Modelling of Groundwater Flow Networks in the Desktop GIS Environment

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Abstract A study of principle processes of flows and pollutant transport in groundwater contaminated sites is described. Details are given of a compartment model and its simulation with GIS tools to predict such processes. The investigation comprises mathematical descriptions of density dependent pollutant transport phenomena, a numerical modelling approach, the creation of digital spatial data sets that reflects the spatio-temporal nature of studied processes, the development of simulation tools in the GIS environment, and a model of radionuclide deposition as an example. The prediction of the spatial and time distribution is described with a dynamic deterministic model. The numerical approach involves the solution of first order differential equations and data management. A desktop GIS' (*ArcView* and its extensions-*Spatial Analyst, 3D Analyst*; *Idrisi*; *MapSheets*; etc.) is used to demonstrate various levels of numerical modelling, data analyses, and graphical presentation. Simulation of a three-dimensional radionuclide transport and its spatio-temporal phenomena illustrates the desktop GIS capabilities to predict and analyse such processes and similar problems.

1. INTRODUCTION

Dynamic groundwater flow models should be standard analysis tools for the evaluation of environmental systems prior to their management. The continuous simulation tools in the environment of the desktop geographic information system (GIS) has been developed for the purpose of modelling systems described by time dependent, nonlinear differential equations and subsequent spatial analysis. The environmental models are used on the increase scale in addition to a typical application area of continuous simulation in control system design, physical and chemical process representation. Both simulation systems and GISs consist of computer hardware and software for entering, storing, transforming and displaying data. Simulation is primary used for time dependent phenomena. The GISs are more concerned on spatial analysis. The analysis of temporal change, which is central to groundwater flow phenomena, is solved with a various GIS extensions, shared database data or special programming modules. GISs also include related technologies such as spatial interpolations, global positioning systems, remote sensing and spatial database management that can be very useful to groundwater flow and pollutant transport modelling.

The continuous simulation system in the desktop GIS *ArcView*'s environment described herein, and referred to as a *AVSim* (*ArcView* Simulation, Matejicek [1999]), is used as an example of integration of time and spatial dependent phenomena. The example includes a compartment model of radionuclide transport and deposition.

2. GROUNDWATER FLOW MODELS

Three-dimensional groundwater flow problems are generally described by systems of partial differential equations. The solutions of the equations arise from numerical approximations. The studied area is usually separated to horizontal layers and then the partial differential equations are integrated vertically across each layer. The results are given in the form of two-dimensional equations that describe groundwater flows in each layer and between adjacent layers. Each layer equation is approximated spatially by a finite element method. The data output can be imported to a GIS for analysis and visualisation.

Another method is to represent the multigrid in a GIS environment, which uses a series of coarser grids to spatially approximate the numerical solution of the partial differential equations. Some of grid-cell-based GISs have internal programming languages, which are capable of manipulating spatial data and handling the results from groundwater simulation problems (as shown by Wesseling et al. [1998]). Execution times for models in the GIS environment usually exceed those of traditional groundwater simulation models due to the more complex data structures and functions. GISs were originally designed to produce maps and perform spatial analysis on static two-dimensional data sets. Modelling of groundwater flow entails the numerical solution of partial differential equations, which arises to enhance the computational capability of the GISs. In the multigrid method, the area is divided into a regular network as the result of the equation discretization. Each grid contains an algebraic equation. Then simulation requires a solution of the large set of algebraic equations.

3. GROUNDWATER FLOW MODEL IN THE GIS ENVIRONMENT

The GIS approach and its application to solving groundwater flow problems presented in this paper is based on an irregular network of points. The points and their attributes form a vector layer. Each point and its attributes represent samples that are taken across a studied area. The location is recorded with a global positioning system (GPS). The compartment model describes the dynamic of pollutant transport phenomena at each point and among its neighbouring points. The compartment model is transformed to a numerical model that involves the solution of first order differential equations. The values of parameters between the points are interpolated with GIS tools and functions.

