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A new composite approach of physical and geostatistical aspects to groundwater modelling

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Abstract This paper proposes a composite groundwater model with physical and geostatistical components to deal with spatial uncertainty in groundwater flow modelling. A hypothetical aquifer, assumed to be a true aquifer, is designed to test the ability of the composite model. The hypothetical aquifer composed of 20 zones with different hydraulic conductivity is represented as groundwater models with different zonation; those are models with one, two, four and 20 different hydraulic conductivity zones, respectively. The proposed scheme to reduce modelling errors is applied to each case, and the changes in the estimated water levels by applying the scheme are assessed. The results show that the composite estimates are reasonable and well in agreement with the true water level.

Key words geostatistical bias; groundwater; modelling error; spatial uncertainty; zonation

INTRODUCTION

Models in classical groundwater flow modelling are of the physically-based, deterministic type. The optimal parameters to be estimated can be obtained when the inverse problem is numerically solved. With such parameters, the calculated hydraulic heads are statistically best fits to the observed hydraulic, while the residuals between the two heads appear because the groundwater model in use is deterministic. They are consequently recognized as modelling errors, which cannot be sufficiently eliminated without a theoretical and sophisticated approach.

A universal and new strategy to completely eliminate modelling errors at the observed points is now needed. The strategy also should take into consideration space–time modelling errors. This paper describes a new theoretical approach to eliminate modelling errors and demonstrates its effectiveness through numerical studies in a hypothetical aquifer.

INTERPRETATION OF SPATIAL UNCERTAINTY IN MODELLING

Calibrations of model paramcters are usually prerequisite to improve the fit between calculated and observed heads. In general, a difference between the above two heads is seen in actual problems. This difference derives from the physical modelling errors, which cannot be represented within the framework of physical modelling in space. For instance, when a true aquifer structure with inhomogeneous hydraulic conductivity is modelled as the one with uniform hydraulic conductivity, the best model with the most likely hydraulic conductivity is equivalently estimated against the true one. In contrast,

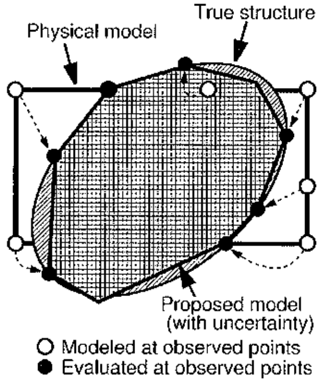

Fig. 1 A schematic view of the proposed model.

larger modelling errors appear in space. In this paper an approach is proposed for a geostatistical evaluation of spatial uncertainty, in particular, the homogeneous modelling error.

Figure 1 shows a schematic view of the relationships among a true structure of a natural phenomenon represented by the inclined ellipse, a corresponding model of the physically-based deterministic type represented by the rectangle, and a corresponding model proposed in this paper, represented by the polygon. Even though parameters in the physical model are identified in advance to fit the phenomenon, the differences between the natural structure and the physical model still remain at some points. A new approach to theoretically fill up the differences is developed and proposed in this paper. In the method, a spatial interpolation using the geostatistical technique of kriging is carried out to make the residuals at all observed points zero. Extensive improvements in the groundwater level estimates would be achieved by incorporating the geostatistical treatment.

MATHEMATICAL DESCRIPTION OF SPATIAL UNCERTAINTY

Spatial uncertainty due to a deterministic use of a numerical model mainly consists of following four kinds of errors the: (a) an error caused by representing a natural phenomenon using a physically-based model; (b) an error caused by representing a physical model using a numerical model; (c) an error caused by boundary conditions in space and time given to a numerical model; and (d) an error in system structure designing, program cording and numerical computing (Hamaguchi *et al.*, 1997a). The errors noted in (a)–(c) are generally defined as the modelling error denoted by $\eta(z,t)$, where z is a vector of space coordinates and t is a time variable. This paper focuses on the second modelling error, especially an error in zoning hydraulic conductivity.

