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Expectations against the modelling practice of groundwater balance and resources

This paper examines recent utilization of numerical modelling in the analysis of hydrogeological water balance and resources. The equations for the flow and mass transport of groundwater, that form the bases of the hydrogeological models' algorithms are presented. The most frequent errors in modelling and in model documentation are discussed. The paper presents the requirements that should be met by properly built models of hydrogeological systems. The urgent need to issue quality certificates for the existing computer codes is a current issue in Poland. This paper proposes that these certificates would be issued by a joint team from The Commission of Hydrogeology (Polish Academy of Science) and from The Commission of Hydrogeological Documentation.

THE STATE OF MODELLING RESEARCH — GENERAL NUMERICAL ALGORITHMS FOR HYDROGEOLOGICAL MODELS

In the 80's modelling techniques became the principal method for evaluation of groundwater resources on the local as well as on the regional scale. Recently it is practically the only method used for the estimation of groundwater resources for a given region. It should be emphasized that in the early 80's every second hydrogeological report did not define a so-called "groundwater-resources-area" at all.

Most of the groundwater resources reports supported by hydrogeological modelling are prepared for regions of 500 to 5000 km^2. Only 15% of these were made for areas larger than 5000 km^2 and 35% for areas less than 500 km^2. It can be noted that this latter group is on the increase — they document large municipal and industrial groundwater intakes in central and western Poland (T. Macioszczyk, B. Kazimierski, 1987).

Based on the analysis of nearly 100 groundwater resources reports, one can conclude that 32% of them apply for the licencing of the resources within the range of 420–2100 m^3/h. 28% of them applied for more than 2100 m^3/h. In the 90's there is a clear downward trend in the volume of groundwater resources submitted for licencing.

It can be easily noted that the largest number of documents (32%) apply for the licencing of Quaternary groundwater resources, with 40% applying for joint Quaternary-Tertiary or lower aquifers. The remaining 28% apply for the licencing of exclusively lower aquifers.

Water-balance-analysis methods dominated groundwater resources development procedures in the 80's (32% of analysed cases). In that time modelling approaches were carried out in 29% of cases. Simple pumping-test analyses accounted for 27% of cases.

In the 90's numerical modelling techniques of groundwater flow have become dominant over all others (T. Macioszczyk, 1991). Analog modelling has been completely given up in the last decades.

As usually happens with the introduction of modern techniques it was observed that hydrogeological modelling served initially as a component of a given report just to make it look nicer for the investor. It also appears recently that many modelers do not care much about proper design, calibration and verification of their models. This damaging tendency leads to the lowering of models' accuracy and creates the lack of trust among those people who would like to apply modelling in groundwater resources development process.

It is worths noting that the purpose of modelling of hydrogeological systems is to get approximate numerical solution of groundwater dispersion and flow equations (T. Macioszczyk, B. Kazimierski, 1990*b*).

$$\delta C_i/\delta t = \mathrm{div}(D_i^*\,\mathrm{grad}C_i) - \mathrm{div}(UC_i) + \Sigma_j F_{ij} + \Sigma_r W_{ir} \qquad [1]$$

$$\beta_i(\delta H/\delta t) = \mathrm{div}(k\ \mathrm{grad}H) + \Sigma_s R_s \qquad [2]$$

where: C_i — concentration of the *i*-th element [ML^{-3}]; D_i^* — dispersion coefficient of the *i*-th element [L^2T^{-1}]; U — pore flow velocity [LT^{-1}]: $U = -k/n_o$ grad H [LT^{-1}]; n_o — effective porosity [1]; k — permeability coefficient [LT^{-1}]; H — hydraulic head [L]; F_{ij} — kinetic function of the *j*-th reaction producing the *i*-th substance concentration [$ML^{-3}T^{-1}$]; W_{ir} — source function of the *r*-th source producing the *i*-th substance concentration [$ML^{-3}T^{-1}$]; R_s — water sources and sinks [L^2T^{-1}]; β_1 — specific yield [L^{-1}]; t — time [T]; i — substance index; j — chemical reaction index; r — mass source/sink index; s — water source/sink index.

Equation [1] describes mass transport in a porous medium and takes into account chemical reactions between substances themselves and between substances and porous matrix. The decay, the ingrowth as well as the processes of molecular diffusion, hydrodynamic dispersion and advection are built into this model.

