; (3) diffusive-dispersive transport is governed by Fick's law.

For solution of water flow and solute transport equations mathematical form of the relationships of water content and hydraulic conductivity to soil water pressure head should be known. *DISNIT2* model uses van Genuchten-Mualem model for this.

For *soil surface boundary condition* the model calculates the amount of water infiltrating into soil from precipitation (rain or snow). *DISNIT2* examines if there is snow on the area, and if so, then it increases the thickness of snow cover in the function of precipitation and air temperature, as well as the amount of water subject to infiltration.
The model calculates the daily total evaporation, as well as the transpiration, if any. This value is determined by a special method in a period when there is no plant on the area in question, distinguishing between cases when evaporation is controlled by receptivity of atmosphere and cases when humidity and moisture capacity of the soil are the limiting factors.
The daily total value of evaporation and transpiration is calculated by Antal formula in the vegetation period. The effect of the calculated evapotranspiration is distributed in the soil profile according to root density of the plant. The depth of root zone as well as root density distribution is calculated on the bases of plant phenological phase. When there is snow cover in the area no evaporation is taken into account.
Infiltration is calculated differently for growing season and non-growing season. The model distinguishes between the period when precipitation intensity exceeds infiltration capacity of the soil profile and the period when it is smaller. The model pays attention to whether or not excess water remains on the area after a calculation period (one day). It determines what portion of that amount of excess water generates run-off.

At the lower boundary of the soil profile either net fluid flux density (which can be constant or time dependent) or zero gradient of the pressure head (for free-draining soil profile) or a given pressure head can be prescribed.

There are two field crops - maize and wheat - in the model for which plant nitrogen uptake is developed and this process is an integrated part of the nitrogen transport calculation. Our assumption in the plant nitrogen uptake calculation is that there are enough nutrients for the plant, but incidental water shortage could limit the nitrogen uptake, which effect is taken into account.

Calculation of the nitrogen transformation processes in the root zone is also part of the complete simulation system. In the course of calculation (i) mineralization, (ii) immobilization, (iii) nitrification as well as denitrification are taken into account in each soil layers.

The basic time step of water and nitrogen transport is one day. However, the water flow model could decrease the calculation time step to the requirements when water pressure head changes sharply. The model is also capable of increasing the calculation time step if the rate of changes makes it possible. By its concept, the model is suitable for calculation of multi-year period processes.

Among the results *DISNIT2* provides water pressure head, volumetric water content, nitrate and ammonium concentrations at points of calculation net. At time level selected for result printing the programme also gives the accumulated amount of infiltrated water, the amount of water that left the soil profile at lower boundary, the total amount of water stored in soil profile, the accumulated amount of nitrate (if it was modelled) leached into soil profile, the amount of nitrate that left the soil at lower boundary, and the total amount of nitrate and ammonia stored in soil profile. There is a possibility to present complimentary results produced by the model. Then the programme gives the internal calculation results of the water- and solute transport dynamics, among others: the daily values of evaporation or evapotranspiration, plant nitrogen uptake, root density distribution, humus content, denitrification, mineralization and nitrification.

For the evaluation of the applicability of *DISNIT2* model I carried out investigations of three different character, gradually more complicated problem areas:

- evaluation of nitrate leaching experiments carried out in undisturbed soil monoliths,
- modelling tritium infiltration process,
- assessing water quality risks of subsurface water resources.

Evaluation of nitrate leaching experiments carried out in undisturbed soil monoliths

I modelled the water content and nitrate concentration changes in soil columns and the accumulated amount of effluents collected at the bottom of the columns. The model calculations were based on the results of water flow and nitrate leaching experiments in undisturbed soil monoliths carried out in laboratory conditions.

It was determined that the simulated conditions during the soil column experiments corresponded to a good approximation for the Hungarian end of winter, early spring conditions, when soil has high or even close to saturation water content and from snow melt or rain additional infiltration could be possible. The measurements and simulations proved that in the case of loamy sand soils even two significant rain events could wash down the major portion of surface applied nitrate fertilizer to 60-80 cm depth, while the nitrate leaching front could reach 120-150 cm depth.

