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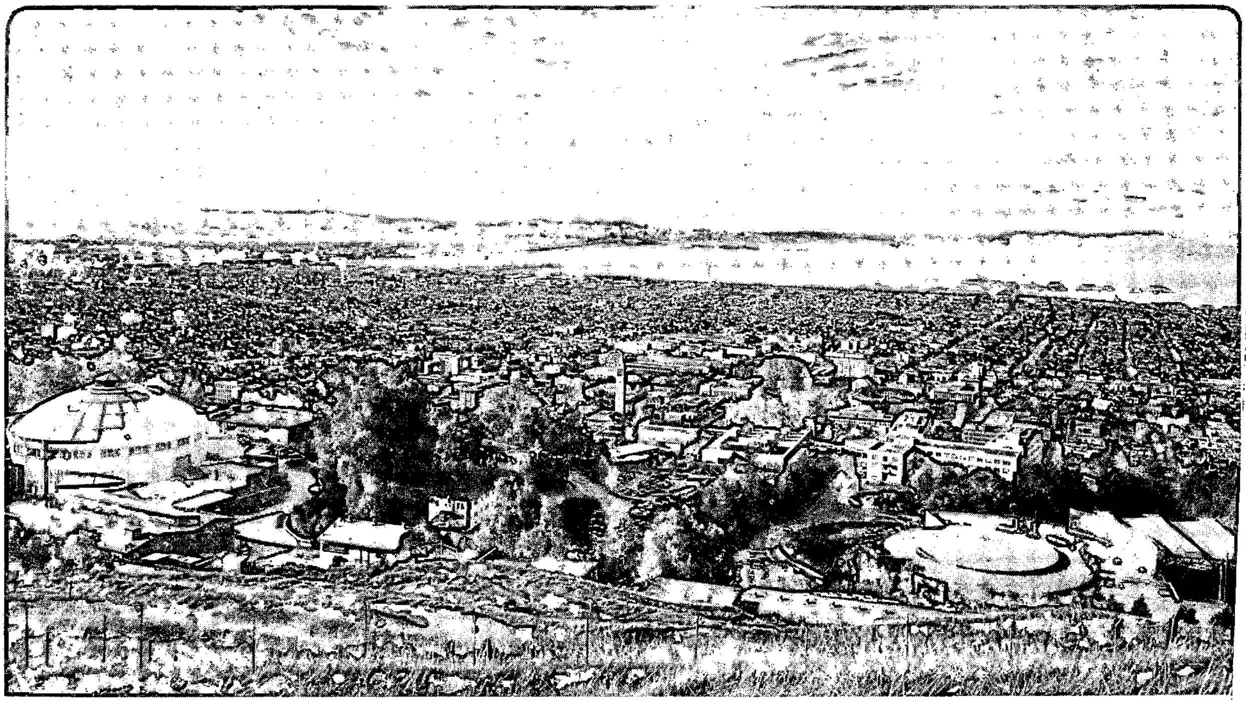

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ABSTRACT

Methodological aspects of the numerical modeling of the groundwater contaminant transport for the Lake Karachay area are discussed. Main features of conditions of the task are the high grade of non-uniformity of the aquifer in the fractured rock massif and the high density of the waste solutions, and also the high volume of the input data: both on the part of parameters of the aquifer (number of pump tests) and on the part of observations of functions of processes (long-time observations by the monitoring well grid). The modeling process for constructing the two dimensional regional model is described, and this model is presented as the basic model for subsequent full three-dimensional modeling in sub-areas of interest. Original powerful mathematical apparatus and computer codes for finite-difference numerical modeling are used.

Table of Contents

List of Figures

Figures **Page**

INTRODUCTION

This report presents a status of the development of the numerical model of the groundwater flow and contaminant transport from the surface radioactive waste reservoirs of PA "Mayak." The primary reservoir is the Reservoir-9 (Lake Karachai, or R-9), which contains high density, radioactive solutions. The groundwater is confined to fractures in a volcanic rock massif which is considered as a complex aquifer. The scope of the development is the modeling process which is composed of: (1) review of the input data, (2) construction of an idealized model with the determined hydrogeological conditions and (3) an application of numerical methods to the non uniform medium with complex conditions. Also the 2-dimensional modeling is presented as the basic regional model for the subsequent full 3-dimensional modeling in the sub-area of interest. The numerical modeling is considered as a tool of hydrogeological exploration; and details of the mathematical developments are not presented here.

The general goals of the modeling are:

- to check the inconsistencies in the independent input data (e.g., the pump test data, flow- and contaminant monitoring data, water balance data of the source reservoirs, etc.);
- to coordinate the input data with the calibration procedures;
- to realize predictive computations.

The main feature of this modeling is that there is a great number of independent input data obtained by hydrogeological surveys, incorporating both the monitoring well grid and the pump test grid. The historical monitoring data cover a period of about 30 years.

The modeling process actually consists of a system of numerical models: (I) the basic regional 2 dimensional model (mainly as the flow model); (2) the internal sub-regional full 3-dimensional model (coupled flow and transport); and (3) local full 3-dimensional models. The system provides direct- and reverse interactions between all the models.

The main problems are associated with the idealization of the hydrogeological conditions, validation and performing the calibration procedures, the respective analysis of the input data, performing the numerical explorations, assessment of the sensitivity and uncertainty of the model, and also with the assessment of the adequacy of the model for simulated natural processes.

It is important that original mathematical methods and software are used for the numerical modeling. We currently have the computer codes to model the time-dependent 2-dimensional flow and to model the contaminant transport for the neutral non-sorbed components. The software for the 3-dimensional modeling is being tested now. The main advantages of the applied finite-difference numerical methods are (1) the large number of cells allowed, and (2) the high computation speed afforded by fast convergence.

The development of the numerical models is one of several tasks of the hydrogeological service for the PA Mayak Area and it is performed by the Group of Dr. Samsonova of PSA "Hydrospetzgeologiya" (input data, modeling process) in collaboration with the Group of Dr. Zinina of IPPE, Obninsk (numerical methods software, code testing, and numerical explorations).

The input data used for the modeling was obtained by several organizations at various times since 1951: PA "Mayak", MINATOM and its divisions as PROMNIIPROEKT and VNIPIET, PSA "Hydrospetzgeologiya", Institute of Biophysics (MINZDRAV), Institute of Physical Chemistry (Russian Academy of Sciences).

The authors would like to acknowledge the permanent support of Dr. Evgeniy Drozhko, Deputy of General Director of PA Mayak. This publication would be impossible without the support and the encouragement of Dr. Chin-Fu Tsang, Group Leader of LBL and Russian-American Center of Contaminant Transport Studies, whose generous assistance will allow this research to continue.

1. BACKGROUND

The systematic hydrogeological service for the Mayak Area was organized in 1964 in connection with the exploration of the existing surface radioactive waste reservoirs that are the contaminant sources for groundwater. These are Lake Karachai, Reservoir-17, and also the cascade of the artificial reservoirs on the Techa River (Reservoirs R-3, R-4, R-10, R-11) (Fig. 1).

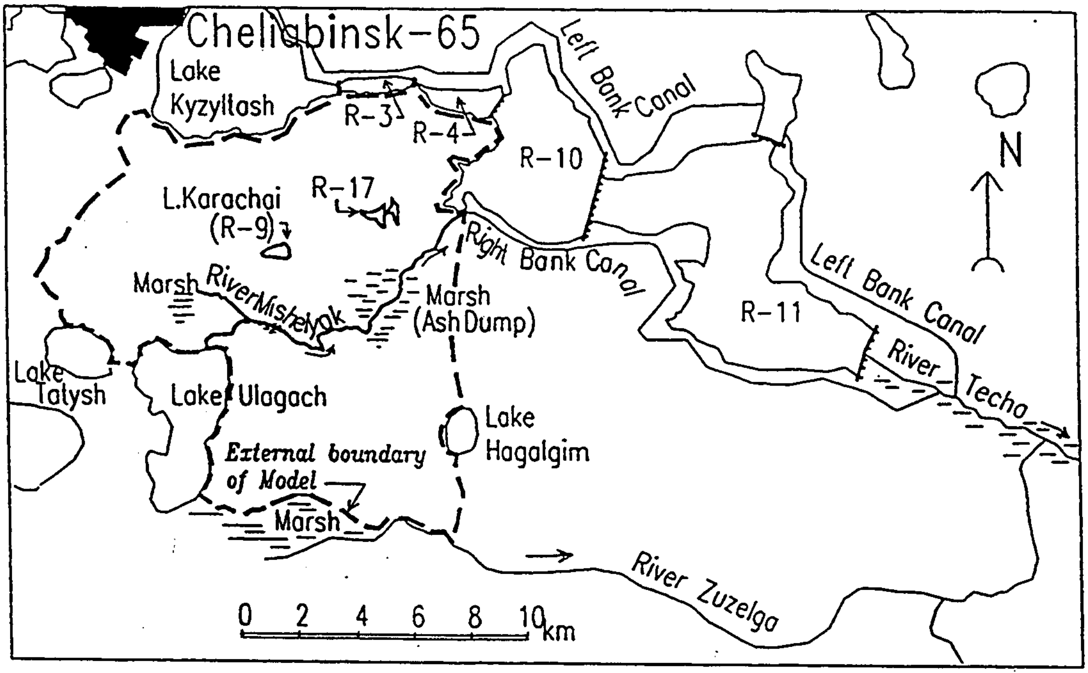

Fig. 1. Geographic elements in vicinity of Lake Karachai, and the model boundary.

Lake Karachai, which contains high density solutions (1.06-1.09S g/cm^3) of complex composition, is the most dangerous from the point of view of contamination of groundwater. Concentration of nitrate-ion is 50–77 g/L, and a wide spectrum of radionuclides are present here.

At the present time the waste disposal into Lake Karachai is reduced very significantly, and the process of covering this lake has started in accordance with the complex program of organizing the closed cycle of radioactive waste reprocessing and the remediation program. However, the big volume of the waste solutions (about 5 million m^3) entered the groundwater in the course of exploitation since 1951, and the contaminant transport process continues in the aquifer. As a consequence a contaminant plume with a dispersion zone has been formed in the groundwater.