Equation [2] constitutes the equation of groundwater flow incorporating sources and sinks. The model described with [1] and [2] is full 3-dimensional mass transport and groundwater flow model. Getting the solution for the above system poses a great problem mainly because of insufficient input data (hydrogeological parameters and identification of the processes involved). This leads to the simplification of the modeled system — reduction of the number of modeled processes (for example neglecting diffusion and dispersion) and even confining the whole problem to equation [2]. Equation [2] constitutes the basis for models of groundwater balances and resources. Even in this simplified case a modeler does encounter serious problems which do not allow him to build proper 3-dimensional models. His knowledge of parameters is usually constrained to the averaged values assigned to particular aquifers and that is why the modeler decides to build quasi-3-dimensional models so-called multi-layered ones.

Multi-layered groundwater flow models are obtained as a 2-dimensional solution of equation [2] for each particular water-bearing layer with the leakage through the semipermeable separating layers. A set of equations describing such a multi-layered system comes from the integration of equation [2] along the z-axis in the interval z_i to z_{i+1} with $z_{i+1} - z_i =$ $= m$ (the water-bearing i-th layer thickness) and averaging within these intervals. So we assign a constant hydraulic gradient within each water-bearing layer as well as assume that parameter values are constant within these along-z-axis intervals. In addition, we change the permeability coefficient k for the transmissivity T ($T = km$) and we change β_1 for β (β $= \beta_1 m$). Applying this approach we get Boussinesq's equation for each i-th water-bearing layer (T. Macioszczyk, B. Kazimierski, 1990*b*):

$$\beta_i \delta H_i/\delta t = \delta/\delta x[k_i(H_i - Z_i)\delta H_i/\delta x] + \delta/\delta y[k_i(H_i - Z_i)\delta H_i/\delta y] + \\ + W_i' + Q_i + k'(H_i - H_{i-1})/m' + k''(H_i - H_{i+1})/m'' \qquad [3]$$

For confined aquifers the thickness function $(H - Z)$ becomes just the aquifer's thickness (m) and equation [3] simplifies to:

$$\beta_i \delta H_i/\delta t = T_i \delta^2 H_i/\delta x^2 + T_i \delta^2 H_i/\delta y^2 + W_i' + Q_i + \\ + k'(H_i - H_{i-1})/m' + k''\,(H_i - H_{i+1})/m'' \qquad [4]$$

where: β_i — specific yield [1]; Z — elevation of the unconfined aquifer's bottom [L]; W_i — surface flux (infiltration) $[LT^{-1}]$; Q — sources and sinks $[LT^{-1}]$; H — hydraulic head [L]; T — aquifer's transmissivity $[L^2T^{-1}]$; k, k', k'' — permeability coefficients of an aquifer and adjacent semipermeable separating layers $[LT^{-1}]$; m — thickness of a confined water-bearing layer [L]; m', m'' — thickness of adjacent semipermeable separating layers [L]; x, y — coordinates [L]; t — time [T]; i — water-bearing layer index.

It should be noted that besides source functions W and Q there are terms modelling leakage through semipermeable layers in, of course, a simplified Hantush's approach. The specific yield of those separating layers is not taken into account in this model.

These equations form the basis of groundwater balance and resources models. To get the solution of these equations the following conditions must be satisfied:

1. The modeler has to have the proper (3-dimensional) knowledge of the hydrogeological system which he intends to model.

2. The modeler has to possess the appropriate knowledge of the space distribution of hydrogeological parameters in the modelled system.

3. The modeler has to possess the appropriate knowledge of the boundary and initial conditions of the modelled system.

After these conditions are satisfied the above mentioned set of equations, i.e., the numerical model, can be solved in an approximate way. It is up to the modeler to choose from available numerical algorithms: finite element or finite difference methods. The distribution of the hydraulic head in the modelled system is produced by application of the given numerical method; getting this distribution is the typical problem that the modeler is faced with.

Getting started with hydrogeological modelling we usually face the problem of inadequate knowledge of the system's structure with little chance to collect all the data that we need (high costs of drillings and pump tests). What makes the problem more reasonable is the possibility of getting relatively reliable information about hydraulic head distribution within the hydrogeological system. It helps to gradually update our knowlege of the internal structure of the modelled system through a series of so-called reverse solutions. This approach helps to identify "the best" set of parameters or structural characteristics of the modelled system. Having got through the above procedure we are able to produce reliable hydrogeological estimations with the help of our calibrated model. So the model becames capable of simulating groundwater balances and resources.