The common assumption is that the trend and random variables are given by the formulation:

$$\phi(z,t) = m(z,t) + w(z,t) \tag{1}$$

where $\phi(z,t)$ denotes a true value, $m(z,t)$ and $w(z,t)$ are trend and random variables, respectively. It is assumed that spatial uncertainty and a random variable are static in time, and it can be rewritten as $\eta(z)$ and $w(z)$, respectively. In the absence of a drift $\hat{b}$, a constant expected value of $\eta(z)$ is proposed as:

$$\eta(z) = \hat{b} + w(z) \tag{2}$$

The specification of the drift indicates spatially uncertain but steady and stationary. The trend variable with the additional drift is then defined as:

$$m(z) = f(z,t) + \hat{b} \tag{3}$$

where $f(z,t)$ is a numerical solution of a physical model. A geostatistical approach of kriging in evaluating spatial uncertainty is proposed as the appropriate method for solving such a problem. The kriged value $w(z)$ can be then presented as:

$$w(z) = k(z)^T K^{-1} \hat{w} \tag{4}$$

with:

$$\hat{b} = \frac{\alpha^T K^{-1} \varphi}{\alpha^T K^{-1} \alpha}, \qquad \hat{w} = \varphi - \alpha \frac{\alpha^T K^{-1} \varphi}{\alpha^T K^{-1} \alpha} \tag{5}$$

where α denotes a constant vector of substituting a scalar 1 for all components, φ designates an observed vector, $k(z)$ describes a covariance vector of $w(z)$ between a given point to be kriged and a observed one, and K represents a covariance matrix of $w(z)$ between the observed points. The resulting evaluation $\eta(z)$ in this framework can be expressed as:

$$\eta(z) = \hat{b} + k(z)^T K^{-1} \hat{w} \tag{6}$$

With the evaluated term $\eta(z)$, the solution to this estimation system $\phi^*(z,t)$ is finally obtained as:

$$\phi^*(z,t) = f(z,t) + \hat{b} + k(z)^T K^{-1} \hat{w} \tag{7}$$

IDENTIFICATION OF EQUIVALENT HYDRAULIC CONDUCTIVITY

The unsteady two-dimensional unconfined groundwater flow in a non-uniform isotropic aquifer is described by:

$$\lambda \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left\{k(h-s)\frac{\partial h}{\partial x}\right\} + \frac{\partial}{\partial y}\left\{k(h-s)\frac{\partial h}{\partial y}\right\} + \varepsilon \tag{8}$$

where λ is effective porosity, h is water head, k is hydraulic conductivity, s is elevation of bedrock, and ε is areal groundwater recharge rate. The groundwater model is numerically analysed by FEM.

The hypothetical example here is designed to satisfy three requirements: (a) sufficient simplicity to allow testing without excessive computation cost and interpretation

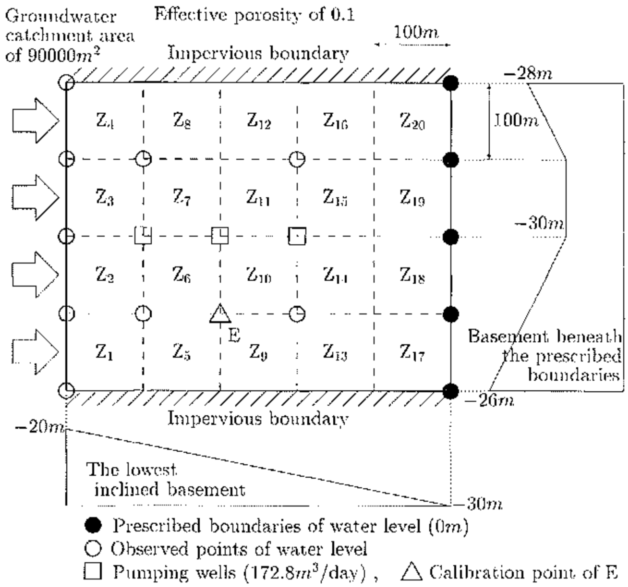

Fig. 2 Hypothetical aquifer modelled in the case studies.