The final goal of the hydrogeological explorations is the assessment of both the necessity and the possibility to localize the contaminant plume in the aquifer by engineering actions, and also to extract some volume of the contaminated water for subsequent cleaning with above-ground technology. At this point it is necessary to predict the spreading of the contaminant plume under the influence of natural factors and to assess consequences of the probable safety measures. Thus the following predicting tasks are defined:

- to predict the contaminant plume behavior (shape, concentrations in time);
- to predict the discharge of the contaminated groundwater into Mishelyak River;
- to predict the efficacy of the safety engineering measures.

It is important to note that we do not try to determine the long-term safety problem (for 10000 year and more). It is only presently possible to predict problems 50-100 years in the future, a period that is comparable to the available historical data (30 years) used for constructing the model.

From 1957 to the present time, a significant volume of independent input data has been obtained and processed. These data characterize the hydrogeological situation and the contaminant transport process from different directions. Considering the processes of interest as the processes in the natural system, we can describe the modeled system:

1) The input conditions of the modeled system: the boundary conditions and the recharge-discharge conditions. These are the historical observation data about the water level of lakes, precipitation, and the ground water supply system;
2) Parameters of the modeled system (the medium parameters). These are the field pump test data, parameters of the flow exchange between the surface water and groundwater, the transport parameters, etc.;
3) The output data of the modeled system, i.e., functions of the processes occurring. These are the groundwater table monitoring data, the contaminant monitoring data, the leakage flow data for Lake Karachai and other reservoirs.

The groundwater of the area is contained in the fractures of the volcanic rock. It is observed that open fracturing decreases with depth, and this zone is restricted to depths of about 50–150 m ("exogenous" fracturing). Thus, we can first consider the concept of a horizontal complex fractured aquifer with a thickness of about 100 m in average [1, 2].

We accept the assumption of a continuous medium, which is typical in hydrogeological practice for fractured rocks, since the scale of processes of interest is usually much larger than the dimensions of any separate fractures that are conducting channels. This assumption has been verified both by the field pump tests and by the monitoring data. All observation wells react to disturbances by cluster tests, and the time-spatial tracing of the disturbance shows that the process behavior does not contradict the Theis model for the "double porosity" medium. Also, monitoring shows that the groundwater flow behavior and the contaminant process behavior correspond to the recharge-discharge conditions of the area if we consider the scale of interest. Thus the processes of interest are defined by the multitude of fractures and may be described with integrated parameters that will be used as the effective parameters in any models of the continuous medium.

In principle the high density of the leaking solutions does not allow us to idealize the process as 2 dimensional, and requires 3-dimensional modeling. However, we have a situation where the considered flow area (about 200 km^2) is much larger than the thickness of the aquifer (100 m). This allows us to consider the groundwater flow as a 2-dimensional process for the test data processing and also for the numerical modeling on this "regional" scale.

The hydrogeological parameters of the aquifer are determined by a number of pump tests including about 100 single tests (a grid of testing) and about 20 cluster tests (Fig. 2). Several interval tests have been performed, and their results have been compared with the fracturing descriptions (including telephotometric data). The grade of the non-uniformity of the medium is very high: the effective transmissivity varies significantly over the area: from 0 to 200-500 m^2/day. The effective value of porosity also varies concordantly, from 0.02 to 2% [2].

The groundwater flow- and contaminant transport observations have been performed since 1957. First, these observations were performed in separate wells near Lake Karachai without a

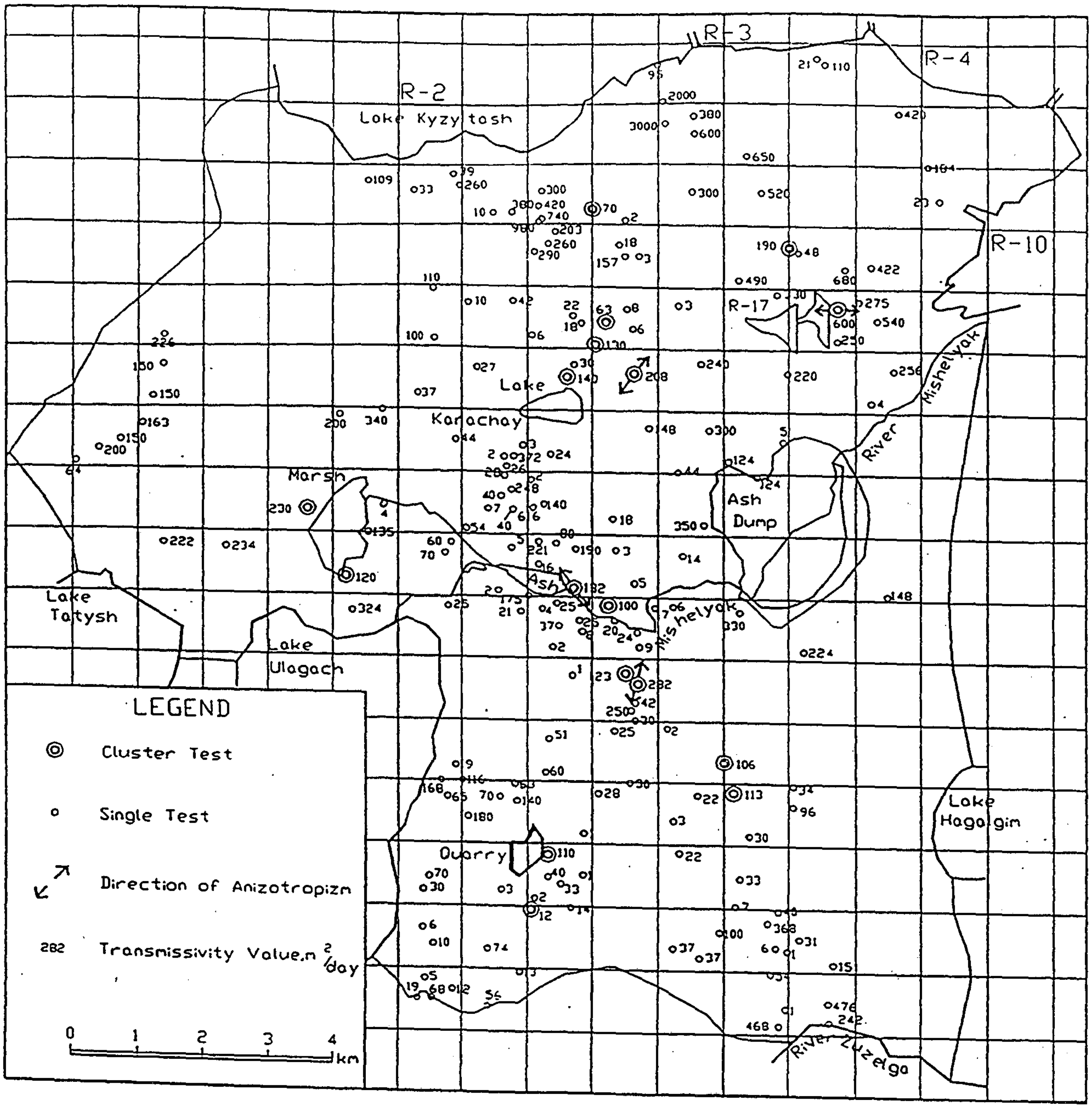

Fig. 2. The modeled area and the array of field pump tests.

well-grid system. However, since 1964 there has been a monitoring well grid which incorporated about 150 wells by 1970 (Fig. 3). The leakage flow data (a calculated value) are shown in Fig. 4, along with the data of observations of atmospheric precipitation and the area of Lake Karachai.

All these data permit definition of the time-spatial regularities (features) of both the groundwater flow- and the high density contaminant transport. Density differences cause the gravitational effects on convection. Near Lake Karachai the convection is defined by the disturbed flow, since the leakage from Lake Karachai substantially affects the natural groundwater flow. The contaminant transport process includes the dispersion, which may be considered in a given case as a result of the influence of such factors as the hydrodynamic dispersion, interactions between the contaminated water and the host rocks (including sorption), and radioactive decay. Thus, the combination of the conditions of contaminant flow entering into the aquifer and conditions of the dispersion lead to forming the contaminant plume as the combination of the "plume body" and the dispersion zone [1, 4].

The conceptual model of the contaminant transport process is as follows. The dense solutions leak down through the lake bottom by gravity-driven flow and displace the fresh groundwater. The reduction of the permeability with depth in the aquifer due to decreasing fracture density defines a situation which tends to cause the contaminant solutions to spread approximately horizontally, as radial flow near a source. Thus, on the one hand, the dense solutions tend to occupy the lowest position in the aquifer, but low permeability restricts their motion. With flow, hydrodynamic dispersion becomes important. Also, there is macrodispersion due to the hydrogeological non-uniformity of aquifer. Any interactions with the host rocks define the total delay of the contaminant transport, and the radioactive decay reduces the concentration of the short-lived as well as long-lived, e.g. Sr, Cs radionuclides. With the distance from the source, the radial flow is strongly changed under influence of both the filtration non-uniformity and the recharge-discharge conditions. This is caused primarily by the infiltration recharge areas, and also any surface lakes, River Mishelyak, and the groundwater-supply systems. The combined influence of all factors has caused the observed evolution and shape of the plume, that has at