Model investigation of tritium leaching

I have used the one-dimensional water and solute transport model to verify tritium profile investigation carried out in Püspökszilágy area. The aim of my investigation was to estimate the infiltration speed of rain water and determine the corresponding dispersion coefficients of soil layers in the profile.

The result of daily time step simulation for the period between 1st January 1952 and 31st December 1989 showed that the infiltration front reached 910 cm depth when equilibrium water pressure head was considered at the start. The speed of infiltration was not uniform during the simulated 38 years. During the first 10 year period between 1st January 1952 and 31st December 1961 the infiltrating water front reached 415 cm depth. Thereafter, during the next 10-year period, between 1st January 1962 and 31st December 1971 the water front moved down only to 500 cm depth according to the calculations. The reason for this is, on one hand that the meteorological conditions were different form the previous period, on the other hand that the soil layers located in the 380-500 cm zone had lower hydraulic conductivity. In the third decade – between 1st January 1972 and 31st December 1981 – the infiltration front advanced faster and by the end of this period it reached 810 cm depth. In the last 8 years the calculated water front reached the 910 cm depth.

Comparing the simulation results with the water profile gained from field measurements when the tritium profile was determined, it was observed that the infiltrated water front was calculated to a bit deeper position than the measured one. The assumed reasons for the difference are the uncertainties in hydraulic conductivity values and retention curves, the non-representative character of soil samples and the possible underestimation of areal evaporation or errors in measurements.

Concerning the determination of dispersion coefficient the model simulation gave very good approximation of the tritium profile (Fig.2). It is especially true if we take into consideration that only approximate initial condition could be used because of the lack of measured data from 1952, and the whole 38-year period was modelled with daily time step.

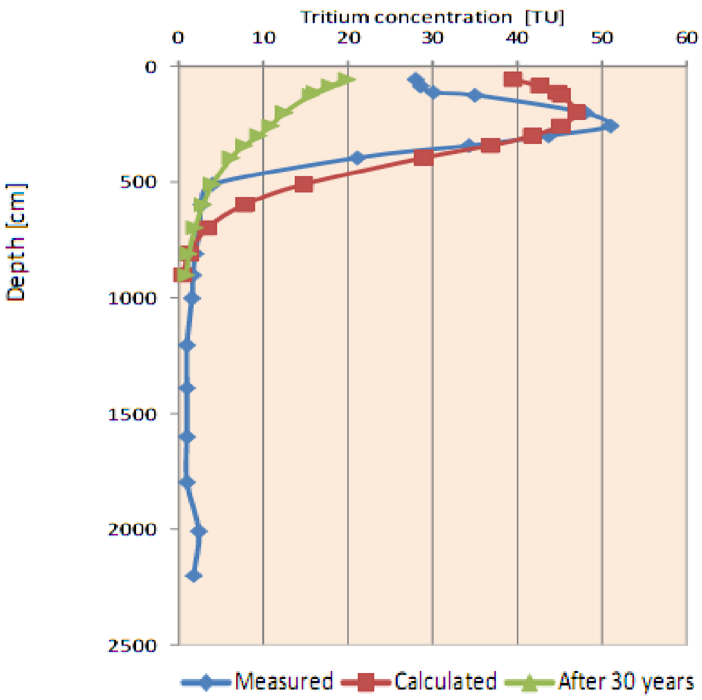

Figure 2. Measured and calculated tritium concentrations in the Püspökszilágy soil profile

Investigation of water quality risk of subsurface water resources by the model

I have carried out a special purpose investigation to estimate risk effects in the territory of water works located near the town of Újkígyós in Békés County and predict the level of risk. A part of the investigations was modelled with *DISNIT2*: (1) how water infiltration front propagated in soil profiles and what rate of infiltrated water reached the groundwater table, (2) what the dynamics of nitrate leaching was and what the nitrate load to the groundwater table was.

