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N. Benoit^{1,2}, D. Marcotte¹, J.W. Molson³, and P. Pasquier²

¹Geological Survey of Canada, 490, rue de la Couronne, Québec, Québec G1K 9A9

²Polytechnique de Montréal, 2900, Boulevard Edouard-Montpetit, Montréal, Québec H3T 1J4

³Université Laval, 1065 avenue de la Médecine, Québec, Québec G1V 0A6

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GEOSTATISTICAL SIMULATIONS OF THE FULL 3D BLOCK HYDRAULIC CONDUCTIVITY TENSOR CONSIDERING INNER LOCAL-SCALE VARIABILITY

N. Benoit^{1,2}, D. Marcotte¹, J.W. Molson³ and P. Pasquier²

¹Geological Survey of Canada/Natural Resources Canada, 490 rue de la Couronne, Québec, Canada, nicolas.benoit@canada.ca

²École Polytechnique de Montréal, 2900 Boul. Edouard-Montpetit, Montréal, Canada

³Université Laval, 1065 avenue de la Médecine, Québec, Canada

Introduction

Heterogeneities in hydraulic conductivity (K) have a major impact on groundwater flow and contaminant transport. Local field measurements, however, typically focus on only one or at most a few local hydrofacies of hydrostratigraphic units (HSUs). This is insufficient to characterize regional hydrostratigraphic systems where numerous HSUs exist, each showing a range of K-values spanning several orders of magnitude. For numerical modelling at the regional scale, the K field is usually discretized in blocks. Quasi-point local conductivities must therefore be upscaled to equivalent block conductivity tensors accounting for the structural connectivity of hydrofacies at the regional scale and textural conductivity correlations at the local scale (Gomez-Hernandez and Journel 1990).

In this study, a multi-step upscaling method was applied to define the spatial distribution of the full 3D hydraulic block conductivity tensor considering the effect of local-scale variability. The approach comprises four main steps: (i) local-scale simulation of K for each HSU, (ii) upscaling of local (point) realizations into the full 3D block K-tensors using a block by block finite element flow simulator, (iii) definition of the spatial covariance and cross-covariance of the block K-tensor, and (iv) direct geostatistical simulation of block K-tensors at the regional scale. The approach was tested for regional groundwater flow in a complex hydrostratigraphic system of the Innisfil Creek watershed, Ontario, Canada (Fig 1) (Benoit et al., 2017). We stress that K-tensor variability effects are studied only within each HSU, as the same deterministic HSU model is used for all realizations. Including uncertainty in the hydrostratigraphic model itself is also possible (Benoit et al. 2017). However, it was our objective to isolate only the effect of K-tensor variability within the HSUs.

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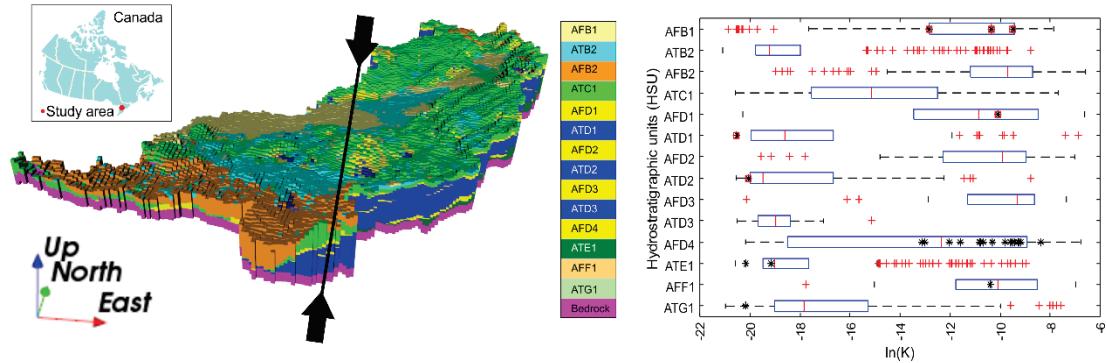


Fig. 1: 3D hydrostratigraphic model of the Innisfil Creek watershed (location of the regional cross-section indicated with arrows) and boxplots of K from grain size analyses (* symbols are laboratory measurements of K).