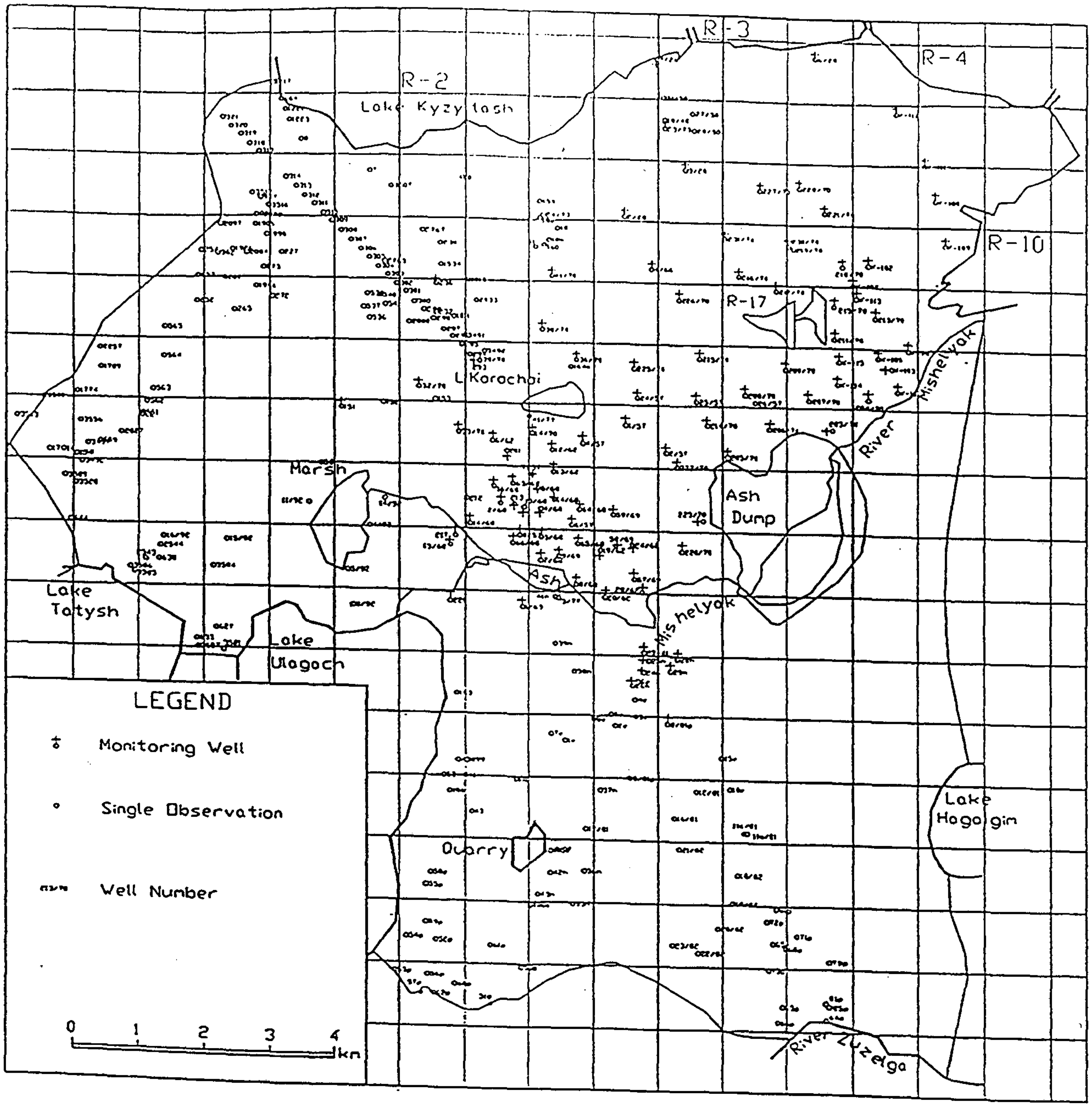

Fig. 3. The modeled area and the array of observation wells.

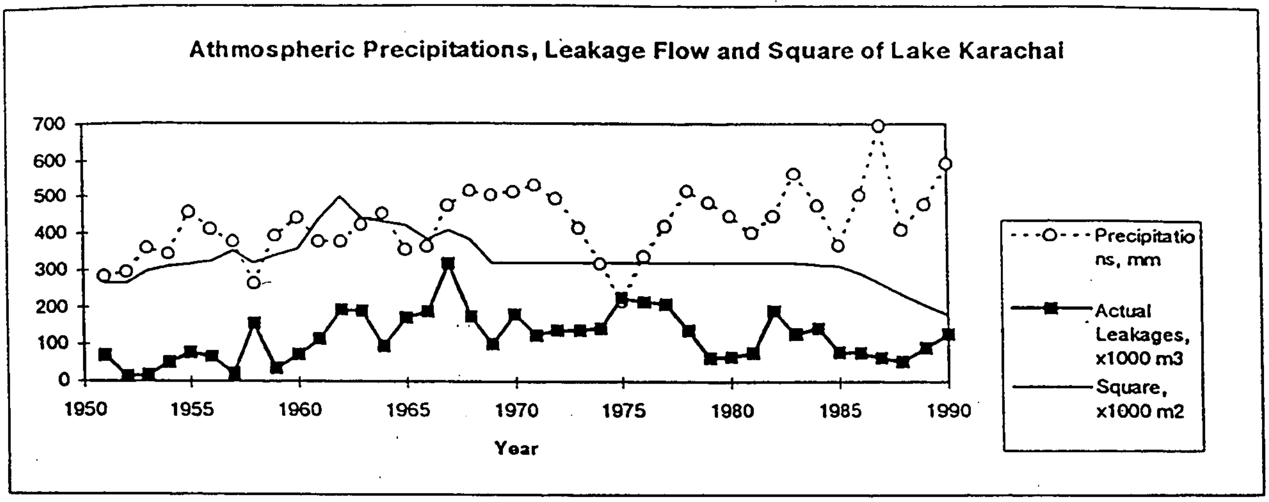

Fig. 4. Dynamics of the leakage flow of Lake Karachai, along with its area and precipitation.

present a north-south orientation. Concentration of the transportable components reduces with distance from the source and increases with depth. At present, most of the contaminated area shows little change over time in concentrations of the contaminant indicators.

The accuracy, reliability and the representative ability of all input data are different. However these data reflect parts of the integrated natural system, and therefore it is necessary to discover possible contradictions in all data and to assess their importance. Thus the place of numerical modeling is sufficiently certain in a given case. It is evident that hydrological conditions are complex and require their adequate reflection in the model. Complexity arises from the spatial non-uniformity of the medium, the spatial distribution of the recharge-discharge conditions and the boundary conditions, etc. As the most flexible modeling tool, numerical modeling allows exploration of the processes of interest in many variations. It allows one to perform sensitivity analyses and to assess the significance of the input data errors, and therefore it allows one to perform necessary calibrations. Finally this method allows one to perform predictive computations and to verify the adequacy of the model for simulated natural process.

However, the significance of this method must not be exaggerated. We understand that although there is a huge volume of input data in our database, nevertheless their quantity and quality may be insufficient to realize the complex modeling that is necessary to most accurately reflect the phenomena of interest. In this case, the modeling process must provide the basis to design subsequent tests and additional observations.

2. THE CONSIDERED SYSTEM OF THE NUMERICAL MODELS

In this section, we consider the following questions. How is a system approach utilized for the given modeling tasks? How are the modeling goals, scales, idealizations and mathematical settings connected?

The necessity to take into account variable density convection requires 3-dimensional modeling in principle. However, it is possible to conduct some explorations of the hydrological processes on a regional scale by using a 2-dimensional model. It is not correct to ignore the 3-dimensional character of the groundwater flow for the contaminated area, nor for the source lakes and for the recharge-discharge areas. This will be the scope of the 3-dimensional modeling. Different scales are required to model the evolution of the plume compared to modeling the local disturbances or recharge-discharge processes.

Several circumstances require consideration of time-dependent conditions. First, it is impossible to ignore or to average correctly the changes of the water level in Lake Karachai and also Reservoir-17 over time. For example, the water level of Lake Karachai was being raised by artificial filling and the water density was increasing during most of the exploitation. Recalculating to the fresh water level, the increase had amounted to about 8 m in the period from 1951 to 1970 (1951–249.3 m, 1970–257.2 m, 1977–256.0 m).

Reservoir-17 began to be filled in 1954 in marsh valley. The increase of the water level is about 6 m (near the dam) compared to the low point of the former marsh (~230 m): 1954–234.2 m, 1962–237.0 m, 1969–236.0 m and further 236–236.5 m. Thus, the sources caused changes of the natural groundwater flow structure. In addition the plume behavior depends on the fluctuations of the infiltration recharge significantly. Also, the mode of the active groundwater supply wells and the possible safety measures are time-dependent.

All these considerations are united with the processes of interest, and therefore an integrated system of interacting models is desired. The developed software allows us to employ the following system of the numerical models (step-by-step):

In the first stage, the problem is to model the regional groundwater flow, to check and to calibrate the parameters regarding the monitoring data, and also to separate the sub-area for the 3-dimensional modeling. In this scale a 2-dimensional flow model is constructed. The transport model for the neutral non-interacting component is performed on this 2-dimensional grid. The high density of the contaminant water is taken into account by recalculating the water level in Lake Karachai to the fresh water level. To provide the possibility of comparing the results with monitoring data, we also recalculate observed levels of the contaminated groundwater compared to the fresh groundwater table for each monitoring well which contains high-density contaminated groundwater. The high degree of idealization by this modeling is obvious, but it is in accordance with the flow modeling goals. Also the usage of the 2-dimensional modeling of contaminant transport is defined by the following limited tasks.

First, the analysis of the plume behavior allows us to assume that the consequences of errors in data may be compared with the 3-dimensional effects, since the plume area is much greater than the effective thickness of the aquifer. In addition, the aquifer bottom may be considered as an approximately horizontal surface. Therefore, after the 3-dimensional modeling we should assess the significance of the 3-dimensional effects and errors of the 2-dimensional idealization. Secondly, transport modeling is a convenient way to illustrate the behavior of the time-dependent flow, since in a given case we trace the front of the flow from the source. Also, exploration of the transport process on a regional scale helps to assess the significance of both the average effective porosity of the medium and the dispersion coefficients. Thus, at the end of this stage we have a 2-dimensional flow model and the border lines of the separated sub-area relevant to the 3-dimensional modeling.

In the second stage this 3-dimensional modeling is performed for the selected sub-area by the dispersion scheme (coupled flow and transport). The main features of the scheme are that it takes into account time dependent processes with variable density convection in an unconfined aquifer interacting with the surface water, and also takes into account the relief of the aquifer bottom.

The following interaction occurs in this model system: the results of the 2-dimensional modeling are used to set the boundary conditions for the desired 3-dimensional sub-area, and results of the 3-dimensional modeling are used to check the adequacy of the averaging of the parameters for the regional model.