The model simulations were divided into two parts. First, the groundwater table level was calculated for the 1980-1989 ten-year period under four soil profiles using the previously estimated initial and boundary conditions (hydraulic investigations). The results showed that with the selected lower boundary conditions for the soil profiles the calculated groundwater levels matched the measured groundwater table fluctuations, which were determined from the groundwater table observation wells of the area. It has to be emphasized that good match did not result when the initial water content of the soil profiles was equal with saturated water content, rather when equilibrium water content was assumed. This fact emphasises that most probably after the rainier, wetter autumn and winter seasons the water content of the unsaturated soil profile would not get close to water capacity.

In order to take into account surface runoff and more precise estimation of flux rate at the lower boundary I have modified the code of *DISNIT2* programme. An alternative calculation method was built in, making it possible in the model to consider the portion of the precipitation which could not infiltrate into the soil remains on the area for the next day infiltration. In this case it was assumed that the area was flat and there was no runoff from it, only surface storage.

Gradually decreasing the water flux at the lower boundary a good match was obtained between the measured and calculated groundwater table time series, when quarter of the originally estimated lower boundary value was applied. Thus the accepted infiltration values were: in 1980 26.25 mm/y; in 1985 35 mm/y and in 1989 30 mm/y in at the 8m deep reference level, while interpolated values were used in these figures. Using these lower boundary conditions as well as the option that rain water could stay on the area if it did not infiltrate, the calculation results showed that the calculated groundwater table was just a few cm higher than the measured groundwater table. It was concluded that the lower boundary condition has significant influence on water dynamics.

In the nitrogen leaching simulation, the above mentioned hydraulic conditions were used. Omission was applied for the sake of safety when the possible maximum possible nitrogen leaching was calculated and plant uptake was neglected and only processes of nitrogen transformations were taken into account. In this simulation I assumed both surface runoff and surface storage as options. The results showed that with application of nitrogen fertilizers at the rate characteristic to the area and given meteorological, soil hydraulic and infiltration circumstances there would be no additional pollution load to the groundwater. The fertilizer applied accumulates in the upper 60-150 cm soil layer. The calculated results were in accord with the soil chemical exploration measurements carried out in the area, which showed that the accumulation could be observed in the upper max. 1 m soil zone, while near to the groundwater table 3-6 mg/kg NO_3-N values were measured.

In summary it can be stated that according to model investigations max. 25-35 mm/y deep infiltration flux could be estimated when lower boundary condition is set at 8 m depth. The surface applied nitrogen fertilizer could not reach the groundwater level under the meteorological and infiltration conditions that are characteristic to the area, even when strong safety omissions were applied.

Expert system (SALINEXP) to predict climate change induced salinization / alkalinisation processes in soils

I developed an expert system knowledge base based on questionnaire survey responses received from a group of specialists. During its development I had to resolve four major problems in order to be able to predict climate change induced changes in the salinity / alkalinity level of soils as well as productivity changes of crops grown on such soils: (i) The variables / parameters that are the most important to characterize salinity / alkalinity level of soils were determined; (ii) The most important variables which significantly influence yields of crops grown on such soils; (iii) I have identified the characteristic variables of climate change scenarios used in the system; (iv) I have elaborated a knowledge base and a rule system to characterize relationships among the variables. Finally, I developed a computer system for the prediction of changes (*SALINEXP*), which used the previously developed knowledge base and rule system.

State variables of soils subject to salinization

Five state variable groups were distinguished for the system in order to characterize the initial state of the salt-affected soil (Table 1).

Group A: Soil characteristics: soil type, soil subtype, depth of the maximum value of exchangeable Na%, cation exchange capacity, texture, organic matter content, bulk density, hydraulic conductivity of the B horizon, maximum value of exchangeable Na% of the B horizon, total salt content, depth of the maximum value of salt content, pH of the B horizon, critical groundwater depth, total porosity, field capacity water content, wilting point water content.

Group B: Ground water parameters: average depth, annual fluctuation, total salt content, Na content (%), sodium adsorption ratio, pH.

Group C: Initial climate characteristics: seasonal average air-temperature, seasonal average potential evapotranspiration, and seasonal average precipitation.

Group D: Plant characteristics: type of plant grown, and average expected yield.

Group E: Irrigation water parameter: annual average amount of water added.