3.1 Mathematical model

The general mathematical description of dynamic phenomena is a first order differential equations:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}(\mathbf{x}(t), \mathbf{r}(t), \mathbf{u}(t), t) \qquad (1)$$
$$\mathbf{x}(0) = \mathbf{x}_0$$

A state vector x contains the mass accumulation of the pollutant. The functions f describe the transport behaviour of mass accumulation. The input vector u includes external mass flows. The vector r contains delayed state variables x. Initial conditions of state variables x are x_0.

The differential equations are extended with output algebraic relations:

$$\mathbf{y}(t) = \mathbf{g}(\mathbf{x}(t), \mathbf{r}(t), \mathbf{u}(t)) \qquad (2)$$

The output vector y includes mass concentrations, which are calculated with algebraic equations.

The delay conditions are:

$$r_{ij}(t) = x_i(t - T_{Dj}) \qquad (3)$$

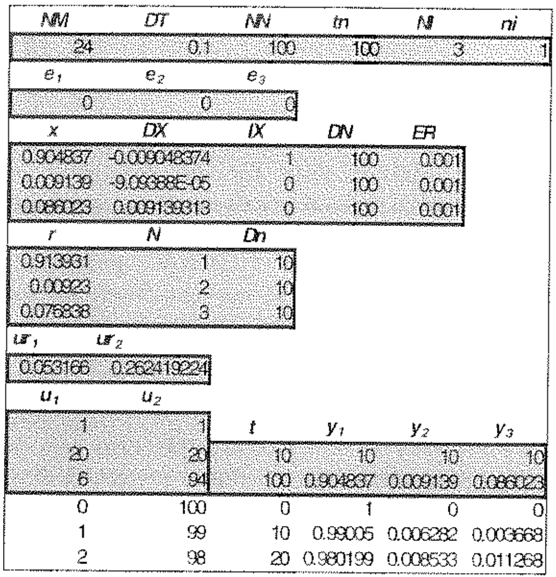
The initial delay functions are:

$$r_{ij}(\tau) = r_{Pi}(\tau)$$
$$\tau \in \langle 0, T_{\max Dj} \rangle; \qquad (4)$$
$$i = 1,2,\ldots,n; \; j = 1,2,\ldots,m$$

Initial functions of delayed state variables are $r_{ij}(\tau)$. The time t is an independent variable. T_{Dj} are time delays of state variables. The mass accumulation x_i and the concentration y_i are described at each point. The number of points is n. The differential equations (1) describe horizontal and vertical transport phenomena of the pollutant in the point layers. The number of layers depends on the vertical structure of the study area.

3.2 Numerical model

The process of numerical solution has two phases. The mathematical model and its simulation parameters are entered as tables in a spreadsheet, as shown in Figure 1.



NM	*DT*	*NN*	*tn*	*NI*	*ni*
24	0.1	100	100	3	1

e_1	e_2	e_3
0	0	0

x	*DX*	*IX*	*DN*	*ER*
0.904837	-0.009048374	1	100	0.001
0.009139	-9.09388E-05	0	100	0.001
0.086023	0.009139313	0	100	0.001

r	*N*	*Dn*
0.913931	1	10
0.00923	2	10
0.076838	3	10

ur_1	ur_2
0.053166	0.262419224

u_1	u_2	*t*	y_1	y_2	y_3
1	1				
20	20	10	10	10	10
6	94	100	0.904837	0.009139	0.086023
0	100	0	1	0	0
1	99	10	0.99005	0.006282	0.003668
2	98	20	0.980199	0.008533	0.011268

Figure 1. Structure of the spreadsheet tables with the mathematical model and its simulation parameters.

The spreadsheet tables are then transferred to an *Avenue* program. *Avenue* is a programming language that provides the customisation and the development environment for the desktop GIS *ArcView*. The numerical solution in the *ArcView* environment is separated into a number of scripts.