In the third stage the proposed safety actions are modeled. This modeling is performed initially with the regional 2-dimensional model to define the borders of the hydrodynamic disturbance and to set the boundary conditions for the subsequent 3-dimensional modeling in the chosen sub-area of interest. This 3-dimensional sub area may contain its own local sub-areas to model the actions in detail. Also at this local scale, we intend to model the interaction between the groundwater and the surface water for Lake Karachai and for the discharge area of the Mishelyak valley. The developed code permits selection of similar local sub-areas dynamically with the 3-dimensional modeling for the larger sub-area.

3. A GENERAL APPROACH TO THE MODELING PROCESS

The modeling process consists of (1) the validation of the model idealization of observed hydrogeological conditions, (2) the calibrations, and (3) the predictive computations.

From the point of view of the general approach we construct a time-dependent model that handles many spatially distributed parameters with many factors affecting the process of interest. The monitoring data of the groundwater table behavior and contaminant behavior, and also the data of the water balance of the source lakes can be used as the quality criteria for the modeling process. The presence of these data implies that we can and must perform not only the model validation but also must bring in accordance all input data using the known calibration method. The main problem here is that the usage of calibrations must be constrained by the limits of the usage and by the criteria of the calibrations' sufficiency. Our efforts are directed to avoid transforming the calibrations into an attempt to solve inverse problems with the artificial selection of parameters, since if there are many spatially distributed parameters in the model then this selecting introduces a great deal of uncertainty.

It is expected that the methodology of calibrations permits this procedure not only to be sufficiently validated (an "uncertain" term), but also to be proven certain and to be repeatable. For example, these procedures are performed for 2-dimensional flow modeling in the following manner. After the first numerical computation of the direct problem, the results (the calculated groundwater table and leakage rate) are compared with the observed data, and the differences are fixed. We are then able to analyze the agreement of the monitored and modeled flow, first qualitatively, since the recharge-discharge areas and general flow directions must correspond. The real leakage rate must also correspond to model values. These are the bases for the initial calibrations. Next, we quantitatively explore the deviations for each monitored point. After the draft sorting of these values we perform the numerical test series to check the model sensitivity to the possible variations of the different parameters. The most important parameters are then determined and the area of influence is defined. On the basis of these computations and respective analyses of the input data, we are able to judge the admissibility of the fixed deviations. Only after this procedure can we validate (a) the list of parameters requiring calibrations and (b) their probable value range. Then the calibration cycle is repeated step by step so that both negative and positive deviations are adjusted until the deviations fall into the admissible range.

The initial scheme of the modeled system was validated and the probable variants and some variations were recognized and prepared for modeling before the first computations. Thus, the calibrations are not a process of the arbitrary selection, but they are a realization of the limited corrections of certain values, which are determined beforehand and independently. By this the probable ranges of the variations are also validated beforehand.

The spatial distribution of the transmissivity is most certain, because we almost have a grid of pump tests. Therefore, calibrations are most limited in this part. However, the density of the grid is not yet sufficient to assess the spatial distribution of transmissivity correctly (e. g., using geostatistical methods). Thus, we use a scheme where each tested point represents one uniform element of the area. In this case, calibrated values of transmissivity must not cross the error range of the pump test data (approximately +/- 30%) for tested points. Obviously, essential calibrations are possible by varying the geometry of the uniform-transmissivity elements of the area, since errors of the interpolation and extrapolation of the test data may be very significant. In doing this the monitoring data show that certain significant elements of non-uniformity may not be discovered directly by pump tests, although these elements can be reflected indirectly in the monitoring data as areas of differing gradient of the groundwater table; for example, in the area to the east of Lake Karachai, where we observe high gradients of the groundwater table. Therefore, we must assume the possibility of considering additional geometric elements of non-uniformity, that are not directly caused by test data. The model explorations have confirmed this situation. Although it is not desired, we have to use elements of the area where the value of transmissivity is selected practically arbitrarily on the basis of modeling, by calibrations only. The initial range selection is limited only by minimum or maximum values of transmissivity for the entire modeled area. Thus, we take into consideration that variations of gradient of the groundwater table are caused by the relative values of transmissivity, but the absolute values are controlled on the average only, through such indices as the value of the leakages.

However, there is the more difficult situation in connection with infiltration recharge conditions, since their input data are much more uncertain and insufficient. Also, data of such transport parameters as porosity and dispersion coefficients may be insufficient.

Thus, the calibrations have the described limits, though these limits have different importance. However, we have too many calibrated parameters to try to calibrate them simultaneously. There are too many uncertainties in such an inverse problem. I is necessary then to divide the problem by separating certain stages of the calibrations.

Finally, we consider the time-dependent processes when in principle both the transmissivity and capacity parameters affect the groundwater flow in a general case. However, the long historical observations of the groundwater table in comparison with the surface water behavior show the periodic character of fluctuations of these conditions in concordance with the fluctuations in precipitation. Because of this the long time trend is insignificant. The historical data then allow us to calculate the reliable average values of all conditions, and we can distinguish the stage of modeling for stationary conditions.

Analyses of fluctuations of the groundwater table in the monitoring wells, fluctuations of the leakage from Lake Karachai, and the analysis of the historical evolution of the contaminant plume in comparison with the precipitation dynamics show that there is insignificant influence of the infiltration recharge at the end of a 2-3 year dry period. We therefore consider the stationary problem first without regard to infiltration recharge. This assumption helps to fix the gross errors of the initial transmissivity scheme and to calibrate this parameter group independently. We use the clear constraints that in this assumption the computed groundwater table must not be higher than the observed groundwater table and the computed leakage rate must not be less than the actual leakage rate.

The calibrations then include the following stages:

1) the preliminary checking and calibrations of the transmissivity map for the dry period (steady mode, no infiltration recharge);
2) checking and calibrations of the infiltration recharge with the transmissivity in couple (steady mode, average conditions);
3) checking of the flow model for the time-dependent conditions; calibrations of the hydraulic capacity parameters (dynamic mode).

In planning to use the calibrations, we took into account that in each stage of this process we compensate for errors that were made in the preceding stage. This compensating role is connected mainly with the infiltration recharge parameters (in combination with the geometry of the recharge areas). We were aware that there is a known risk of losing the real physical sense of the model. A cause is that if the model has a number of spatially distributed parameters, then calibrations may lead to gross errors in some of the parameters, even though the model may remain in sufficient agreement with the control data. In this case, the model may still be useful for quantitative predicting (within narrow limits), but the physical sense will be distorted, and we will obtain the wrong idea about values of any effects in connection with any separate parameters.

Thus, although we have a number of tests and monitoring data, the total grade of uncertainty of the model remains sufficiently high and requires an assessment. Finally it is desirable to quantify the grade of uncertainty of the model or to illustrate this problem by a sufficient number of the modeled variants. The main method is to use special numerical tests to perform the sensitivity analysis. However, the conditions for these tests are not determined easily and the process is very difficult. This section presently uses the methods of perturbation theory.

A significant problem is the assessment of agreement between the model and natural processes, though it is clear that errors in the model are explained approximately by arbitrary errors of input data. However, such an approach is not as critical if we use calibrations. If the calibrations are applied, then the adequacy of the model is defined by the modeling process itself. However, experience of the modeling shows that possibilities of the calibrations may be limited. This is a reflection of both the imperfection of the accepted conceptual model and the insufficiency of the input data. Thus, one can pose two following questions: a) how do we determine that the calibration process is adequate, and, b) what is the grade of realization of these procedures ?

The second question is only significant with respect to the principal possibilities of calibrations, and the resulting assessment is problematic. However, the first question is critical, since it is difficult to complete the calibrations without knowing when to stop (if reasonable expenses of the work time are taken into account). At this point an analysis of the groundwater table range in the modeled system, gradients, and the test modeling results (using the different densities of the computation grid) show that any calibrations are not reasonable if the deviations are less than 0.5 m. For the separate high gradient area, we agree if the deviations are about 1-3 m. Deviations less than 1 m may be acceptable.

4. A SHORT REVIEW OF THE MATHEMATICAL SETTINGS, METHODS AND SOFTWARE

The validation of the 2-dimensional setting with the separated solution of the flow and transport tasks was covered when the accepted system of the numerical models was described. The flow process is described by the differential equation using the Dupuit-Forcheimer-Boussinesq approximation relatively to the fresh groundwater table:

$$\mu^* \, dH/dt = d(km^* \, dH)/dx + d(km^* \, dH)/dy + w$$

(or $\mu * dH/dt = d(kH * dH)/dx + d(kH \sim dH)/dy + w$, when we model conditions of high fluctuations of the groundwater level with respective significant changes of the aquifer thickness, e.g., to assess consequences of the engineering hydrodynamic actions with significant depression or repression of the groundwater table)

where: km- transmissivity, (m*m/day),

k - coefficient of conductivity, (m/day),

m - thickness of aquifer, (m),

μ - hydraulic diffusivity,

$\mu = km/a$, a - hydraulic diffusivity coefficient, (m*m/day),

w - rate of a recharge-discharge, (m/day),

H - level of the groundwater table, relative to the fresh water, (m),

t - time, (day).

The density is taken into account by recalculation of the water level in Lake Karachai (flow exchange condition at Lake Karachai in the model):

$$H=(\Sigma(m_i*\rho_i))/\rho+Z$$

where: H - the fresh groundwater level, m;

m_i - thickness of the separate contaminated interval in vertical section, m,

ρ_i - density of the contaminated groundwater in this interval, kg/m3,

ρ - density of the fresh water, $\rho \sim 1000$ kg/m^3,

Z - elevation of the conventional aquifer bottom, m, (Z = 150 m).

The transport process is described by the respective transport equation with dispersion.

The initial differential equations of both flow and transport are approximated by systems of linear algebraic equations with the Euler implicit scheme and the control volume method. These systems are solved by the conjunct gradient method, preconditioned by an incomplete factorization scheme (basic development by Dr. N.I. Buleev, 1965). The geometry is described as the integration of zones of uniform properties.