METHODOLOGICAL INADEQUACIES AND DOCUMENTATION ERRORS IN HYDROGEOLOGICAL MODELS

1. Inappropriate definition of the hydrogeological system, its boundaries and boundary conditions.

2. Inappropriate documentation and justification of the accepted hydrogeological scheme (no reliable maps, no cross-sections, no analysis of parameters).

3. Inappropriate definition of the relationship between the real system and its simplified model.

4. Inappropriate superimposition of the constant-head boundary condition (type I). Excessively long sections of the model's boundary are assigned that type of boundary condition and this error makes the model unable to estimate groundwater resources properly. The constant-head boundary condition implies that the modelled region gets as much water from across that type of boundary as the groundwater intake pumps out of the domain. The proper definition and the placement of the constant-head boundary condition dramatically influences the reliability of the groundwater balance and resources model.

5. Superimposition of the constant-head boundary condition (type I) along lake and river banks instead of type III. This error is now less frequent. The proper estimate of the river bed hydraulic resistance does not happen very often.

6. Determination of the boundary conditions for production aquifers only or assigning, without any justification, the same boundary conditions to non-productive aquifers incorporated into the model.

7. The lack of a unique method to simulate the infiltration, the aquifer-river water exchange and groundwater intakes. The data in the analysed hydrogeological reports show serious inadequacies in this field. It happens that estimates of these factors based on the water balance infiltration differs as much as 50% from that superimposed on the model.

8. Incomplete and unclear documentation of the hydrogeological model covering the definition, calibration and verification as well as incomplete and poor documentation of the modelling procedure outcome.

Table 1

An example of an incorrect water balance

Water balance components	Simulation results for 1992		Simulated forecast	
	+	–	+	–
Aquifer A (60 km^2)				
— effective infiltration	370.9	–	370.9	–
— influx from surface waters	0	0	0	0
—influx/outflux through the model's boundary	157.2	0	986.5	0
— leakage from/to aquifer B	0*	217.1**	0***	306.6****
— groundwater production rate	–	3.4	–	15.6
— the sum	528.1 ←	→ 220.5	1357.4 ←	→ 322.2
Aquifer B (515 km^2)				
— effective infiltration	481.3	–	481.3	–
— influx from surface waters	0	0	0	0
— influx/outflux through the model's boundary	0.2	47.6	142.2	0
— leakage from/to aquifer A	262.3**	0*	410.4****	0***
— groundwater production rate	–	649.1	–	1191.0
— the sum	743.8 ←	→ 696.7	1033.9 ←	→ 1191.0

The values coupled with ↔ should differ no more than 1%; * –**** — values that should be the same but with opposite sign

9. Lack of justification of the model as well as no accuracy assessment of the model's results.

10. Incorrect presentation of the model's results.

Examples:

— presentation of the selected water balance components only instead of the whole balance;

— presentation of the differences between input and output balance components without presenting input and output values themselves;

— presentation of the integrated water balance with no information about water balances for each particular water-bearing layer. In the application for the licence there is usually no word on how the resources are to be distributed among production aquifers within the hydrogeological system. The curious example of a groundwater balance with nearly the all abovementioned inadequacies is shown in Table 1.

11. Inappropriate verification of the model resulting in unbalanced inputs and outputs as well as incorrect model structure.

In a considerable number of cases water balances of the models show unacceptably large differences between the inputs and outputs for each particular water-bearing layer. These differences should not exceed a fraction of one percent. Differences larger than 2–4% disqualify the model; nevertheless there are models with these differences above tens or even hundreds percent. These discrepancies could suggest the existance of errors in the algorithms applied for calculating the water balances in the model subdomains. For example, the amount of water drained from aquifer A into adjacent aquifer B should be equal to the water flux that aquifer B receives from aquifer A. These fluxes should only differ in sign.

12. Illogical structure of water balance compared against the approved flow system. For example, two aquifer system have a separating semipermeable layer (till). There are "hydrogeological windows" in this layer. In the case of groundwater pumping from the lower aquifer there has to be a non-zero flow through these "windows". The model showing a zero flow through the "windows" should be rejected.

