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Spatial–temporal models to monitor groundwater data

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Abstract Spatial-temporal models are used (a) for the interpolation of hydrographs to locations without observations, and (b) for the definition of boundary values for a transient finite element groundwater flow model. If the first principal component—resulting from a principal component transformation performed on the data set—explains more than 95% of the whole variance, this can be used to analyse the spatial structure of the data set with respect to the temporal behaviour. Kriging can be used to estimate the spatial distribution and the error variance of the first principal component. Using the calculated kriging weights of unobserved grid points and the time series information from its explanatory observation wells, water table hydrographs can be estimated, using the error variance as an indicator of the estimation error. Using the proposed spatial-temporal models the definition of initial boundary values for transient finite element flow models is possible.

INTRODUCTION

Data sets holding information about the elevation of a groundwater table, gathered from monitoring networks, can be characterized as "time rich—space poor". To analyse the spatio-temporal structure of such data sets, to get information at unsampled locations or to reconstruct time periods not measured, it is necessary to combine the spatial and the temporal components of the data. One possible method for the analysis of spatio-temporal data is use of a one-dimensional spatial overall variogram which contains all of the temporal information.

The investigation site, the so-called "Leibnitzer Feld", is located in the lower Mur valley (Styria, Austria), where 10–15 m depth of Quaternary gravels and sands of relatively high permeability occur. They represent an important aquifer which is intensively used for water supply. The groundwater table monitoring network is described in Fuchs *et al.* (1995). For part of the Leibnitzer Feld (extending to up to 15 km^2) a transient finite element groundwater flow model shall be developed. To apply the groundwater flow model, the definition of initial boundary values (hydraulic head) for the solution of the partial differential flow equations is needed. The data set for the calibration of the model consists of 26 wells, where the groundwater table was measured from 1992 to 1996 at weekly intervals.

PRINCIPAL COMPONENT ANALYSIS

The PCA (principal component analysis, Flury & Riedwyl, 1983) is a mathematical transformation of the variables x_{ij} and can be used to reduce highly correlated data sets to an uncorrelated form for the characterization and visualization of their real structure. The measured p hydrographs $\mathbf{x} = (x_{1j}, \ldots, x_{pj})', j = 1, \ldots, n$ are calculated as linear functions of new vectors $\mathbf{y} = (y_{1j}, \ldots, y_{pj})'$:

$$x_{ij} = \sum_{l=1}^{p} u_{il} y_{lj} \quad \text{with} \quad u_l = (u_{1j}, \ldots, u_{pj}) \qquad (1)$$

The vectors $\mathbf{y}_i$, the PC (principal components), are calculated after the transformation (equation (1)) solving the special eigenvalue problem $(\mathbf{S} - \lambda\mathbf{E})\mathbf{u} = 0$, having the real

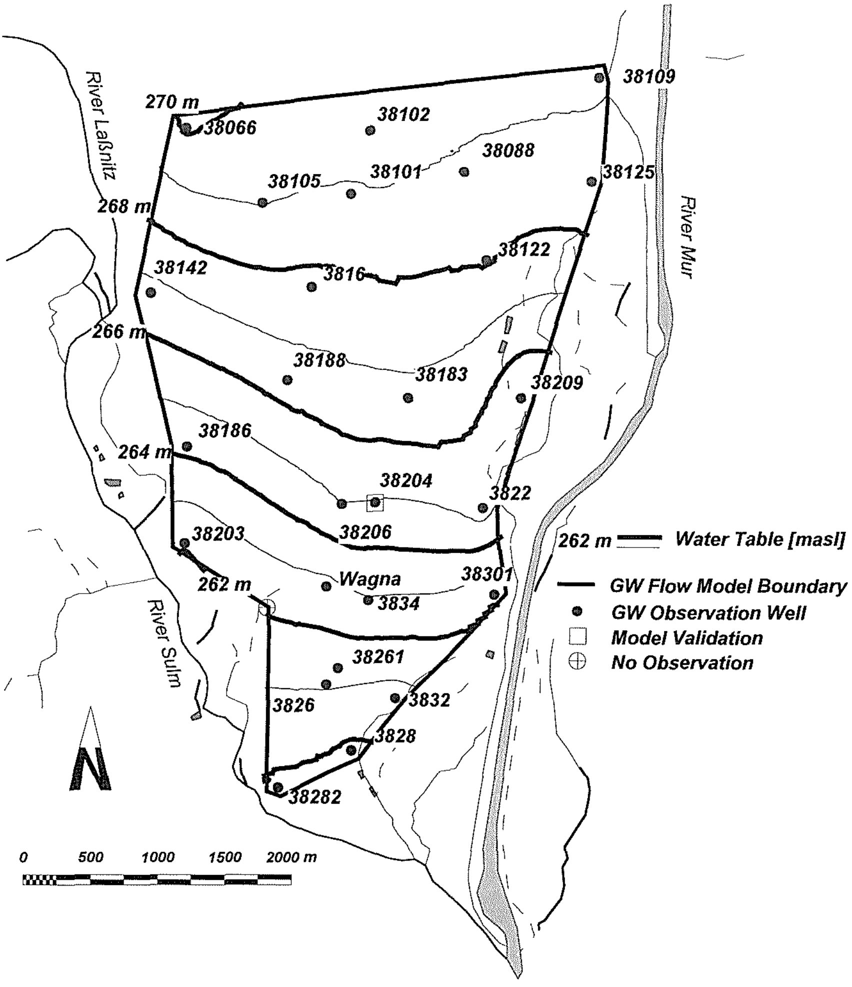

Fig. 1 Investigation area with the isolines of a mean groundwater table, groundwater flow model boundary, groundwater observation wells, observation point for spatio-temporal model validation and a marked unobserved point.

eigenvalues $\lambda_1 \geq \ldots \geq \lambda_p$ (**S** is the estimated covariance matrix from the n observations x_{ij} and **E** the $p \times p$ identity matrix). The sum p of the eigenvalues λ describes the total variability, the part of the variance explained by the first PC can be calculated (λ_1/p).