The main advantages of the finite-difference numerical methods used in the software are the high power of the computation grid (number of cells) and the high computation speed (fast convergence). These iterations usually converge for any complex combinations of input data and conditions, when other numerical methods may not give convergence. For example, the Intel 486 CPU (66 MHz) requires about 1-1.5 minute of computation time for one time step by solution on an irregular grid with about 40000 cells (the protected mode of CPU is used, 4 Mb RAM are required). The computer makes about 2 iterations per second. Usually 100-200 iterations are required for one time step, about 400 iterations are required for a stationary solution (hydrodynamic task) from zero-approximation of the field, and less than 100 iterations are required for a one time step of the transport task.

The geometrical input data have a vector representation, and transferring of these vector data to the model grid is performed automatically by the special averaging procedure.

The program GEON-2D (developed in 1991-92) addresses the time-dependent flow and transport tasks (neutral non-sorpted components) in a two-dimensional setting. This code was developed for IBM PC/AT 386 (and more) using MS DOS and consists of several functional-complete modules that are connected about the data by the common structure. The program components, that require the dialogue user interface, provide the following functions: the input of the graphical and digital data; showing and editing the initial maps; presentation of the computation results; and checking of the balance for the areas of interest.

The GEON-2D code was used for the 2-dimensional flow and transport modeling of Lake Karachai, Reservoir-17, and the Techa River cascade.

In 1993 the GEON-3D full three-dimensional modeling code was developed and is now being tested. This code utilizes the dispersion scheme, taking into account time-dependent flow, density convection, the free groundwater table interacting with the surface water, aquifer bottom relief, and the flow exchange occurring through the bottom of the aquifer.

5. THE TWO-DIMENSIONAL MODELING

5.1. THE MODEL INPUT DATA AND THE IDEALIZATION OF THE HYDROGEOLOGICAL CONDITIONS.

The numerical model requires certain sets of the input data which include the data on the properties of the medium, recharge-discharge conditions, boundary conditions, and respective parameters to describe these conditions. It is difficult to provide the multi-parametrical model with necessary input data.

This problem has two aspects:

First, the process involves several physically heterogeneous parameters and conditions that are included in the initial differential equations. These are the water transmissivity, the hydrogeological diffusivity, the parameters to describe the hydraulic connection between the surface water and groundwater (the flow exchange parameters), the recharge-discharge conditions, the porosity, and coefficients of hydrodynamic dispersion.

Secondly, all these parameters (and also the conditions) are spatially distributed in a non-uniform area, which creates a huge group of geometric parameters. This situation multiplies the number of the model parameters many times. The main input errors are associated with the discrete character of data and arise from errors of the interpolation and extrapolation of the test data. It is also obvious that methods of processing the test data also have limited precision, since the solved inverse problems are incorrect mathematically. However, the uncertainties become higher if any indirect data are used.

In addition, the known problems are associated with both preparing and using the historical data for calibrations. The time-dependent setting expects validation of the time approximation. A value of the time step is first defined by the time scale of the features of processes of interest.

Analyses of the monitoring data, the hydrological data and the water balance data show that it is necessary to take into account the fluctuations of the infiltration recharge that reflect the 10-12 year cycle of atmospheric precipitation. It is then possible to ignore seasons in each year, and a one-year step is sufficient to reflect desired fluctuations. Other discussed time-dependent processes tolerate this discretization of the time axis. Secondly, it is necessary to take into account the time resolution of the input data. Here the frequency of the observations amounts to several points per month, which allows us to obtain reliable annual average values.

In connection with the errors of the monitoring data used for respective comparisons, it is possible to note the following: The water table measurements are precise obviously, and the error of averaging about the time-step is insignificant. However the recalculated (about density) hydraulic heads take part in the computation scheme for the contaminated area. These recalculations may have significant errors as is shown by the substitution of the extreme values for the area near Lake Karachai.

In connection with calculations of the water balance of Lake Karachai for obtaining the leakage value (see Fig. 4) we can make the following note: This value is calculated as a difference between the input flow rate (the liquid waste disposal, adding fresh water to support the water level in Lake Karachai permanently as a constant value, atmospheric precipitation) and the evaporation rate. Considering the respective probable errors of these calculated components we see that the total error may be approximately 30-50% for the separate time step (1 year).

Therefore, the considered hydrogeological data are characterized by typical objective errors of the input data. However, the high quality level of these input data is defined by the high density of both the pump-test grid and the monitoring well grid, and also by the unique term of the monitoring. These features of input data allow us to hope that the desired model system will be realized and will satisfy the requirements that are established by solving the engineering problems.

External boundary conditions. The outline of the computed area was chosen so that external boundaries depend on natural features (Fig. 5): the Techa's cascade (Reservoirs #2 - #10), Lakes Ulagach, Tatysh, Hagalgim and River Zyuzelga. There are no problems with the outlines or with the data about the surface water levels here. However, these borders are imperfect relative to the grade and to the character of the exposure of the aquifer and require parameters of the flow exchange. For the given scheme, this is expressed as the additional resistance value which depends on the effective relation of the aquifer transmissivity to the conditionally additional distance. However, the monitoring data show, indirectly, that the additional resistance of the bed of the lakes is insignificant. Besides as it was shown by the subsequent modeling, these borders are sufficiently distant and these parameters do not affect significantly the groundwater flow in the area of interest. It is possible to ignore this parameter and to set practically the condition of the given head on these borders (a type I condition). An exception is the boundary condition associated with River Zyuzelga. An analogy with the Mishelyak River prompted us to assume a sufficiently large value of the flow exchange parameter.

Therefore we take it into account by setting a boundary condition of type III. It is necessary to note that the fluctuations of the annual average values of the water level of the lakes are insignificant (usually less than -/+ 0.5 m), especially when considering the cascade of the Techa's reservoirs, which are stabilized by dams.

In the remaining cases (outside of the surface waters) the conventionally stationary flow lines were admitted as "non-permeable" borders (a variant of the condition of the type II kind). The error due to groundwater flow interpolation enters here. These borders have the known conventional character, since the groundwater flow is not stationary, and there are some errors from averaging.

A scheme of the idealization of hydrogeological conditions is given below.

Internal boundary conditions and recharge-discharge conditions. The Mishelyak River belongs to the computed area and this river is considered as the internal border with type III conditions. The effective value of additional resistance was evaluated by the monitoring data about observation wells that are placed approximately along a flow line and across the river. The range is from 100 m (insignificant) to 2000 m for the different segments. The fluctuations of the water level are characterized about several points, but these fluctuations are less than +/- 0.5-0.7 m, and also the level is stabilized now by dams.

The recharge-discharge conditions are influenced mainly by the source lakes, the marshes and the ash dumps, and also by the infiltration recharge areas and by the groundwater supply systems (Fig. 5). The groundwater supply systems are modeled by the assignment of the local discharge area. To do this, the respective discharge rate is calculated by dividing the pump rate by the area of the respective model cell. From the point of view of the probable errors these discharge conditions are reliably defined. The existing errors in flow rate average values are insignificant in relation to other errors. However, the uncertainty of the infiltration recharge conditions is much higher. The significance of these conditions is very high as shown by the monitoring and modeling. The errors of the geometrization of the infiltration areas are most significant, because the concept of this process is mostly schematic; there is no quantitative evaluation here, since direct testing is practically impossible.

The initial approximation of the average recharge may be the approximate general data of the water balance of this area, or such data for any similar area with analogous hydrological and hydrogeological conditions. However, it is important to emphasize that such data can not reduce the uncertainty of the problem significantly, even if we knew this general water balance accurately. So the modeling shows us that in a given case the spatial non-uniformity of the recharge conditions is very significant. Areas of the different recharge value may be approximately the same size as the contaminant plume area; so this non-uniformity alone affects and defines the features of the flow network in this scale and it defines the plume shape and the contaminant distribution. However, for the same average values of the area water balance, variations from site to site may be very significant. For example, the temporary surface flows may lead to the situation where the recharge may be even greater than the atmospheric precipitation. Thus, for the schematization of the infiltration recharge it is necessary to use such indirect data as the amplitude of the flood elevations