13. Aggregating local models to get a regional model usually results in the accumulation of local models' errors.

14. Modelers tend to avoid the clarification of existing constraints like the intake's maximal production rate.

The overwhelming majority of hydrogeological models do not take into account the question of ensuring certain minimal flow in rivers while simulating groundwater intakes in the modelled domain.

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The review of the existing hydrogeological models shows that the abovementioned errors are caused (T. Macioszczyk, 1985; T. Macioszczyk, B. Kazimierski, 1987, 1990*a*) by:

— lack of appropriate knowledge of the modelled system;

— wrong software;

— wrong modelling strategy;

— wrong groundwater management concept.

The only way to improve this gloomy picture is exposure of errors and detailed discussion of their origin.

For example, discussion with the authors of the HYDRYLIB library used by groundwater modelers in Poland (J. Szymanko, 1977–1989, 1980) will soon result in the elimination of the encountered problems.

Full and reliable documentation of hydrogeological models will always serve as an extremely helpful tool in analysing and eliminating potential errors. A calibrated model which produces heads with ±0.5 cm accuracy is useless unless we know what heads: piezometric or topographic and unless we know how these heads are dated and what infiltration and its distribution was taken as the input.

The documentation of the model should cover the following four stages of construction and exploitation of that model.

A. Definition of the modelled system (T. Macioszczyk, B. Kazimierski, 1989, 1990*a, b*):

— the system's description with all assumptions, description of the main and neglected processes within the system, justification of all these assumptions;

— the model's description, its structure, and applied numerical algorithms;

— synthesis of the geological and hydrogeological data with the determination of its reliability and internal cohesion.

B. Calibration of the model. Documentation of this stage should define the so-called object function as well as include is local and global calibration record, and what parameters and in what sequence they were identified. Despite getting an acceptable correspondence between calculated and measured heads the modeler should produce the distribution of balance residuals within each aquifer in the modelled system. The distribution of the surface recharge ought to be included as well. It is known that in low permeability zones the modelled heads can easily be raised by increasing the recharge (in reality the recharge is less than its value obtained in this way). Local modifications of hydraulic gradients are usually done by applying variable recharge although such a recharge pattern often seems to be highly unlikely to occur in reality.

C. Verification of the model. To verify the model so-called independent data should be used. In this case the independent data means data not used in the model's calibration. If there is no independent data it should be explained why is that so (T. Macioszczyk, B. Kazimierski, 1990*b*).

The crucial point is the confrontation of the modelled groundwater balance with the groundwater balance obtained from hydrological methods. This is especially important for the proper estimation of such balance components like drainage from rivers or surface recharge.

What is also important is to discuss the differences between the parameter values from the model's calibration and those values from pumping tests. The modeler should also test the model's behaviour under extreme conditions. The verification results can serve as a measure of the model's quality.

D. Simulation. The modeler should test the influence of different groundwater production schemes on particular water balance components. At this stage all modelling has to be very carefully documented.

The documentation must contain the justification of boundary conditions (stresses) and assumed constraints as well as detailed explanation of the groundwater balance structure. This documentation has to address all a model's components (water-bearing layers) as well as so-called water-resources-area. The boundaries of this area will mark the extent of the intake protection zone according to present regulations. It must be stressed that the term water-resources-area has to be properly understood to avoid very common mistakes in this field.

The water-resources-area has to be defined as the area from within which water flows to the groundwater intake. From this area intake gets at least 80–85% of its licenced exploitation resources. At the same time outflow across the boundaries of an area defined in this way should not be decreased by more than 20–25% provided there are no other groundwater intakes downgradient. Another constraint is to ensure local river flow above a certain limit.

This paper formed the basis for the discussion during the meeting of the Commission of Hydrogeological Documentation and of the Commission of Hydrogeology of the Commitee of Geological Sciences of the Polish Academy of Sciences. These sessions addressed the question of application of modelling methods in groundwater management policies. The need to enhance the contribution of proper modelling techniques was strongly raised. What is of prime importance is the verification of hydrogeological software utilized in Poland. It was recommended that this verification should be carried out in recognized foreign modelling centres. Another proposed method of verification is to run already existing models using various hydrogeological software including software with the IGWMC certificate. It was decided that this initiative will be submitted to the Departments of Science and Geology. It was decided that instead of placing orders for models of standard catchments, a contest for the best model of a particular catchment is to be organized.