Zone	Z_4	Z_8	Z_{12}	Z_{16}	Z_{20}
	Z_3	Z_7	Z_{11}	Z_{15}	Z_{19}
	Z_2	Z_6	Z_{10}	Z_{14}	Z_{18}
	Z_1	Z_5	Z_9	Z_{13}	Z_{17}
Exact	215.3322	255.5558	321.1791	400.0000	383.3276
	173.9983	200.0000	272.5400	329.4123	346.6049
	136.6654	171.4817	226.1393	273.9904	300.0000
	100.0000	146.4934	194.3980	235.9593	265.2360

Unit: m/day

Fig. 3 Original zonation of true hydraulic conductivity.

of the results; (b) sufficient complexity to allow testing various aspects of modelling errors; (c) a realistic representation of transient groundwater recharge by using the tank model. A rectangular domain of an unconfined aquifer having the area of 400 m × 500 m as shown in Fig. 2, was chosen for the case study. The domain has impervious boundaries at the top and bottom, a constant head boundary (0 m) at the right side, and a prescribed flow rate boundary based on the tank model at the left side. The groundwater recharge takes place at variable rates based on the tank model over the whole domain. A true aquifer has continuous properties in space, i.e. hydraulic conductivity, effective porosity, and so on. In preprocessing a numerical analysis by FEM, we need to discretize the two-dimensional domain of the aquifer by triangle or quadrangle elements. Representative model parameters on integrated average at each element are thus needed. The original aquifer in this study is subdivided into 20 constant-hydraulic conductivity zones with 4 × 5 square elements, as seen in Fig. 3. Here, the aquifer is represented by models with one constant-hydraulic conductivity zone (case 1), two zones (case 2), four zones (case 3), and 20 zones (case 4),

Case 1	221.5426				
Case 2	154.8059		335.7763		
Case 3	206.6947		354.0413		
	118.2425		293.4447		
Case 4	219.3408	263.1140	289.9044	382.6352	380.4207
	168.8113	224.7142	254.9413	348.1349	352.3683
	135.8332	185.8441	215.4022	273.9089	295.5448
	101.7502	144.2885	180.1621	237.3977	260.8399

Unit: m/day

Fig. 4 Results of identified hydraulic conductivity in each case.

respectively, as shown in Fig. 4. Three wells pump up water at a rate of 172.8 m^3 day^{-1} each to create strongly transient conditions. Head measurements are made at the nine observation wells.

The primary purpose of this study is to optimally describe a model with some equivalent hydraulic conductivity in an inhomogeneous aquifer. To identify the parameters from the observed head data, the extended Kalman filtering system in conjunction with FEM (Hasegawa *et al.*, 1994; Hamaguchi *et al.*, 1997b) is used in the framework of inverse analysis processing. The solutions of $\bar{k}_j$, the equivalent hydraulic conductivity in the *j*th zone, in each case are obtained by using the method with FEM computation. The results are arranged in Fig. 4.

The second purpose is to evaluate a geostatistical term added to the groundwater heads obtained by a groundwater model based on the proposed approach. The groundwater heads are numerically solved by using the models with equivalent hydraulic conductivity. After calculating the model heads, geostatistical estimates of the residuals of groundwater heads based on head measurements are obtained. The improved heads are obtained by adding the kriged residual heads with uncertainty to the modelled ones.