Data and methods

The regional geological model of the Innisfil Creek watershed was provided by the Ontario Geological Survey (Bajc, personal communication 2016). This model includes 14 HSUs of unconsolidated sediments, discretized into $200 \times 200 \times 1$ m block HSUs. Each block is assumed to be part of only a single HSU. Each HSU includes different hydrofacies described by a specific distribution of local K values (Fig. 1). The K database was built using 1,086 transmissivity measurements extracted from public wells, 32 soil samples recovered from boreholes analysed in the laboratory with constant and falling head permeability tests (Pasquier et al. 2016) and 1,694 grain size analyses from soil sampling in 15 boreholes located in the study area (Bajc et al. 2015). These field data were used for local scale assessments of K, which produced a highly variable K distribution both between and within the HSUs (Fig. 1). From the K boxplots, six HSUs are characteristic of aquitards, six of aquifers, and two appear transitional.

Herein, the collected grain size samples provide the only high-resolution information. Different methods for assessment of K values exist in the literature based on grain size analysis. Among the several tested methods, Sauerbrei's method (Vuković and Soro, 1992) was selected as it allows enough flexibility to cover the wide range of laboratory K measurements (see * symbols in boxplots in Fig.1).

The collected grain size samples have high resolution in the vertical directions along the boreholes. Vertical variograms of $\ln(K)$ were modelled separately for each of the 14 HSUs. These variograms were modelled either by spherical (12 HSUs) or exponential (2 HSUs) structures with a nugget effect (9 HSUs) representing 1-49% of the total variance. The practical vertical ranges vary between 1.1 and 19.5 m. Due to the large distances between the boreholes, the horizontal variograms could not be defined based on the grain size analyses. Instead, a global horizontal range of about 1,800 m was estimated from K values based on specific capacity tests with relatively dense spatial coverage, which represents a horizontal/vertical range anisotropy ratio of about 300. This ratio was applied to each HSU, with the anisotropy ratio of 300 being comparable to the horizontal/vertical block length ratio in the model.

Scalar K fields were simulated using a non-conditional turning band simulation (TBS) algorithm (Emery and Lantuéjoul 2006) over a grid of $120 \times 120 \times 120$ points on a mesh of size $2 \text{ m} \times 2 \text{ m} \times 0.01 \text{ m}$. This simulation grid was divided into $12 \times 12 \times 12$ blocks. 3D hydraulic conductivity tensors for each block were obtained by upscaling the local-scale simulation to the block scale (Fig. 2). Each individual block was upscaled with a block skin on each side. Thus, nine blocks were needed with the flow simulator to calculate the K tensor of the centre block. The method proposed by Zhou et al. (2010) was used with different sets of prescribed head conditions (three for flow between opposing faces, three for flow between opposing corners and two for flow between opposing edges). The Saltflow simulator (Molson and Frind, 2017) was used to obtain the 3D velocity and head fields. Mean 3D components of flux (q_x, q_y, q_z) and gradients ($\nabla h_x, \nabla h_y, \nabla h_z$) were calculated and used with Darcy's law to solve the full 3D K tensor.

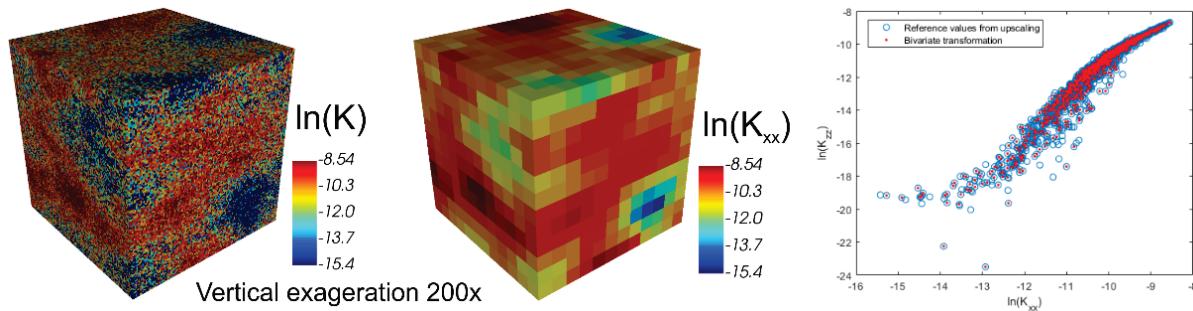


Fig. 2: Local-scale scalar K fields of unit AFB1 obtained from non-conditional TBS; the corresponding upscaled K_{xx} tensorial component and bivariate transformation of the K_{zz} component from a realization generated with LMC TBS.