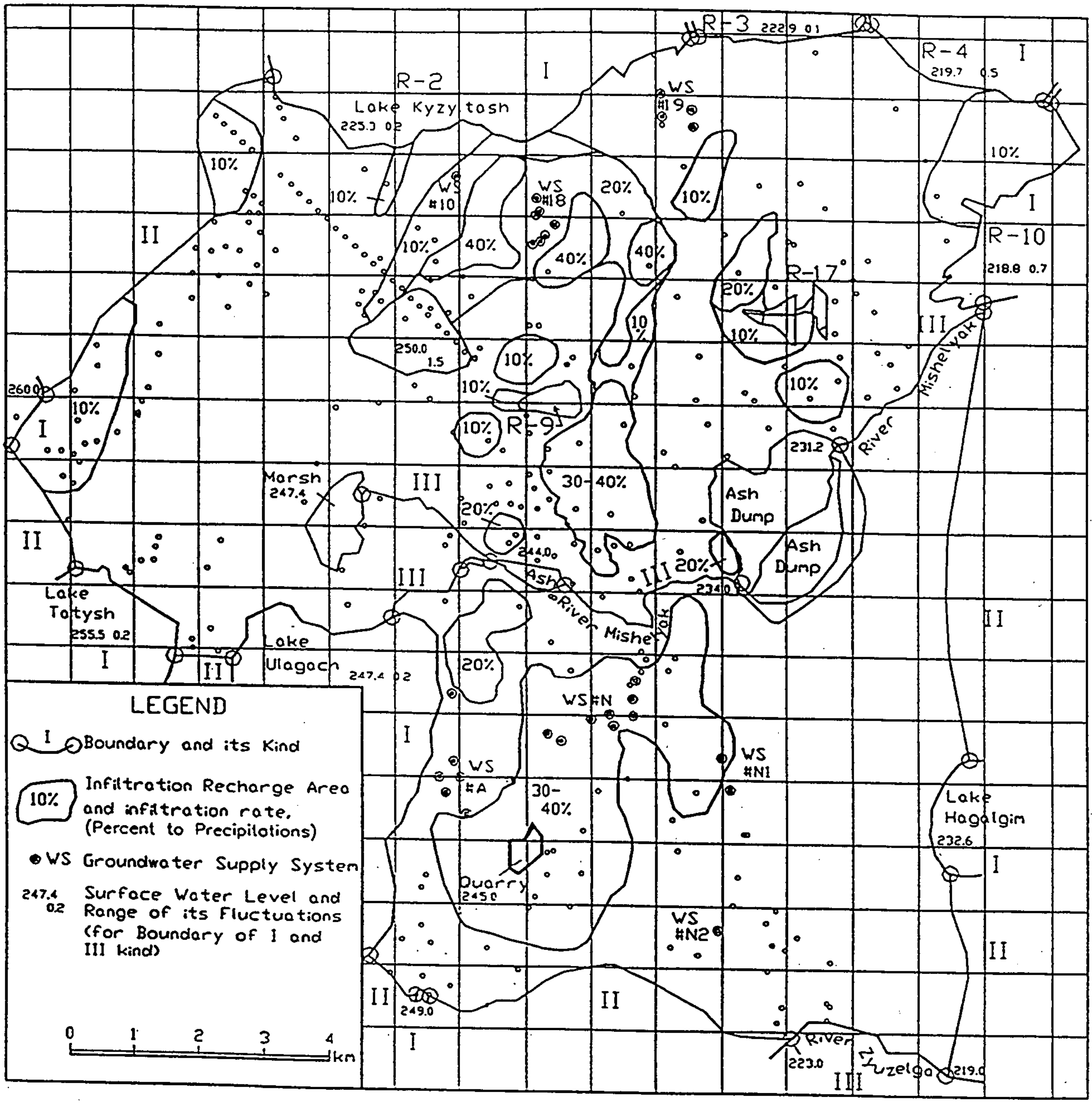

Fig. 5. Recharge-discharge conditions and the boundary conditions (after calibrations).

of the groundwater table, the correlation with the atmospheric precipitation for different wells, the thickness and the properties of the cover sediments, and geomorphologic data of qualitative character [2].

contaminant plume area; so this non-uniformity alone affects and defines the features of the flow network in this scale and it defines the plume shape and the contaminant distribution. However, for the same average values of the area water balance, variations from site to site may be very significant. For example, the temporary surface flows may lead to the situation where the recharge may be even greater than the atmospheric precipitation. Thus, for the schematization of the infiltration recharge it is necessary to use such indirect data as the amplitude of the flood elevations of the groundwater table, the correlation with the atmospheric precipitation for different wells, the thickness and the properties of the cover sediments, and geomorphologic data of qualitative character [2].

It is important that the fluctuations of the observed groundwater table occur later than the precipitation fluctuations. The value of this delay amounts about 1 year for the annual discretization of the time axis (data of the analysis of correlation). The rare exclusions concern single wells. Obviously this phenomenon must be reflected by the modeling of the time-dependent process.

For the initial quantitative approximation, the data of an analogy were used. It is known that the infiltration rate amounts to about 20-40% of the precipitation value for areas with similar hydrological and geographical conditions. We assume the following range of this value to reflect its probable spatial variations: 0–40% by the draft discretization (0, 10, 20, 40%). To quantify the fixed one-year delay we calculate this percentage in relation to the precipitation value of the preceding year. The historical data of atmospheric precipitation for PA Mayak Site are presented in Fig. 4.

The surface waters are included in the computed area by the scheme of the "hard" flow exchange. Here the flow exchange parameter is defined as the effective relation of the water conductivity of the bed layer to its thickness. We define these parameters using such indirect data as the monitoring data and also the laboratory conductivity test data for the core samples together with the thickness determined from shallow drilling data.

Reservoirs that are sources of hydrodynamic disturbance and contamination. The conditions in connection with the source reservoirs require a separate discussion in more detail. To assign the flow-exchange conditions for the source lakes we recognize that there is a direct hydraulic connection with groundwater here [2]. The data of the shallow drilling that was performed on Karachai marsh before the waste disposal show the sharp non-uniform structure of the lake bed in plan and in cross section. The sediments are composed mainly of interbedded clays and loams [2]. The total thickness of the layer of loose sediments (excluding the weathered porphyrite) varies from 4-7 m to 0.5 m and less. Places with low thickness and where the weathered rock chips making up the sediments of this layer work as filtration "windows," are the main areas where contaminant solutions leak into the aquifer (Fig. 6a).

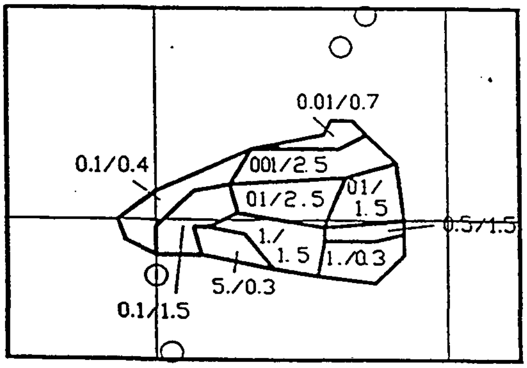

Fig. 6a. A scheme of the flow exchange parameters (conductivity/thickness of the bed of Lake).

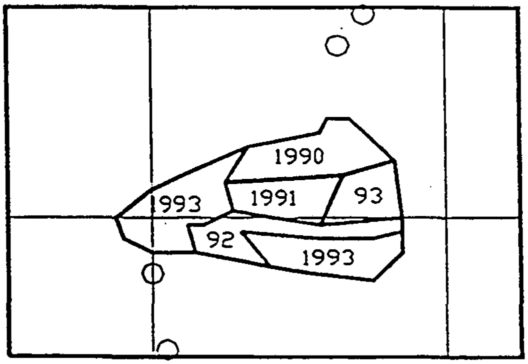

Fig 6b. A scheme for the covering of Lake Karachai.

It is an important feature that the thickness of the bed layer of Reservoir-17 (which occupies the bottom of a former small valley) is much greater than at Lake Karachai. This value varies from about 10 m (the north side of the valley) to 20-30 m (the south side). The structure of the Reservoir bed is non-uniform also.

To construct the geometrical scheme of the model the area of each source lake was divided in several zones, which allow us to assign both the constant average thickness of the bed layer and the calculated average conductivity coefficient. The laboratory test data and the published data about analogous sedimentary rocks are used for these calculations.

The geometrical scheme of the Karachai conditions takes into account the change of the coast line due to the step-by-step covering of this Lake. For modeling we accept the draft scheme of covering that was proposed for the period 1992-1995 (Fig. 6b). This scheme will be corrected relative to the real situation. Thus the two initial schemes were taken into account for modeling the flow exchange in the Lake-Aquifer system: the scheme of the flow exchange parameters and the scheme of the covering.

The flow exchange conditions for Reservoir-17 are described in a similar manner. Changing of geometrical structure (during constructing the dam and filling the reservoir) may be ignored here. This is because the water surface area developed quickly during the first years after construction of the dam (1954). Subsequently, the area of the reservoir grew insignificantly if we take into attention the scale and the detail grade of the constructed model.

Constructing the scheme of the areal distribution of the medium parameters. This is the final part of the idealization. The main feature of our input data is the number of the field pump tests, that are distributed in the area of interest. In the contaminant plume area we have an approximately regular grid of these tests. In this case, we must use interpolation rather than extrapolation of the data, and the data processing is similar to the mapping. For this the block-uniform structure is accepted (Fig. 7). The use of indirect and uncertain data such as geological data or other similar data has a secondary significance here. However, this relates mainly to the data set for the 2-dimensional modeling. The data base of the vertical distribution of parameters that is necessary for the 3-dimensional modeling has fewer of the direct data such as the pump tests on the different depth intervals (about 30 tests). So we also must use such indirect methods as the telephotometry and the geological description to extrapolate these data.

Fig. 7. A scheme of transmissivity of the modeled area.

For the time-dependent flow modeling the hydraulic capacity parameters can be very significant. However, for the accepted time step (1 year) the capacity properties do not play an important role. Therefore, based on the direct correlation between the transmissivity and the hydraulic diffusivity we assume the simple relation: the hydraulic diffusivity coefficient is constant and equal to the average value, which was calculated by the pump test data. However, a stronger initial assumption is accepted for the transport modeling: the porosity is equal the hydraulic diffusivity. Coefficients of the hydrodynamic dispersion are checked by modeling for a wide range (10 – 100). In particular, one of conclusions is that the probable variations of the longitudinal dispersion (even very significant) do not have any significant effect. Such a result was expected, since we had the results of earlier explorations of the transport processes [1, 4]. We do not discuss the transport task in-detail here because this task is secondary for the 2-dimensional modeling. It is possible to note that the transport parameters are not yet a strong factor in the input data.

To reflect the spatial non-uniformity of the parameters and conditions, we accept the idea that the modeled area consists of blocks (pieces), each of which has the same parameters and conditions inside. One conventionally uniform block of the model is the zone that is contoured as the geometrical intersection of the contours of the two initial schemes: the scheme of the recharge-discharge (and boundary) conditions and the scheme of the parameters. Thus, each zone is characterized by its own transmissivity (with the diffusivity and porosity) and also the infiltration recharge value, discharge value, or the flow-exchange conditions and parameters

The generated model grid (Fig. 8) is adapted to the features of the initial scheme and to the required scale resolution. The resolution of the grid is much higher than the dimensions of the respective zones, a necessary requirement for the spatial approximation. The chosen density of the grid is sufficient to reduce the numerical dispersion. The latter was tested and verified by numerical explorations with different grid resolution, from 70x70 to 200x200 cells.