Investigated soil types

Three soil types were considered in the system, such as meadow solonetz, meadow soil and meadow chernozem, while five soil subtypes were identified to the selected soil types, as medium, deep, steppe, solonetz-like and deep-salt. The characteristic soil textures considered were sand, loamy sand, sandy loam, loam, clay loam, loamy clay and clay. Plant types considered were wheat, maize, sunflower, sugar-beet, oilseed rape and soybean.

Characteristic climate change variables

In SALINEXP, climate change is characterized by four parameters: (a) change in seasonal average air-temperature, (b) change in seasonal average potential evapotranspiration, (c) change in seasonal average precipitation and (d) change in average ground water depth.

Table 1 Soil salinization / alkalinisation changes due to different climate change scenarios

			Climate change scenarios					
			1	2	3	4	5	6
		C.1 Air-temperature	No change	No change	No change	+ 2,5 ºC	+ 2,5 ºC	+ 2,5 ºC
		C.2 Pot. evapotransp.	No change	No change	No change	+ 25%	+ 25%	+ 25%
		C.3 Precip-itation	No change	No change	No change	- 25%	- 25% + irrigation	- 25% + irrigation
		C.4 Ground-water depth	No change	Decrease	Increase	No change	No change	Decrease
A.1	Soil type	[verbal]	–	–	–	–	–	–
A.2	Soil subtype	[verbal]	–	–	–	–	–	–
A.3	Depth of max. exchangeable Na% in B horizon	[cm]	–	⇘	⇗	–	–	⇘
A.4	Cation exchange capacity	[mg eq/100 g]	–	–	–	–	–	–
A.5	Texture	[verbal]	–	–	–	–	–	–
A.6	Humus content	[%]	–	⇘	⇗	⇘	–	⇘
A.7	Bulk density	[g/cm^3]	–	⇗	⇘	–	–	⇗
A.8	Hydraulic conductivity	[cm/d]	–	⇘	⇗	–	–	⇘
A.9	Max. of exchangeable Na% in B horizon	[%]	–	⇗	⇘	–	–	⇗
A.10	Total salt content	[%]	–	⇗	⇘	–	–	⇗
A.11	Depth of max. of salt content	[cm]	–	⇘	⇗	–	–	⇘
A.12	pH in B horizon	[-]	–	⇗	⇘	–	–	⇗
A.13	Critical groundwater depth	[cm]	–	–	–	⇗	–	⊖
A.14	Total porosity	[vol. %]	–	⇗	⇘	–	–	⇗
A.15	Field capacity water content	[vol. %]	–	⇗	⇘	–	–	⊖
A.16	Wilting point water content	[vol. %]	–	⇗	⇘	–	–	⊖
B1.	Average groundwater depth	[cm]	–	⇗	⇘	–	–	⇗
B.2	Annual groundwater fluctuation	[cm]	–	⇘	⇗	–	–	⇘
B.3	Total salt content of groundwater	[mS/cm]	–	high	high	–	–	high
B.4	Na% of groundwater	[%]	–	high	high	–	–	high
B.5	SAR of groundwater	[$mg\ eq/l^{1/2}$]	–	high	high	–	–	high
B.6	pH of groundwater	[-]	–	high	high	–	–	high
D.1	Type of plant grown	[verbal]	–	less plant type	more plant type	less plant type	more plant type	less plant type
D.2	Average expected yield	[t/y]	–	⇘	⇗	⇘	⇗	⇘
E.1	Annual average irrigation	[mm/y]	–	–	–		⇗	⇗

Legend: – = No change; ⇘ = Decrease; ⇗ = Increase.