Analysis of the upscaled K-tensor components revealed a clear control of principal components with strong correlations between them. Off-diagonal tensor components were negligible for all HSUs. The K-tensors of the different HSUs showed correlation ranges of a few to several blocks with no nugget effect. The variogram behaviour at the origin appears parabolic due to the large change of support from quasi-point to block scale. Simple correlations (at $h=0$) between $\ln(K_{xx})$ and $\ln(K_{yy})$ components vary between $0.75 < r < 0.99$. Correlations between horizontal components and $\ln(K_{zz})$ were also strong (10 HSUs showed $r > 0.91$). A linear model of coregionalisation (LMC) adequately describes the variograms and cross-variograms of $\ln(K_{xx})$, $\ln(K_{yy})$ and $\ln(K_{zz})$ in each HSU. Based on the upscaling results, two constraints were imposed: $\ln(K_{yy}) = \ln(K_{xx})$ and $\ln(K_{zz}) \leq \ln(K_{xx})$. The latter constraint was applied a posteriori using the transformation of the $\ln(K_{zz})$ realisation to the reference bi-variate distribution ($\ln(K_{xx}), \ln(K_{zz})$) of the upscaling results (Fig. 2, right).

Application

The developed block tensor coregionalisation model was used to assess regional 3D groundwater model of the Innisfil creek watershed (in development). For the application example, we present results

based on a large 2D vertical groundwater flow model extracted from the watershed (Fig. 3), chosen parallel to the flow direction based on the kriged head field. This regional cross-section includes five streams and cuts through the main physiographic features in the watershed: lowlands (north), uplands (south-central) and the highly permeable Oak Ridges Moraine (south). Although the model is based on real data, the assumption that the cross-section is aligned parallel to regional flow direction is a potential limitation. The study can thus be seen as a partially conceptual exercise.

Groundwater flow was simulated using homogeneous (deterministic) and stochastic HSU K_{xx} and K_{zz} fields. The model boundary conditions are: no-flow conditions for the lateral boundaries corresponding to the watershed divide, a no-flow condition at the model base, seepage conditions to simulate streams, and imposed flux (recharge) conditions at the surface of the model. The recharge rates were adjusted based on expected values for surficial material, which values correspond respectively to 200 mm/y and 20 mm/y for coarse and fine soil deposits. Initial K_{xx} and K_{zz} values were corresponding to the upscaled geometric mean. First, the calibration was conducted on the deterministic model by adjusting K_{xx} per HSU using the kriged regional zero-pressure surface as a calibration target. The K_{xx} parameter was adjusted by applying numerical inversion with Pest algorithm (Doherty, 2005). The K_{zz} values were derived from this updated K_{xx} field using the K_{xx} and K_{zz} ratio from the initial values. Next, stochastic modelling was conducted varying the K_{xx} and K_{zz} fields and keeping the other settings unchanged. No further calibration was conducted in this modelling. However, for each realization, K_{xx} field was modified based to the HSU ratio obtained for the calibration of the deterministic model ($K_{xx_PEST}/K_{xx_initial}$). Bedrock was not included in the upscaling process. A constant K value of 10^{-5} m/s was assigned on its top decreasing linearly with depth to 10^{-10} m/s.

Stochastic models with variable K tensors generated zero pressure surfaces comparable to that of the calibrated deterministic model (Fig 3). The impact of the K-tensor uncertainty on a typical flow simulation was assessed and proved non-negligible as shown with the simulations of the mean groundwater age. The stochastic simulations show that the mean age variation is indeed affected by the K tensors' variation within the HSUs.