The top table *MODEL* sets the numerical method *NM* and its integration step *DT*. *NN* specifies the number of time steps in a simulation period. *tn* indicates the actual number of integration steps. Parameters *NI* and *ni* indicate the maximum and the actual number of cycles for the implicit numerical methods. The terminating conditions e_1, e_2 and e_3 are set in the *EVENT* table. The functions f and the initial conditions in the equations (1) are specified in the *INTEG* table as the column *DX* and *IX*. The column *DN* sets the maximum number of saved data points needed to represent the delay of the state variables $\boldsymbol{x}$. *ER*s are the estimates of maximum numerical errors. The delayed state variables $\boldsymbol{r}$ (3) are set in the *DELAY* table. The columns *N* and *Dn* specify the index of delayed state variable and the delay in the number of integration steps. The delayed values are in the column r. Cells ur_1 and ur_2 set random inputs in the table *RANDOM*. The actual model inputs u_1, u_2 and outputs t, y_1, y_2, y_3 during the simulation period are set in the tables *INPUT* and *OUTPUT*.

In Figure 1, the actual values are set each 20th integration step for inputs and each 10th integration step for outputs. The time series of inputs and outputs are under the tables *INPUT* and *OUTPUT*. The number 1 sets the approximation of input values in each integration step to linear interpolation. The number of columns in the *EVENT* table, the *INPUT* table, the *OUTPUT* table and the *RANDOM* table depends on the mathematical model and the parameter set in the spreadsheet program. The number of the rows in the *INTEG* table and the *DELAY* table depends on a set of the differential equations (1) and the number of the delay conditions (3). The model structure in Figure 1 is transferred to *Avenue* scripts.

Figure 2 outlines the flow of the continuous simulation system *AVSim*. The structure of the *SIMULATION* script includes *INPUT*, *MODEL* and *OUTPUT* scripts. The main script *SIMULATION* is activated from the *ArcView* environment. The program proceeds sequentially through the initial code block, the section for definition of internal data lists and variables. After initialisation, the program evaluates initial inputs $\boldsymbol{u}$ in the *INPUT* script and creates a new point theme with the attributes $\boldsymbol{y}$ in the *OUTPUT* script. The coordinate information of each point is read from the specified file that is produced by GPS software. After initial *INPUT* and *OUTPUT* script section has been executed, the condition flag is tested. If the flag is true, the integration routine is asked to integrate over an integration step dt using the *INPUT* script to set the actual inputs $\boldsymbol{u}$, and the *MODEL* script to evaluate the state variable derivatives. The integration routine returns with the states $\boldsymbol{x}$ advanced through the integration step. After the increment tn and the output script *OUTPUT* has been evaluated, the program loops and re-executes the condition flag. If the condition flag is false, program control transfers to the terminal code block. On passing out of the section, control returns to the *ArcView* executive, which can processes any further scripts or analysis.

3.3 Spatial data and simulation tools in the GIS environment

The data structure of the continuous simulation system *AVSim* is illustrated in Figure 3. The model structure is developed as a set of spreadsheet tables. The spreadsheet contains a macro that allows model conversion and construction of *AVSim* scripts.