Table 1 (continued)

			Climate change scenarios				
			7	8	9	10	11
		C.1 Air-temperature	+ 2,5 °C	+ 2,5 °C	+ 2,5 °C	No change	No change
		C.2 Pot. evapo-transp.	+ 25%	+ 25%	+ 25%	Slightly increase	Slightly increase
		C.3 Precipitation	No change	No change	No change	+ 25%	+ 25%
		C.4 Groundwater depth	No change	Increase	Decrease	Decrease	Increase
A.1	Soil type	[verbal]	–	–	–	–	–
A.2	Soil subtype	[verbal]	–	–	–	–	–
A.3	Depth of max. exchangeable Na% in B horizon	[cm]	–	–	↘	↘	↗
A.4	Cation exchange capacity	[mg eq/100 g]	–	–	–	–	–
A.5	Texture	[verbal]	–	–	–	–	–
A.6	Humus content	[%]	–	–	↘	↘	↗
A.7	Bulk density	[g/cm^3]	–	↘	↗	↗	↘
A.8	Hydraulic conductivity	[cm/d]	–	↗	↘	↘	↗
A.9	Max. of exchangeable Na% in B horizon	[%]	–	↘	↗	↗	↘
A.10	Total salt content	[%]	–	–	↗	↗	↘
A.11	Depth of max. of salt content	[cm]	–	↗	↘	↘	↗
A.12	pH in B horizon	[-]	–	–	↗	↗	↘
A.13	Critical groundwater depth	[cm]	–	–	–	–	–
A.14	Total porosity	[vol. %]	–	↘	↗	↗	↘
A.15	Field capacity water content	[vol. %]	–	↘	↗	↗	↘
A.16	Wilting point water content	[vol. %]	–	↘	↗	↗	↘
B1.	Average groundwater depth	[cm]	–	↘	↗	↗	↘
B.2	Annual groundwater fluctuation	[cm]	↘	↘	↗	↗	↘
B.3	Total salt content of groundwater	[mS/cm]	–	–	high	high	–
B.4	Na% of groundwater	[%]	–	–	high	high	–
B.5	SAR of groundwater	[mg eq/l$^{1/2}$]	–	–	high	high	–
B.6	pH of groundwater	[-]	–	–	high	high	–
D.1	Type of plant grown	[verbal]	less plant type	–	more plant type	more plant type	less plant type
D.2	Average expected yield	[t/y]	↘	–	↗	↗	↗
E.1	Annual average irrigation	[mm/y]					

Legend: – = No change; ↘ = Decrease; ↗ = Increase.

Table 1 summarizes the expected direction of changes of soil characteristic parameters due to different climate change scenarios. Red arrows mark decreasing changes, while green arrows indicate increases. The direction of changes reflects the average opinion of the expert group members.

Variables for prediction of salinization processes

From the initial state parameters SALINEXP predicts the new salinity / alkalinity state, which is represented by five objective variables: (i) change in the amount of exchangeable Na%, (ii) change in depth of the maximum value of the exchangeable Na%, (iii) change in the total amount of salt at the salt accumulation level, (iv) change in depth of total salt content, and (v) change in average expected yield (Table 2).

Several assumptions are made when the prediction is evaluated:

a) The maximum depth of the pedon (soil profile) considered is 1,5 m or down to permanent ground water level if this is shallower than 1,5 m.

b) A pedon consists of layers, and each layer is regarded as homogeneous. It is assumed that a larger region can be characterized by horizontally homogeneous, vertically layered soil profiles, or in other words, by pedons.

c) The change in the salinity / alkalinity of the soil and the probability of these changes are dependent only on climate change phenomena. No salinization / alkalinisation is considered in the program due to the effect of irrigation water, which means that no secondary salinization was taken into account.

d) The long term effect of soil cultivation is also not considered in the programme. It is assumed that all parameters characterizing the soil layers are characteristic of naturally settled layers. Artificial compaction is not considered.

e) It is also assumed that the new climatic situation will affect the soil for at least 15 years continuously, and that the given scenario parameters represent an average value for the entire period. 11 different scenarios were taken into consideration in the system.

I made analysis for the Hungarian Middle-Tisza region to predict the effect of a feasible climate change scenario on the probable yield of maize and wheat. It was assumed for the climate change scenario that the average air-temperature – and the consequence of it – the potential evapotranspiration will increase, the amount of precipitation will decrease and the level of groundwater will basically not change.

After running the expert system programme for the Middle-Tisza Region soils, the prediction in the majority of the cases were as follows:

- the salinity/alkalinity level will increase only slightly, but the cropping potential will decrease;
- there would be no significant change in the state of salinity/alkalinity in the soils located in the region;
- the expected cropping potential decrease will occur as a consequence of water and soil moisture shortage in the soils. It can be compensated by irrigation, but this will increase production costs and raise the likelihood of secondary salinization of the soils.