Such a model would fully satisfy expectations of institutions responsible for licencing of groundwater resources, their management, distribution and protection. This approach would lead to standarization of models of groundwater balance and resources.

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OCZEKIWANIA A PRAKTYKA MODELOWANIA BILANSÓW I ZASOBÓW WÓD PODZIEMNYCH

Streszczenie

Po przedstawieniu rozwoju i aktualnego stanu regionalnych opracowań zasobowo-bilansowych wykonywanych w Polsce (ostatnio wyłącznie za pomocą modelowania numerycznego) omówiono ogólne równania transportu masy i ruchu wód podziemnych z uwzględnieniem szczególnej ich pozycji dla modeli wielowarstwowych w stosunku do modeli przestrzennych oraz warunków koniecznych dla ich rozwiązań oraz zasad estymacji parametrów modelu, określania obszaru jego zasadności itp.

Na tym tle przedstawiono najczęściej spotykane (niestety liczne) niedopracowania metodyczne i błędy dokumentacyjne modeli hydrogeologicznych.

Oprócz wadliwego i niestarannego definiowania formy przestrzennej systemu, jego schematu, relacji systemu do prototypu modelu, niepoprawnej dokumentacji modelu itp., wymieniono bezkrytyczne operowanie warunkiem brzegowym I rodzaju na znacznej przestrzeni lub na wszystkich granicach modelu oraz przemilczanie istotnych informacji o sposobach symulacji zasilania infiltracyjnego. Dość istotnym mankamentem jest pomijanie omówienia obszaru zasadności modelu, dokładności prognoz oraz zachowania się modelu w warunkach ekstremalnych wymuszeń. Zwrócono też uwagę na wadliwy sposób przedstawiania wyników badań modelowych (niepełny bilans, bilans zagregowany zamiast wszystkich składników dla wszystkich warstw, różnice bilansowe wybranych składników oraz bilans łączny dla całego modelu, pominięcie bilansu obszaru zasobowego) oraz przerywanie badań modelowych bez uzyskania dostatecznego zbilansowania modelu w ustalonych warunkach. Przykład kuriozalnego bilansu obszaru zasobowego systemu dwuwarstwowego przedstawiono w tab. 1. Omówiono potencjalne przyczyny braku zbilansowania modeli. Powinny one być zidentyfikowane przez hydrogeologa oraz usunięte tak, aby model mógł być uznany za poprawny i zasadny do spełnienia celu, dla którego go skonstruowano. Systematyczne błędy modelu mogą się też ujawnić w nielogicznej strukturze bilansu, dlatego każdorazowo struktura ta powinna być przeanalizowana. Na koniec zwrócono uwagę na metodycznie niedopuszczalną technologię „zszywania" modeli lokalnych w celu otrzymania modelu regionalnego oraz na bezwzględną konieczność jasnego i pełnego określania ograniczeń, przy których wyznaczano zasoby wód podziemnych, np. przy kontrolowaniu zachowania przepływów nienaruszalnych w ciekach.

Większość nieprawidłowości w badaniach modelowych może mieć swe źródło bądź w niedostatkach rozpoznania hydrogeologicznego, w błędach syntetyzowania wyników rozpoznania, błędach algorytmów programów i/lub poprawności ich wykorzystania, błędach modelowania oraz w nieracjonalności koncepcji zagospodarowania zasobów. Dla uniknięcia tych błędów lub identyfikacji przyczyn ich występowania konieczna jest pełna dokumentacja badań modelowych, która musi objąć wszystkie ich etapy, a więc: specyfikację systemu i modelu, identyfikację i tarowanie modelu, weryfikację modelu oraz badania symulacyjne bilansu i zasobów. Przy okazji podano też propozycję definicji tzw. obszaru zasobowego.

Uznaje się potrzebę weryfikacji wykorzystywanych w Polsce systemów programowych w ośrodkach zagranicznych lub przynajmniej przez testowe porównywanie rozwiązań dla tych samych modeli za pomocą różnych programów polskich i zagranicznych. Proponuje się też zorganizowanie konkursu na model wybranej zlewni (np. Kamiennej), który spełniałby najlepiej czekiwania instytucji zatwierdzających zasoby oraz odpowiedzialnych za ich rozrząd, pozwolenia wodno-prawne, ochronę zasobów i kataster zasobów.