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The program system GEOFIM for the digital simulation of subsurface water movement and transport

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Abstract The program system is used for the simulation of subsurface water movement and transport based on space discretization, a differential equation system is established using the balance method. The solutions of the direct task as well as of the inverse task make the program system applicable to problems of exploration, design and management.

SIGNIFICANCE AND STATE-OF-THE-ART OF SUBSURFACE WATER MOVEMENT AND TRANSPORT PROBLEMS: THE REASONS WHY THE SYSTEM HAS BEEN DEVELOPED

Mastering the subsurface water movement is a relevant factor in the national economy of the German Democratic Republic (GDR). The complexity of natural conditions and human impacts requires modelling and simulation. A number of the symposium papers are dedicated to such problems.

The past decade has shown that mathematical simulation models, established as computer codes, can provide effective instruments for multiple use.

Although a great number of different codes have been developed to solve subsurface water movement problems, it has to be mentioned that due to objective and subjective factors parallel developments happened and solutions which are incompatible to each other have resulted from the use of different computers and programming language.

The application of these codes often requires profound program and data processing knowledge. The operator's error handling, computation abortion and restart rarely matches the wishes of the user or at best meets only few of the requirements. That is why it seemed reasonable and necessary to integrate the knowledge of subsurface water movement and transport simulation available in the GDR into one universal program system.

The program system was developed with the following objectives:

- to solve all subsurface water movement and transport problems of practical relevance while offering the possibility of coupling groundwater and surface water flow models;
- to separate the tasks of preprocessing, processing and postprocessing;
- to develop the system for ESER computers, thus allowing their general application in the GDR and in CMEA countries;

- to structure the program system into a control program with user-oriented problem description and modules.

STRUCTURE OF GEOFIM

The general structure of GEOFIM is shown in Fig. 1. The following three main components may be distinguished:

- problem description (PROBLEM)
- numerical solution (COMPUTATION)
- representation of results (RESULTS)

The interrelation between the modules of the different levels is established by defined data interfaces (problem data storage, result data storage). The tasks and solution principles of the modules are shown in a survey below.

THE OPTIONS OF GEOFIM

GEOFIM can solve two typical tasks:

The direct task

Initial:	Initial values (e.g. groundwater level, ...); characteristics of the area under investigation (e.g. permeability, storage coefficient, groundwater recharge, ...); boundary conditions (at grid points; special ones at freely chosen points, rivers, lakes, ...)
Results:	time and space variations of the groundwater level, flow rates, ...

The inverse task

Input:	Distribution of groundwater levels and of flow rates in time and space; characteristics of the area under investigation; boundary conditions
Results:	space distribution of the unknown parameters

Thus, GEOFIM is applicable for solving exploration, design and management tasks.

Table 1 gives an overview of the model types and their typical fields of application. By means of defined words the user selects the model that is next suited to his problem. A simple model concept has advantages in terms of data supply and running times. That it why it is preferable to select a plane/plane-layered model to a three-dimensional model.

MATHEMATICAL MODEL AND COMPUTATIONAL PROCEDURE

A system of partial differential equations is established for every planning element using the well-tested mathematical model concept of filtration and balance analyses.