Table 2 Soil salinization/alkalinisation changes predicted by the SALINEXP expert system in the case of different climate change scenarios

			Climate change scenarios					
			1	**2**	**3**	**4**	**5**	**6**
		C.1 Air-temperature	No change	No change	No change	+ 2,5 °C	+ 2,5 °C	+ 2,5 °C
		C.2 Pot. evapotranspiration	No change	No change	No change	+ 25%	+ 25%	+ 25%
		C.3 Precipitation	No change	No change	No change	- 25%	- 25% + irrigation	- 25% + irrigation
		C.4 Groundwater depth	No change	Decrease	Increase	No change	No change	Decrease
OV.1 (A.9)	Change in the amount of exchangeable Na%		–	⇗ (red)	⇘ (green)	–	–	⇗ (red)
OV.2 (A.3)	Change in the depth of maximum value of the exchangeable Na%		–	⇘ (red)	⇗ (green)	–	–	⇘ (red)
OV.3 (A.10)	Change in the total amount of salt at the salt accumulation level		–	⇗ (red)	⇘ (green)	–	–	⇗ (red)
OV.4 (A.11)	Change in the depth of total salt content		–	⇘ (red)	⇗ (green)	–	–	⇘ (red)
OV.5 (D.2)	Change in the average expected yield, if the plant is **maize**		–	⇘ (red)	⇗ (green)	⇘ (red)	⇗ (green)	⇘ (red)
OV.5 (D.2)	Change in the average expected yield (**wheat**)		–	–	⇗ (green)	–	⇗ (green)	–
OV.5 (D.2)	Change in the average expected yield (**rape**)		–	–	⇗ (green)	–	⇗ (green)	–
OV.5 (D.2)	Change in the average expected yield (**sunflower**)		–	–	⇗ (green)	⇘ (red)	⇗ (green)	–

			Climate change scenarios				
			7	**8**	**9**	**10**	**11**
		C.1 Air-temperature	+ 2,5 °C	+ 2,5 °C	+ 2,5 °C	No change	No change
		C.2 Pot. evapotransp.	+ 25%	+ 25%	+ 25%	Slightly increase	Slightly increase
		C.3 Precipitation	No change	No change	No change	+ 25%	+ 25%
		C.4 Groundwater depth	No change	Increase	Decrease	Decrease	Increase
OV.1 (A.9)	Change in the amount of exchangeable Na%		–	⇘ (green)	⬈ (red, full)	⇗ (red)	⬊ (green, full)
OV.2 (A.3)	Change in the depth of maximum value of the exchangeable Na%		–	–	⬊ (red, full)	⇘ (red)	⬈ (green, full)
OV.3 (A.10)	Change in the total amount of salt at the salt accumulation level		–	–	⬈ (red, full)	⇗ (red)	⬊ (green, full)
OV.4 (A.11)	Change in the depth of total salt content		–	⇗ (green)	⬊ (red, full)	⇘ (red)	⬈ (green, full)
OV.5 (D.2)	Change in the average expected yield, if the plant is **maize**		⇘ (red)	⇘ (red)	⬊ (red, full)	⇘ (red)	⬈ (green, full)
OV.5 (D.2)	Change in the average expected yield (**wheat**)		–	–	–	–	⇗ (green)
OV.5 (D.2)	Change in the average expected yield (**rape**)		–	–	–	–	⇗ (green)
OV.5 (D.2)	Change in the average expected yield (**sunflower**)		–	⇘ (red)	–	–	⇗ (green)

Legend: – = No change; **Red arrow** represents change direction, which reflects salinity increase as well as plant yield decrease. **Green arrow** represents change direction, which reflects salinity decrease, as well as plant yield increase. **Full coloured arrow** represents high intensity change.