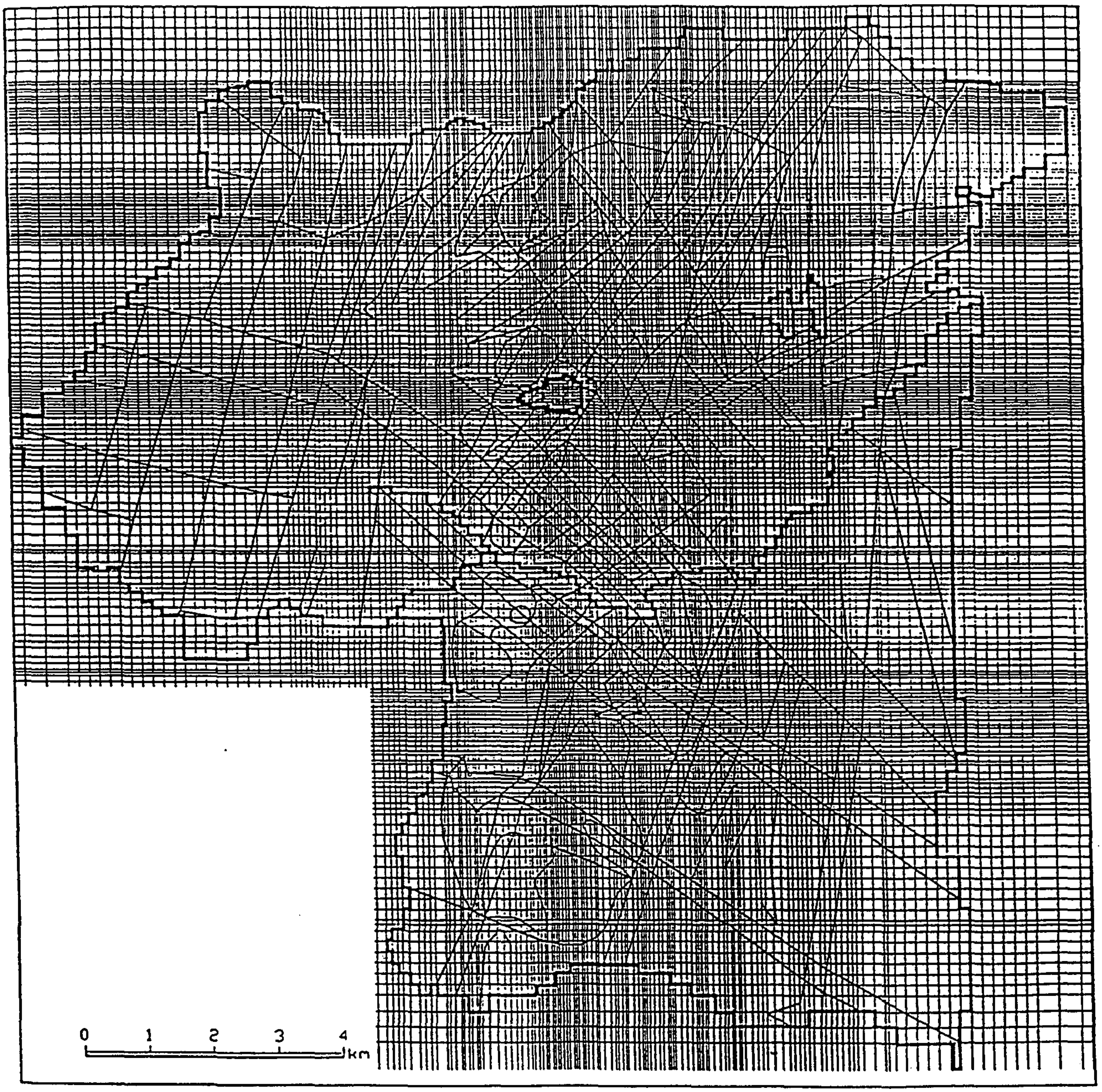

Fig. 8. Geometry of the uniform zones of the 2-dimensional numerical model, and the finite-difference grid.

5.2. CONSTRUCTING THE REGIONAL MODEL. CALIBRATIONS AND ASSESSMENT OF ADEQUACY OF THE MODEL

In accordance with the accepted approach we first limit the task by the stationary conditions. First the stationary process is modeled with conditions from 1976, a year which ended the anomalous dry period (1974-1976). It was assumed that the disturbing influence of the infiltration recharge in the preceding wet period (before 1974) is least, and therefore the groundwater table reflects the spatial distribution of the transmissivity only.

Initial computations with the prepared initial data show the following results. The modeled flow network was in accordance with the observed flow network. The absolute values of the deviations were different and amounted to about 1-3 m. However, several anomalous deviations (to 5 m and more) were recognized. This was characteristic for the area east of Lake Karachai and for the separate sites between Lake Karachai and River Mishelyak. These anomalies were significant and caused the essential differences of the flow network, e.g., gradients of the groundwater table. From this, the computed value of Lake Karachai's leakage was higher, by 30%, than the estimate with the water balance. In particular, near Lake Karachai the flow network was distorted: a significant flow was computed for the easterly direction that contradicted the contaminant monitoring data. Therefore, these results were not included.

Thus, the main conclusion was that the initial assigned scheme required additional refinement. The analysis of the computation's results provided directions for the calibration. Some sites were determined, where the computed groundwater table was above the observed table. Obviously, these positive deviations could only increase further if we took into account the addition of the infiltration recharge. Therefore, such sites were separated from the calibration of the transmissivity map. At the same time, there is no such simple situation for the sites where the negative anomalies were determined. They could result from the condition that some infiltration recharge occurs in nature even in relatively dry periods, but this recharge was excluded from a list of the modeled conditions at this stage. This situation could occur in the area east-south-east of

Lake Karachai. This was in accordance with the concept of the morphology of the infiltration area, and also with the monitoring data.

Before the calibration, we perform a series of test computations to define the sensitivity of the model relative to the parameters of the areas of interest, and to define the areas of influence of the probable variations. The analysis of the results showed that the transmissivity variations weakly affect the leakage value. It is clear that this value is defined by the average transmissivity of the whole groundwater flow area. However, the transmissivity map does not have sufficient uncertainties to assume that the average transmissivity could be changed significantly. The less certain situation results from deviations of the calculated field from the observed groundwater table. The sensitivities of the separate sites are very different. The groundwater table of some zones is influenced by variations of transmissivity, but for other zones it is not possible to obtain the change in groundwater level by more than 0.2–0.5 m if we vary the transmissivity values even (+/- 100%) for the desired zones and their vicinity. Thus, the numerical explorations showed that the calibrations would be sufficiently complex, since this procedure must concern not only the parameter values but also the geometrical structure, i. e. non-uniformity of the morphology of the area.

We also performed some direct calibrations. Beginning with the highest inconsistencies, we were able to coordinate the parameters, but we had to compute many hundreds of the probable variants. In any case, we had to use the assumed geometrical structures with the respective assumed transmissivity value, for example, in the area of low transmissivity east of Lake Karachai and at local sites near Mishelyak River. At the same time, areas were delineated where the calibration was not successful by using the reasonable variations of the parameter values and geometry. These sites were marked for subsequent calibrations using the infiltration recharge. By this manner we obtained the calibrated transmissivity map, which was then used for the calibration of the infiltration recharge.

We then performed the computations for the stationary conditions, which were assigned as the average values relative to the entire observation period. The infiltration recharge was also taken into account based on the average values determined from the different values for the respective sites. These values depended heavily on values of the atmospheric precipitation in accordance with the previously described approach (see Section 5.1). To calibrate the recharge conditions we performed a series of computations which assume unreasonable high values of the infiltration recharge in the large area. These numerical explorations allowed us to check the reliability of the assumed scheme of the infiltration and also to define the areas with different sensitivity of the flow network relative to the recharge conditions. It is significant that the some low sensitivity areas may have a large infiltration recharge, and this will be reflected in the contaminant transport process, but we may not see significant reflections in the flow network.

We also assessed the influence of the infiltration recharge conditions on the leakage value. This influence was very significant relative to the total leakage value, especially as to the flow rate at various directions from Lake Karachai. The latter is very significant for the given task and requires the most attention by calibrations of the recharge conditions near Lake Karachai.

We then checked the capabilities of the model in time-dependent conditions. First, a limited time interval was used. We used the situation that the 1976 year is anomalously dry, 1977 is average and 1978 is very wet. So the interval 1976–78 includes practically a full range of precipitation values. Modeling the flow network over this interval we detected the following: The values of the infiltration recharge that was selected by calibration based on stationary conditions do not usually provide the observed increase of the groundwater table. Besides the leakage flow is not reduced in the required grade, especially in the easterly direction from Lake Karachai. Therefore, in the given case we must couple the recharge conditions with the transmissivity.

As a result, the deviations were finally reduced so that the model flow network was practically in accordance with the monitoring data for the time-dependent conditions. The rate of the modeled leakage was then usually within the limits of the balance assessments, and its directional distribution was in accordance with the control data.

The results allowed us to perform the modeling for the entire period of interest from 1951. Such computations may be one of the ways to check the adequacy of the model. During the computations the comparison of the modeled and observed flow network was performed for the period including dry, average, and wet conditions. The modeled flow structure reflected the features of the observed flow satisfactorily. The solution was checked quantitatively about the deviations for each observation point and for each year. An average, deviations were not over 1–1.5 m. Also, the modeled leakage flow was checked against the water balance for each year (Fig. 9).

Sufficient convergence between actual data and modeling results is observed (+/- 30%) for each time step. The exclusions are single. The difference between the actual total value of the leakage for the entire modeled period (1951-1989) and the modeled value then does not exceed 20%.

The results of the transport modeling are illustrated on Fig. 10, and an example of the modeled groundwater flow is presented on Fig. 11. We can see that even using the aforementioned idealizations and assumptions, the modeled plume shape corresponds with observations over the monitored period. This shows that the main feature of the transport process is the mechanism of flow convection, and groundwater flow may be approximated as horizontal flow for the scale of the contaminated area. This feature is satisfactorily reproduced by the 2-dimensional model. The real flow rate is defined by the porosity that is determined very approximately, as we noted above. Then to obtain accordance with the observed transport velocity we had to select the appropriate diffusivity coefficient that defines the porosity strictly in the accepted idealization (see Section 5.1).