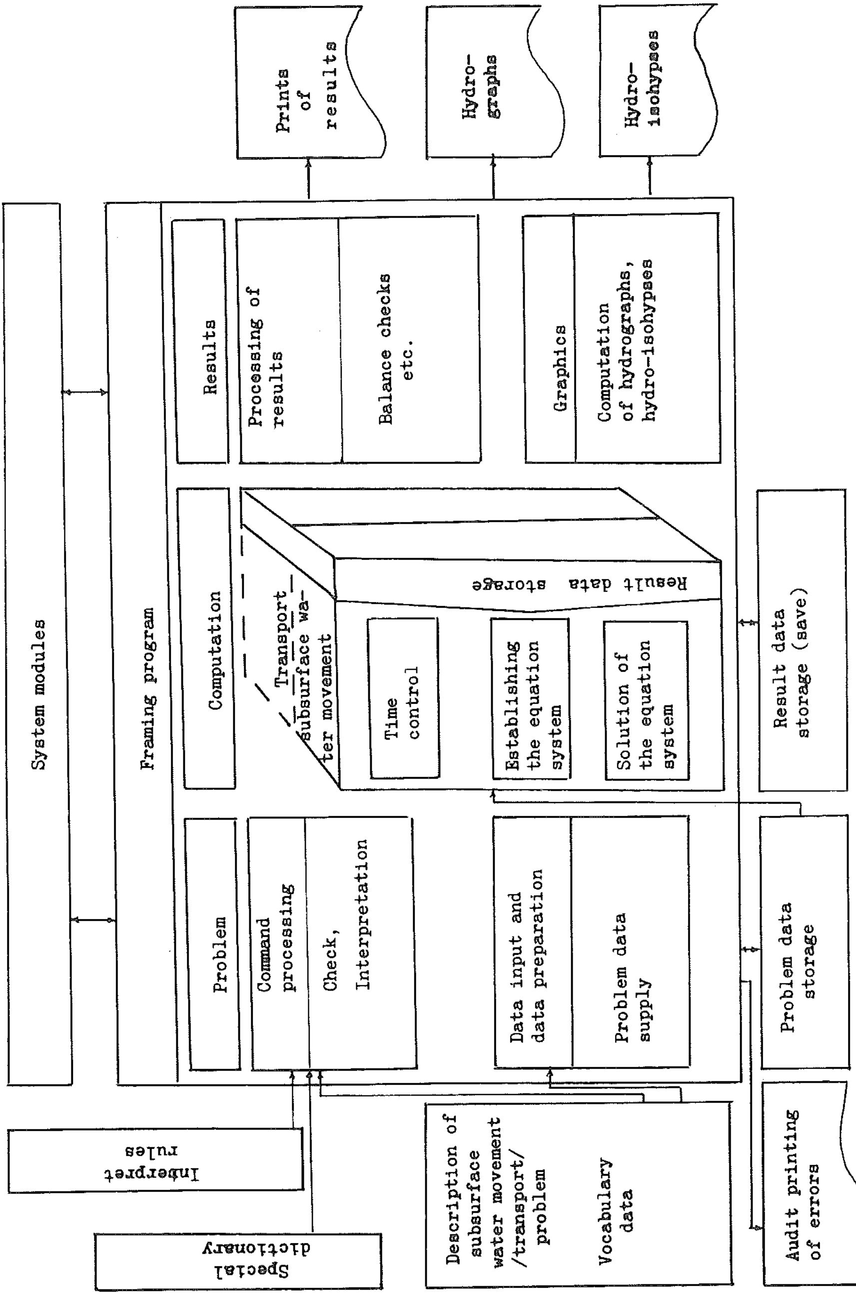

Fig. 1 General structure of GEOFIM.

Table 1 Models and applications

Type of model	*Groundwater management*	*Open-cast mine drainage*	*Hydrogeology*	*Geohydromechanics*	*Irrigation and drainage*
Horizontal-plane	*X*	*X*	*X*	*X*	*(X)*
Horizontal-plane layered	*X*	*X*	*X*	*(X)*	
Vertical-plane	*(X)*			*X*	*X*
Three-dimensional		*X*	*(X)*	*(X)*	
Parameter identification	*X*		*X*		

In the important case of horizontal-plane groundwater flow the vertical integration of the Darcy law gives:

equation of motion:

$$\vec{q} = -T \cdot \text{grad} \;\; h\,(x,y,t)$$

or

$$\vec{q} = -k \;\text{grad}\; \phi$$

equation of continuity:

$$\text{div}\, \vec{q} = S \cdot \frac{\partial z^*_R}{\partial t} - w$$

or

$$\text{div}\,(K \cdot \text{grad}\; \phi) = S - \frac{\partial^*_R}{\partial t} - w$$

with

T = transmissivity,

K = permeability,

S = storage coefficient,

h = piezometric head,

w = groundwater recharge,

ϕ = Girinskij potential,

$$z^*_R = \begin{cases} z^*_R: & \text{unconfined water table;} \\ h: & \text{confined water table.} \end{cases}$$

To simplify the solution of the system of differential equations thus obtained, the geohydrological properties (T, K, S, ...) are assumed constant in time and the initial and boundary conditions have to be formulated.

The system of differential equations is transformed by means of discretization in space and time into a corresponding system of difference equations. The discretization of the flow field in space is defined by the user.

The discretization in time results from:

- the time points at which the solution is desired,
- time characteristics of boundary conditions,
- automatic splitting of time steps in the cases of
  - * inadmissibly great changes of the piezometric head (may be defined in advance),
  - * consideration of a (given) maximum time step (standard value: one month).

The resulting nonlinear equation system is solved by iteration for every time step with the method of "ordered elimination". This method is based on a special Gauss algorithm for symmetric positive definite sparse linear equation systems. By this method, acceptable running times for the system were achieved for smaller and medium-sized problems (several hundred to a few thousand grid points).