NEW AND NOVEL SCIENTIFIC RESULTS

1) In my dissertation I made a survey of the general setting up of decision support systems, their main elements and applications in agro-environment protection focusing on water resources protection. I presented how water resources protection oriented decision support systems can utilize the knowledge that is formulated in mathematical and non-mathematical forms, and the knowledge of different professions which could be a useful element in the decision-making process. I pointed out that rule based knowledge bases should be necessary elements of expert systems, especially for relationships which could not be formulated mathematically.

2) I developed a rule-based algorithm system for the optimal selection of models which describe solute transport processes in unsaturated soil zones. Based on the rule-based model selection algorithm I developed an expert system (*EXSOLUTE*), which can assist the users is selection of solute transport model(s) for special problems which depend on the soil physical characteristics of unsaturated soil layer(s), the geometry of the modelled domain, characteristics of the pollutant to be modelled and the initial and boundary conditions.

3) For modelling work of solute transport processes in unsaturated soil zone I developed an agricultural field level, management oriented model concept and model structure to describe unsaturated zone solute transport and nitrate leaching. The model can calculate, in daily time step, the nitrate leaching process from manure and fertilizer applied on the agricultural field taking into account the infiltration from precipitation (rain or snow) as well as storage or run-off (*DISNIT2* model).

4) For the evaluation of the usability of the *DISNIT2* model I have carried out simulations for three different, gradually more complicated cases. In the first case I made model calculations to describe water content and nitrate concentration distributions within undisturbed soil columns and the accumulated amount of drainage water and leached amount of nitrate at the bottom of these columns using results of water and nitrate leaching experiments, which were carried out under laboratory conditions. It was determined that the simulated conditions during the soil column experiments corresponded to a good approximation for the Hungarian end of winter, early spring conditions, when soil has high or even close to saturation water content and from snow melt or rain additional infiltration could be possible. I proved with model simulation that in the case of loamy sand soils only with two heavier rainfall events the surface applied nitrate could be washed down to 60-80 cm depth and the nitrate from could reach 120-150 cm in the soil.

5) In the second case I investigated the speed of the infiltration process in the soils in the Püspökszilágy area. Using the multi-decade long tritium concentration time series of the precipitation I made a model analysis. I estimated what dispersion parameters characterized the soil profile in the area. Based on the determined dispersion coefficients the speed of downwards moving infiltration water front was modelled for a 38-year period. As a result of the model analysis the total depth of infiltration front was 910 cm for that period. During the 38-year period different infiltration speed periods – by 10-year periods and depending on meteorological conditions – could be separated.

6) In the third case an investigation was also carried out for the Újkígyós subsurface water resources area located on the South Great Hungarian Plain. I have proved that taking into account a long period the nitrate load originating from fertilizer usage would not cause additional load to subsurface water resources when the meteorological, soil hydraulic and infiltration circumstances are considered that are characteristic to the area. Compounds of applied fertilizers accumulate in the top 60-150 cm soil zone.

7) I determined a method – using questionnaire survey responses received from a group of specialists - how parameters, which predict the salinity / alkalinity change caused by climate change in different soil types, and parameters (exchangeable Na%, depth of maximum value of the exchangeable Na%, change in the total amount of salt at the salt accumulation level, change in the depth of total salt content) best influencing the expected cropping potential, can be applied in expert systems.

8) I worked out a relationship system – based on questionnaire survey responses received from a group of specialists – which describes how salinity/alkalinity levels of soils change as well as how the expected average crop yields of most important arable land crops (maize, wheat, rape and sunflower) produced on such soils change in the case of 11 climate change scenarios. Using the determined relationship system I developed an expert system programme (*SALINEXP*) which gave the increasing or decreasing direction of salinity/alkalinity changes fro the different climate change scenarios.

9) After running the expert system programme (*SALINEXP*) for the Middle-Tisza Region soils, the prediction in the majority of the cases were as follows:

- the salinity/alkalinity level will increase only slightly, but the cropping potential will decrease;
- there would be no significant change in the state of salinity/alkalinity in the soils located in the region;
- the expected cropping potential decrease will occur as a consequence of water and soil moisture shortage in the soils. It can be compensated by irrigation, but this will increase production costs and raise the likelihood of secondary salinization of the soils.

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I. PUBLICATIONS IN THE SUBJECT OF DISSERTATION

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