The PCA of the 26 groundwater hydrographs in the investigation area (Fig. 1) for the period 1992–1996 shows that the first PC explains more than 95% of the whole temporal variance. Therefore the factor scores of the first PC can be used for the analyses of the spatial structure with respect to the temporal behaviour of the groundwater table. Using VARIOWIN™ (Pannatier, 1996) the spatial structure of the factor scores of the first PC has been investigated and a linear variogram model was fitted to the experimental variograms.

ESTIMATION OF GROUNDWATER HYDROGRAPHS

The kriging interpolation of the values of the first PC for every grid element gives a system of linear equations which include the contribution of every observation point (kriging weights) to the resulting estimation value. The first PC is an overall variogram over observation time, therefore this model can be used for all the observed time points with an error resulting from the unexplained part of the hydrograph through the first PC. Using this model and the groundwater hydrographs at the observed points, it is possible to estimate a groundwater hydrograph for every grid element in the investigation area. Therefore this method can be used to estimate a groundwater hydrograph at every boundary node of a groundwater flow model, too. The estimated hydrographs may be used as initial boundary conditions for a transient groundwater flow model.

The PCA and the kriging interpolation were done twice: first using all the groundwater observation wells, and secondly without well 38 204 (Fig. 1) for model

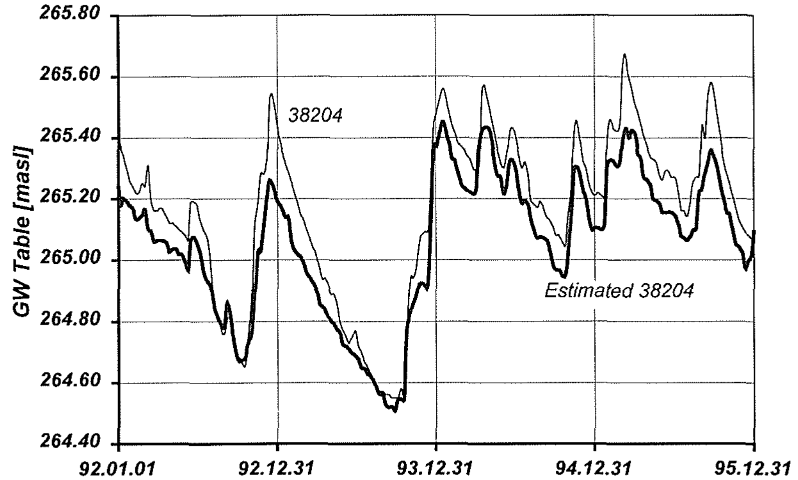

Fig. 2 Measured and re-estimated hydrograph (thick line) for the observation point 38 204 (for model validation this point was not included in the spatio-temporal model).

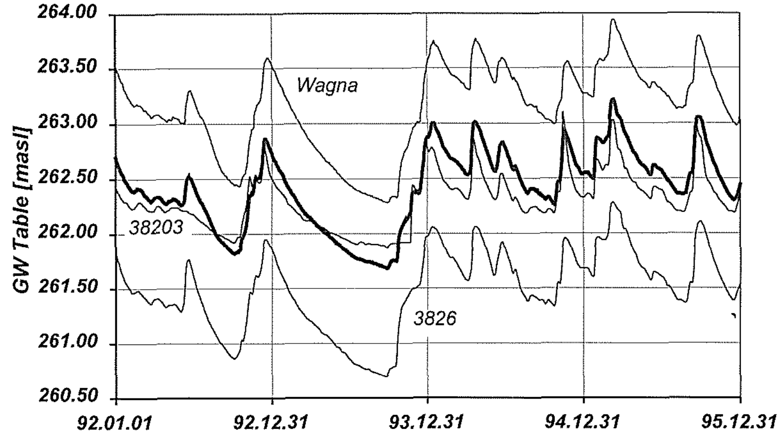

Fig. 3 Estimated hydrograph (thick line) for the point without observation and neighbouring observed hydrographs.

validation. Using this second spatio-temporal model for 38 204 a hydrograph was estimated and compared to the observed hydrograph (Fig. 2).

Using the first model, a hydrograph for a point at the flow model boundary without observations, was estimated and compared to the neighbouring observed hydrographs (Fig. 3).

ESTIMATION ERROR IN THE HYDROGRAPH

The krige-variance σ^2_{ok} of every grid element, calculated after Journel & Huijbregts (1978), is a measure of the quality of the spatial estimation of the first PC. If the centre of a grid element is identical with an observation point the estimation value equals the observed value. The krige-variance is $\sigma^2_{ok} = 0$. The error in the estimated hydrograph results from the unexplained part in the PCA of the observed hydrograph. The krige-system and the krige-variance of a grid element depends on the structure of the variogram $\gamma(h)$ and on the relative distribution of the observation points used for the estimation but not on the particular values.

A 95% confidence interval for the true value z of the factor score of the first PC estimated by z^* can be expressed as $[z^* \pm 2\sigma_{ok}]$. The value of σ_{ok} at observation point 38 204 using the model without observations at point 38 204 is 0.192. The factor score z at this point is 1.8903 and lies between the confidence interval $[1.636 \pm 0.384]$.

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