The following practical example may give some idea of the computation time needed:

Computer:	EC 1055	
Operating system:	OS	
Model type:	horizontal plane	
Discretization in space:	400 points	
Boundary conditions:	Dirichlet-type	75 s
	Neumann-type	65 s with 2,...,10 check points in time
	Robin-type	85 s
Computational period:		2 years
Language analysis and problem preparation:		53 s
Preparation of boundary conditions:		35 s
Mesh generation		9 s
1st call: solution of the equation system, Topography:		32 s
27 calls: solution of the equation system		16,...,17 s
Total CPU time		743 s

At present, faster solution methods are being developed (decomposition methods, multi-grid methods) to apply the program system to future large-scale models (5000, ..., 20 000 planning elements).

The input of all data for the description of the problem, of the flow field and its coefficients (height, thickness, permeability values, ...) of initial and boundary conditions by the user is facilitated as far as possible by defined terminology and a number of possibilities (unformatted input, DO loops, repetition factors).

Characteristics and initial conditions can be given for grid points or any other point. In the latter case and in the case of incomplete data input an interpolation routine ensures a complete "input" of data for the whole grid.

Boundary conditions may be of Dirichlet-type (potential), Neumann-type (flow) or Robin-type (potential-dependent flow).

Special attention was devoted to the consideration of wells, because they are important technological elements both in water management and in mining (open-cast mine drainage).

Vertical filter wells may be treated as a single well, a group of wells, or as a battery of wells:

Single well:	The potentials of the neighbouring grid points are taken into the discharge formula; partially penetrating wells and interrelations with neighbouring single wells are taken into account.
Group of wells and battery of wells:	The planning element contains *n* wells which are designed in the same way; well spacing is small against the size of the element; partially penetrating and interrelation between wells of the group/battery are taken into account.

The operational regime of the wells is controlled by a given well operation function. The control of the well water level or control is made by the discharge of the well. Well water level and/or well discharge may be limited. Thus it is possible to include or exclude wells automatically during the computation.

While the coefficients of the flow field are considered to be constant in time, the boundary values may be describe in the form of potential-dependent or time functions as step functions or polygonal ones.

The solution of the equation system gives a piezometric head value for every grid point which represents the respective planning element.

RESULT OF THE SIMULATION

The user may determine the time points for which the results are printed and the extent of results. At defined moments of time a print-out of selected results is possible in variable extents.

Besides the direct solution of the equation system, namely the piezometric head, the program system indicates:

- potentials or discharges of sources and sinks,
- velocities of flow,
- specific discharge,
- boundary values at grid points,
- vertical filter wells,
- balance of inflows and discharges,
- balances for sub-areas,
- piezometric head values for defined sites of observation wells,
- hydrographs,
- isolines etc.

Each simulation run is supplemented by a balance analysis of the storage variation and of inflow and discharge values as well as by a model error assessment.

In the interactive operation, the user may have intermediate results (complete data fields or sections from them) displayed or printed.