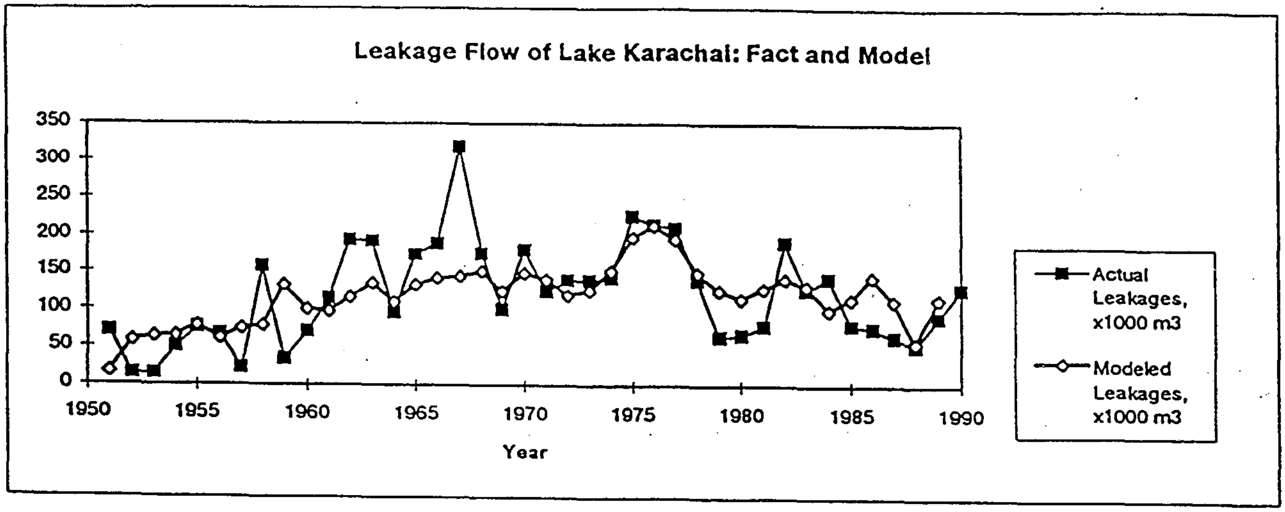

Fig. 9. The leakage flow through the bottom of Lake Karachai: actual and modeled values.

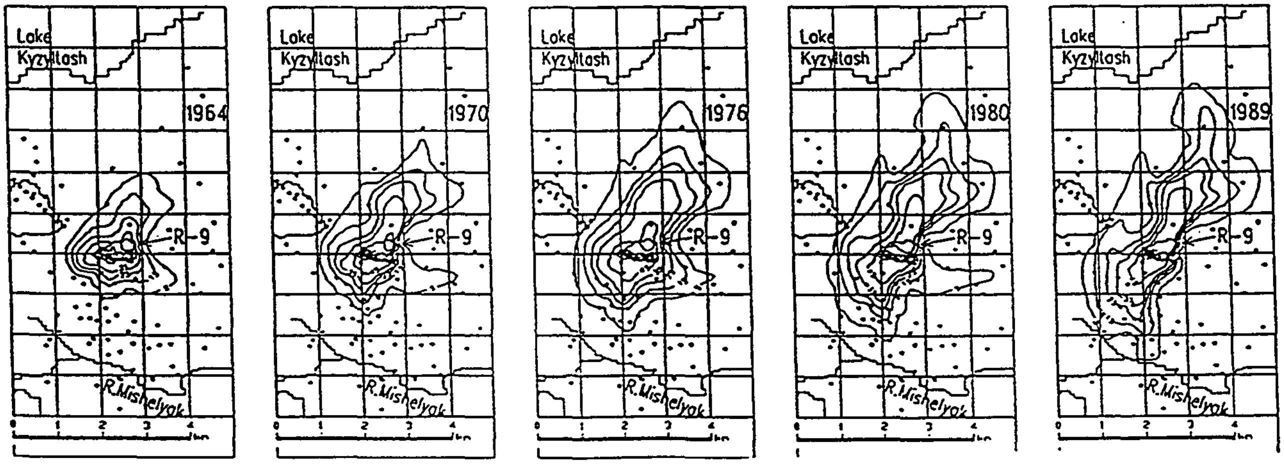

Fig. 10. An example of the modeling results: evolution of the contaminant plume from 1964 to 1989 (relative to the neutral indicator NO_3^{--}).

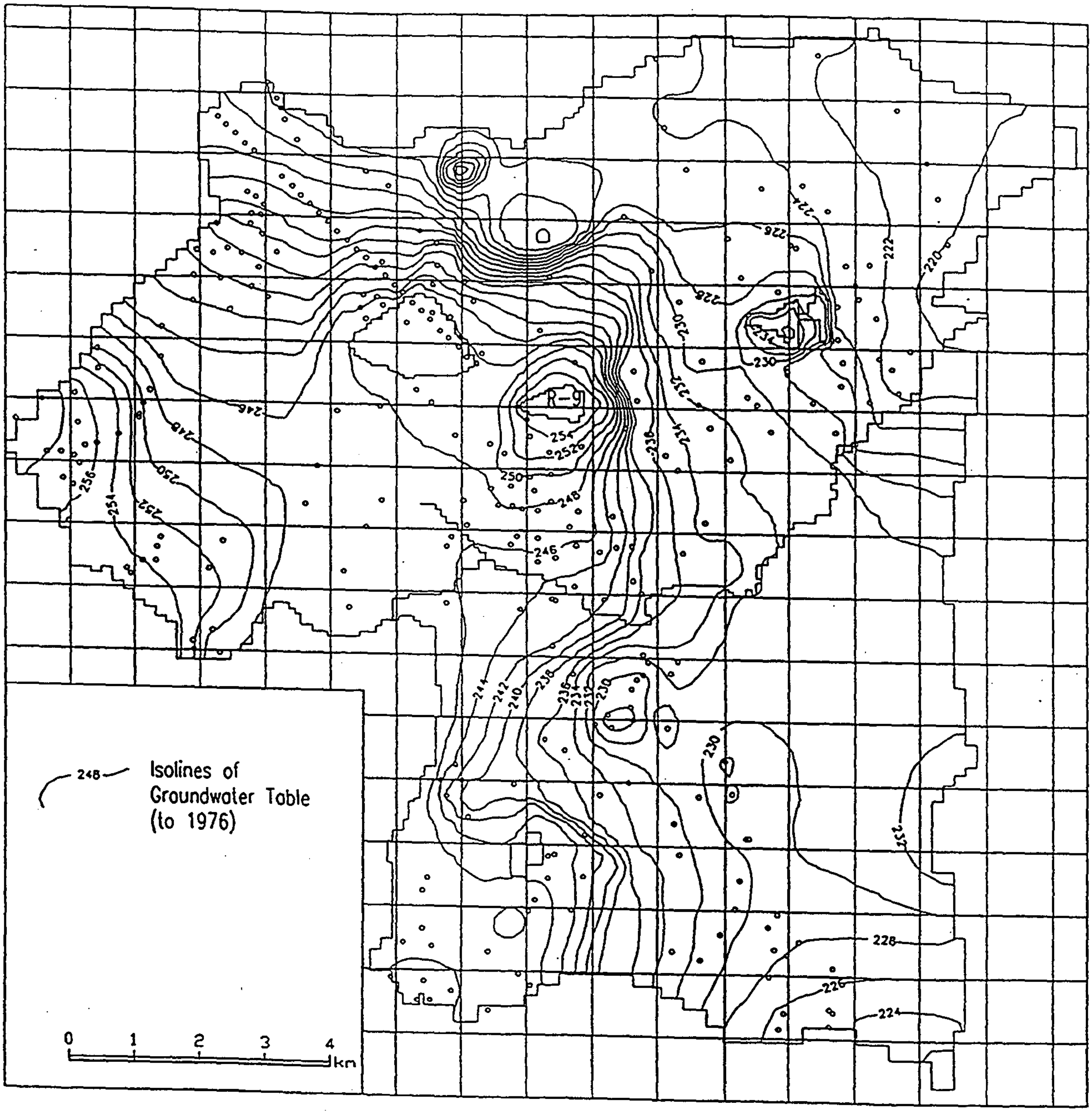

Fig. 11. An example of the modeling results: isolines of the groundwater table to 1976.

CONCLUSIONS

The primary goal of the work described in this report was to develop the methodology of using numerical modeling to explore the groundwater contaminant transport in the Lake Karachai area.

First the tasks, scales and mathematical settings were validated and linked in the interacting system of the numerical models: from the 2-dimensional regional model with the separated flow and transport task to the full 3-dimensional model of the sub-area. Then the analyses of the contents and quality of the input data were performed, and the calibration procedures were validated, including objects of calibrations, limits of variation, the optimum sequence of calibrations and criteria of their sufficiency. The checking-calibration cycles were conducted in three steps: the stationary dry conditions, average conditions and time-dependent conditions.

The second goal was to develop the 2-dimensional regional model, an accepted approach in numerical modeling. In this stage the modeling goals were to check the concordance of all input data relative to the regional 2-dimensional scheme (with defined assumptions) and to coordinate the probable inconsistencies. The hydrogeological idealization was first performed to obtain the initial scheme for numerical explorations. In this, the alternative variants and the probable variations were considered. Subsequent checking by modeling on each step allowed us to discover some deficiencies in the initial scheme of the medium and conditions, allowing us to illustrate the sensitivity of the model and to assess the significance of these deficiencies, taking into account the objective errors and uncertainties. In each step the possibilities to coordinate input data were validated, and the respective calibrations were subsequently performed.

Finally, the comparison of the modeled characteristics against the control data (the flow network dynamics and the leakage flow rate, and also the data of the groundwater transport of the neutral indicator) allowed us to conclude that the resulting 2-dimensional flow model describes the observed regional flow structure satisfactorily. Thus, the first stage of the modeling process has been accomplished. This model may be used to explore the groundwater flow dynamics on the regional scale, and in particular to assess the probable regional consequences of the proposed artificial remedial measures.

We have already used this model to localize the outline and contours of the contaminant plume sub-area and to establish the boundary conditions of this sub-area planned for the 3-dimensional modeling. The calibrated 2 dimensional map of the parameters and conditions is used now to prepare the 3-dimensional initial idealization of the selected sub-area.

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