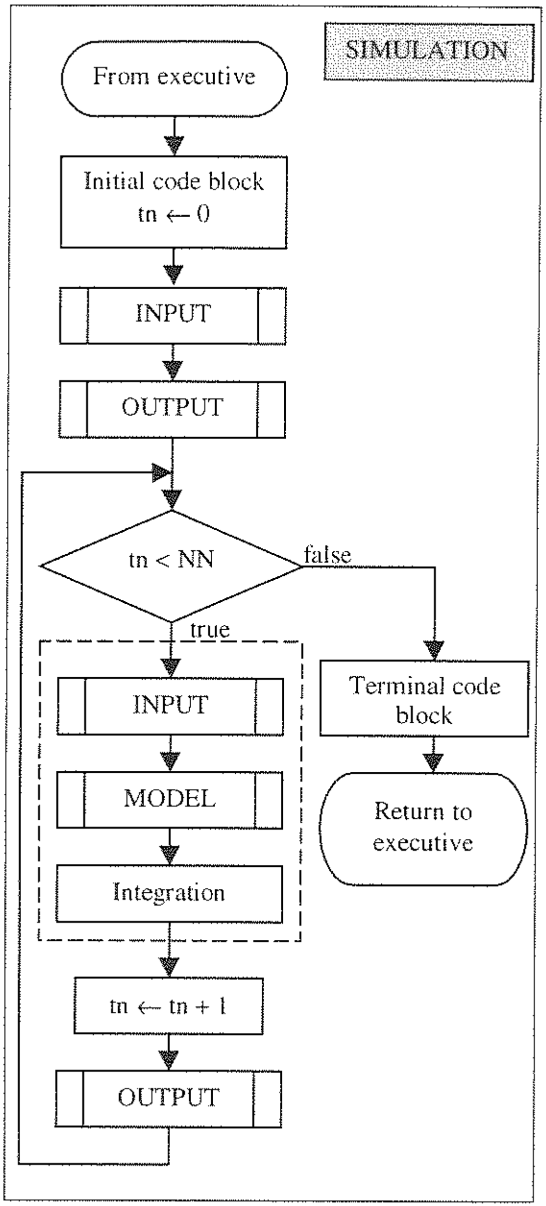


Figure 2. Main program loop of the *AVSim* model

After the scripts have been developed, their program code can be executed in the *ArcView* environment. The *OUTPUT* script assumes that the file with GPS coordinate information will contain comma-delimited coordinates in the format: *id*-identification number, *x*-coordinate; *y*-coordinate. New point themes are created as a result of the simulation. The themes are created and output data are recorded at each communication interval. The communication interval is set as a number of integration steps. Each point theme is converted to a grid theme. The polygon theme can be used as a boundary of the grid themes for the studied area. The interpolation of grid themes can be carried out with a few methods: inverse distance weighted, spline and kriging methods and trend interpolation. The mass concentrations in specified point locations are written in the attributes of point themes and, using the surface-creation functions, an estimated values is assigned to all other locations in the grid.

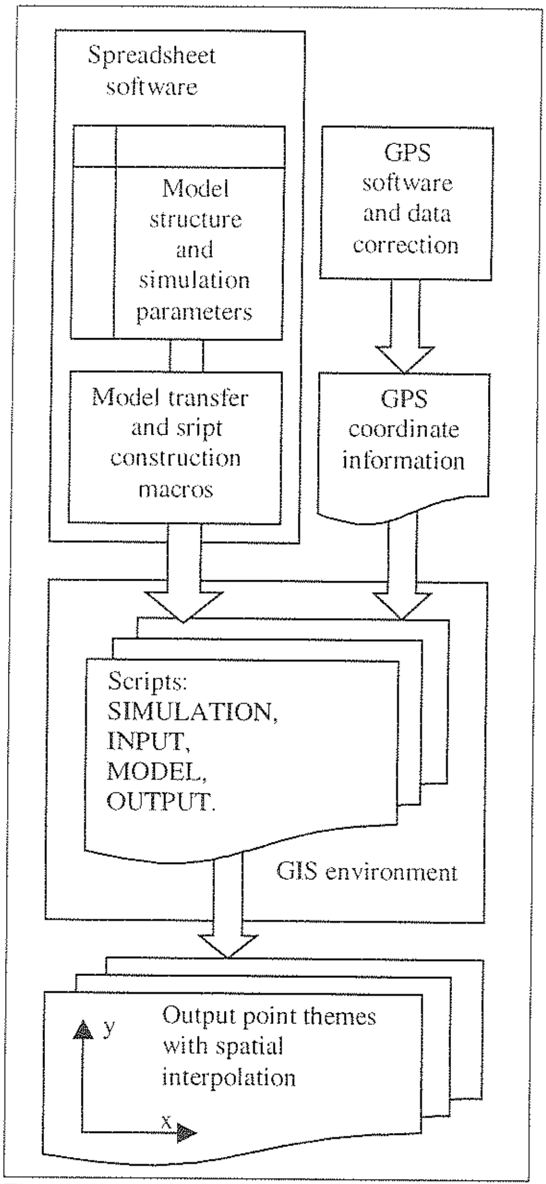


Figure 3. Data structure of the continuous simulation system *AVSim*

3.4 Simulation of the three-dimensional radionuclide transport and its spatio-temporal phenomena

A few mathematical models have been described to predict radionuclide distribution as described by Kershaw [1992]. The dynamic models in the GIS environment are used to integrate dynamic and spatial phenomena. The desktop GISs can visualise and analyse data samples and model predictions as shown by Matejicek [1996, 1997]. Figure 4 shows a model scheme of radionuclide deposition.