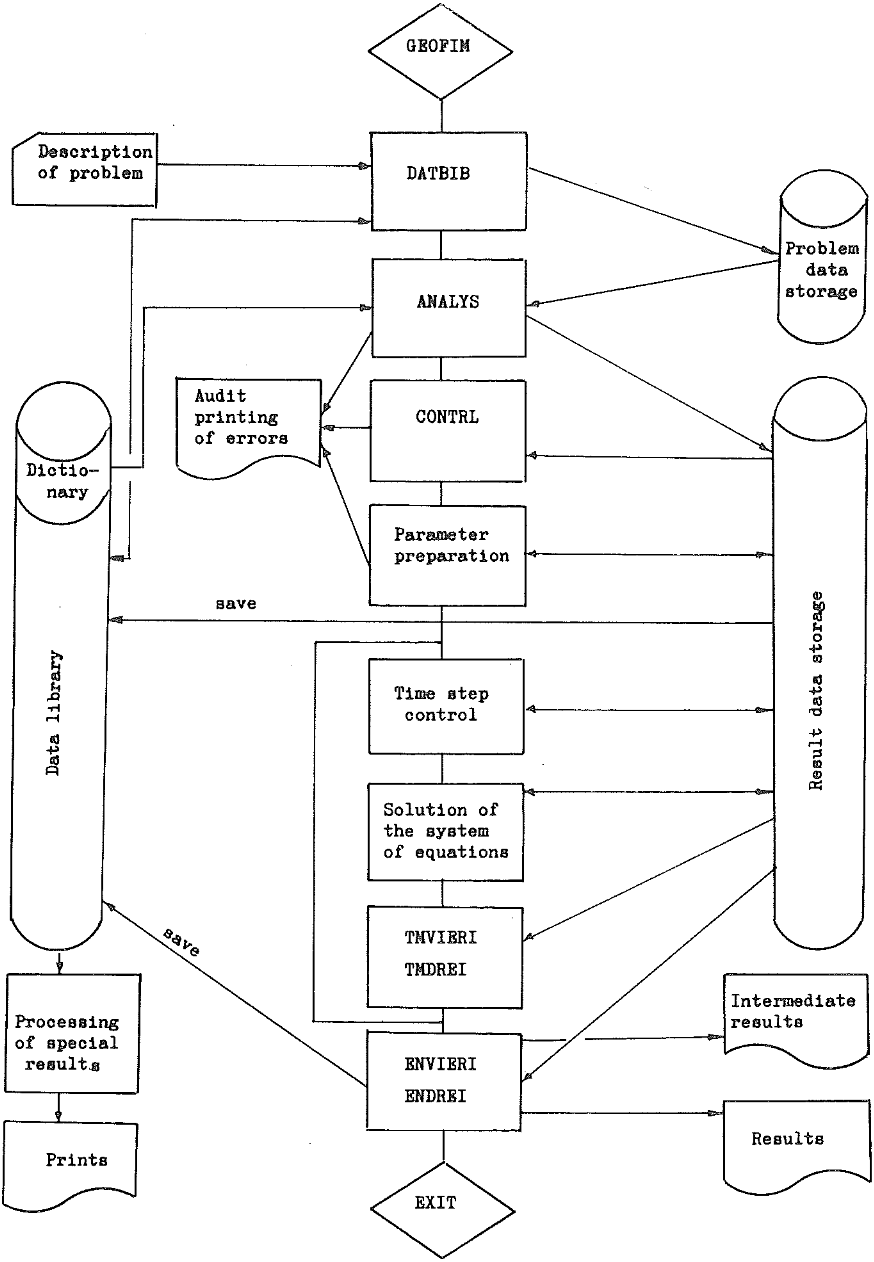

Fig. 2 Scheme of data flow "GEOFIM".

```
#JOB  testbeispiel...
 #PROBLEM
  #START
  #AUFGABE
   #MENGE
   #HORIZONTALEBEN
   #ZEITEINHEIT  d              time unit for data input
  #DISKRETISIERUNG
   #VIERECK
   #DIMENSION  10  20
   #X
    (1:10, 1:20) ...           coordinates of the grid points
   #Y
    ...
   #Z                           heights of the bottom and
    ...                         thickness of the aquifer
   #M
    ...
  #PARAMETER
   #KF                          geohydrological properties
    ...                         of the aquifer
   .
   .
  #ANFANGSBEDINGUNGEN           initial values of the
   #H                           piezometric head
    ...
  #RANDBEDINGUNGEN
   #KLASSEN ...
    #HRAND  ...                 description of boundary
    #QRAND  ...                 conditions
    #LRAND  ...
  #BERECHNUNG
   #BEGINN    0                 simulation time
   #ENDE    730                 0 - 730 days
   #DTMAX    60
  #ERGEBNISSE
   #KLASSEN                     classes for prints
    #H
     .
     .
     .
#END
```

Fig. 3 Example of the sequence of keywords for a prepared problem of groundwater flow.

APPLICATION OF THE PROGRAM SYSTEM GEOFIM

GEOFIM is run on ESER computers EC 1040- EC 1055 under the operating system OS. Figure 2 shows the flow of data. Data preparation and simulation (smaller and medium-sized problems) may be run in interactive mode or in batch-processing mode. The simulation of larger problems is done in batch-processing mode.

Problem description, preparation of all input data, control of the computations/simulation and selection of volume and frequency of print-out of results are made by the user by means of defined vocabulary. Figure 3 shows an example for the data input of a groundwater flow problem.

Comprehensive documentation is available on the setting up of a "GEOGIM-JOB", and on the definitions and the use of the vocabulary on the utilization of the numerous facilities for easier data input.

The program system is a joint development by institutes of water management, mining, geology and higher education and it is hoped it will be of general application.

It is possible to purchase the program system GEOFIM from the Institute of Water Management, Berlin.