EFFECTIVENESS OF ADDITIONAL MODELLING ERRORS

To demonstrate the effectiveness of the improvement of the optimized groundwater model, the validity of its improvement is illustrated by the water level variation at point E (Fig. 2). Figure 5 shows the estimated water levels simulated by the physical models (marked by +, ×, Δ and ◊), those obtained by the proposed model with spatial uncertainty (marked by □, pentagon, ∇ and ○) in cases 1 to 4, and the true groundwater level drawn by the solid line. This figure reveals that the improvement of estimations by adding the modelling errors to the modelled solutions is greatly performed in all cases because all the geostatistically improved solutions are in better agreement with

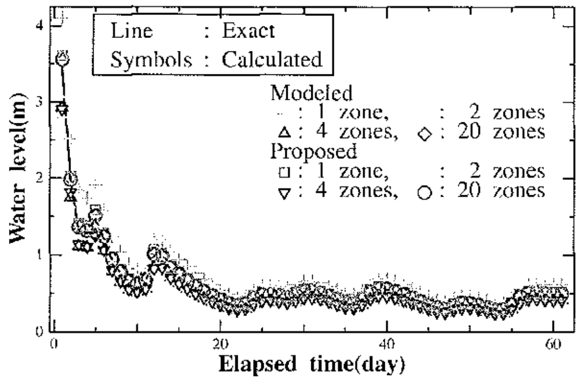

Fig. 5 Comparison of water level variations.

the true values than physically modelled ones. A striking feature of the fact in those studies is that the resulting variation in case 4 is the most accurate in estimating the true heads due to its similarity to the original zonation shown in Fig. 3. The improved variation in case 1 is in reasonable agreement with true variation, and it proves the proposed method effectively works to eliminate the modelling error.

EFFECTIVENESS OF A BIAS OF SPATIAL UNCERTAINTY

Introducing a drift term $\hat{b}$ in the proposed method is discussed in the section. To show the effectiveness of introducing $\hat{b}$, the index, a reciprocal number of a coefficient of variation

$$\frac{1}{|\delta_t|} = \frac{|\hat{b}|}{\sigma_t} \tag{9}$$

is used, where δ_t is a coefficient of variation, σ_t is a standard deviation of $w(z)$, and $|\bullet|$ indicates an absolute value of the variable. This index has two interesting properties in that a relative and absolute comparison among the variations at any time can be made, and that the effectiveness of $|\hat{b}|$ is increased in the geostatistical component when a value of $1/|\delta_t|$ becomes larger.

Figure 6 shows the temporal changes of $1/|\delta_t|$ in each case. The result of $1/|\delta_t|$ in case 1 keeps higher at any time than that in any other cases except case 4. The results in case 4 is higher than any other results, but this evaluation is practically overestimated because any values of σ_t are essentially smaller than the corresponding drifts. This means that the overall value of $\hat{b}$ computed in case 1 is most effectively worked to eliminate the model error corresponding to spatial uncertainty. As mentioned above, it is proved that a drift term of $\hat{b}$ is effective in decreasing the model error in the process of geostatistically describing spatial uncertainty.

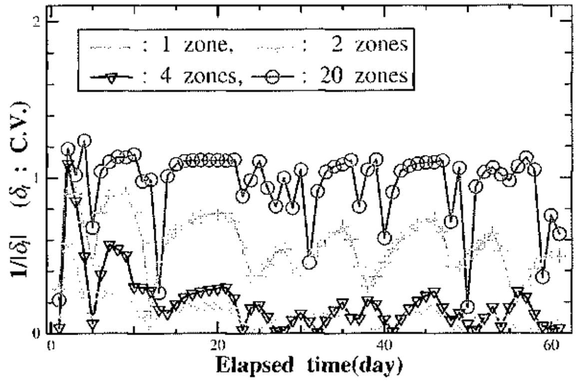

Fig. 6 Effectiveness of a drift term.

CONCLUSIONS

The proposed approach for groundwater modelling statistically assesses spatial uncertainty, which is added to the physically described spatial variability. The advantage of this scheme is the ability to fill up the differences between simulated and observed values. The study demonstrated four hypothetical cases, where a geostatistical calibration was applied successfully to model the aquifer behaviour under unsteady conditions. From these case studies, it was shown that drift term information was greatly helpful and effective in improving the physical model. The major conclusion is that a successful complement to spatial uncertainty due to modelling errors is performed for groundwater flow modelling.

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