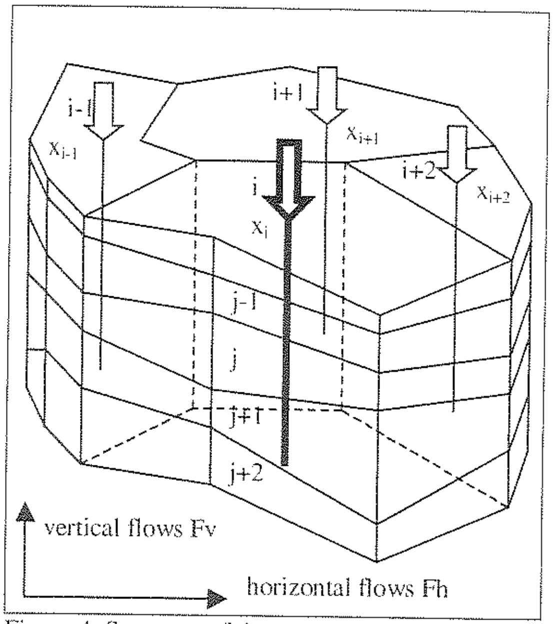


Figure 4. Structure of the compartment model

The description of a model for the region *i* in the vertical layer *j* is:

$$
\begin{aligned}
&\frac{dx_{ij}}{dt} = -\lambda x_{ij} + \sum F_{hkj} + \sum F_{vil} + \sum u_m \\
&F_{hkj} = F_{hkj}\left(x_{ij}, r_{kj}, t\right) \\
&F_{vil} = F_{vil}\left(x_{ij}, r_{il}, t\right) \\
&x_{ij}(0) = x_{0ij} \qquad (5) \\
&y_{ij} = \frac{x_{ij}}{V_{ij}} \\
&r_{kj}(t) = x_{kj}\left(t - T_{Dn}\right) \\
&r_{il}(t) = x_{il}\left(t - T_{Dn}\right)
\end{aligned}
$$

where x_{ij} is the amount of radionuclide in the stack of the region *i* in the layer *j*. Fh_{kj} and Fv_{il} are interactions with horizontal and vertical neighbour stacks. λ is a positive constant of proportionality independent of time *t*. u_m are external inputs of radionuclide in the stack ij. The estimate of concentration in the stack ij is calculated as y_{ij}. Variables r_{kj} and r_{il} implement the transport delay of radionuclide in the horizontal and the vertical direction. x_{0ij} are the initial amounts of radionuclide. The simulation model of the system (4) was extended with other rules and special properties in the *AVSim* environment. As a result, time series of vertical layers was generated. Each *ArcView* theme with the layer was converted and interpolated in the grid theme. The desktop GIS *ArcView* (with its tools *Spatial Analyst* and *3D Analyst*) was used for interpolation, drawing and other analysis. After development of the GIS project, the graphic schemes were exported to various GIS software (*ARC/INFO* version 7.2.2, *Idrisi*, *MapSheets*, etc.).

4. CONCLUSIONS

Integrated environmental systems for modelling of groundwater flow are tools to support environmental planning and protection. The GIS platform can bring the best knowledge to bear on decision-making processes and is easy to use and understand. The desktop GIS is able to access large volumes of various data formats and a set of tools for their analysis and interpretation. Spatially distributed data represent an important aspect in environmental problems and their management. Levels of integration of GIS functionality and mathematical modelling vary widely not only in sophistication, but also in the price of the software. The desktop GIS modelling tools *AVSim* consists of a combined vector-grid based topological data model. Spatial features are represented as point themes and spatial interpolations as grid themes. The attributes of those themes are stored in a database. The GPS coordinates, data samples and model outputs are entered, stored and analysed prior to being interpolated and transferred to the grid themes. The results can be exported to other information systems.

Acknowledgements

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