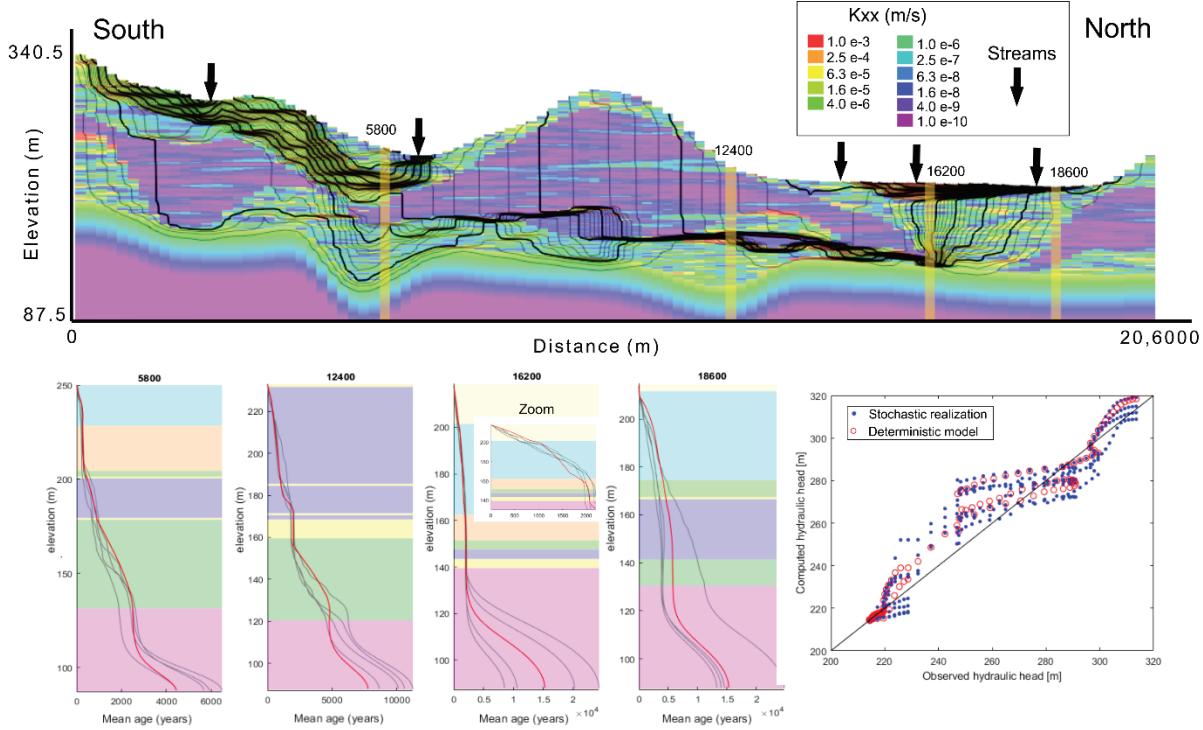


Fig. 3: Top row: simulated K_{xx} with stream function isolines via vorticity equation; Bottom row: HSU units and computed mean groundwater age for four realizations (left) along cut lines (yellow lines in top row) and computed vs observed hydraulic heads (right) for four realization and the deterministic model.

The stochastic models were also used to calculate the capture zones of the simulated streams and their uncertainty using the backward-in-time transport equation (Cornaton and Perrochet, 2006) (Fig. 4).

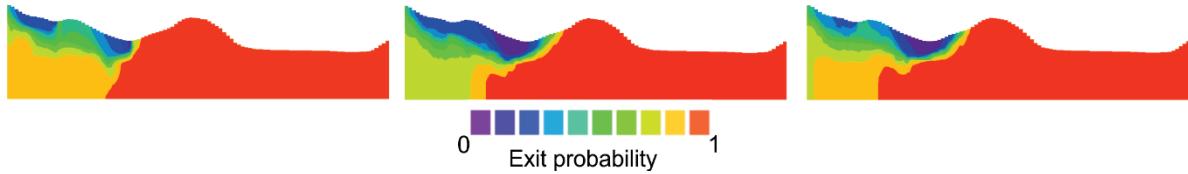


Fig. 4: Capture zones of the streams located in lowland area (North) for the deterministic model (left) and two realizations (centre and right). The capture zones were defined by the exit probability (0.1 colour intervals) of the random walk particles path toward the lowland streams.

Fig. 4 shows that capture zones of the lowland are well defined with current information. Note that the current assessment probably underestimates uncertainty as the same deterministic HSU model was used for all realizations. Nevertheless, the effect of the alternative models define different capture zones. Combining capture zones with mean groundwater age or its mean life expectancy, one can assess the vulnerability of each stream to a land contamination event and therefore determine possible land usage restrictions.

Conclusion

An efficient method was developed for regional characterisation of HSUs using 3D K tensors and was tested with 2D cross-sectional deterministic and stochastic groundwater flow simulations. It was found that within each HSU, K-tensor variability has a moderate effect on groundwater ages computed by the flow simulator but a relatively stronger effect on the definition of the stream capture zones. The results emphasize the different effects of homogeneous and heterogeneous HSU K-tensors under the same hydrogeologic settings and boundary conditions. These effects were quantified by simulating the groundwater age distribution and the capture zones of the streams. The proposed methodology appears well suited for determining the uncertainty of groundwater flow and transport models including aquifer vulnerability.

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