THINKING SCALE
IN UNSATURATED FLOW PARAMETER ESTIMATION

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ABSTRACT
Applying hydraulic parameters to the matrix model is the very decisive moment in unsaturated flow modelling. Observations and measurements must be related to scale, geometry and flow conditions in order to be rightly comprehended and transformed into adequate model parameters. We will use the data from the Gardermoen airport area in an attempt to identify the parameter disestimation that may arise when not considering the impact of these factors. In special we will look at the upscaling of parameters from a model with a multiple dipping layer structure into a model with this structure homogenized, applying flow simulation results from the multiple layer model as observation input for a homogenized inverse modelling. This has implications both for the transformation of soil sample measurements into regional soil hydraulic parameters, and for the use of field tracer experiments in calibrating the same.

INTRODUCTION
The omnipresent heterogeneity of the subsurface makes the question of scale fundamental in hydrology. Observations reflect in general a magnitude of different scales, while the opposite is true for hydrological models. Due to limited computer resources, numerical models are usually made for one or at best a limited number of scales. A flow model therefore usually represents a homogenization of the sub-elemental scale. Because of the ubiquitous heterogeneity, this disparity of scales makes hydrological forecast a risky business.

The subsurface represents also another challenge: It is inaccessible for direct observations. In particular this is true with respect to transport of contaminants. The most critical variable, namely the residence time of pollutants in the subsurface, is extremely expensive to monitor. Calibration is therefore usually based on observations obtained at lower costs. Lower costs imply more observations, and the question arises: What is best; a few observations with a lot of information, or a lot of observations that carry less information? In practice a trade-off has to be done.

In this paper we focus on flow in the unsaturated zone. Unsaturated flow represents an interesting challenge, namely the highly non-linear relation
between degree of saturation, pressure and permeability. Due to heterogeneities these non-linear relations are also connected to scale.

We limit the scope of this paper furthermore to unsaturated flow in dipping layers. Dipping layers are of interest mainly because of the economical interest connected to delta structures. Delta deposits are important reservoirs around the world, not only for water extraction, but also for mineral oil and gas. In this study we use observations from the Gardermoen deposit, which probably is the best-studied delta structure of mainland Norway. Flow in dipping structures is of more general interest than flow in horizontal layers, the latter being but a special case of the former. Unsaturated flow in horizontal layers might be modelled as one-dimensional flow, while flow in dipping layers is two-dimensional. In this study we use the same dip angle as observed at the distal parts of the Gardermoen delta. In general the dip angle is a function of the mean grain size of the sediment, but in this study we limit ourselves to one constant dip angle.

The purpose of this paper is twofold; firstly we generate a synthetic heterogeneous flow model with very high spatial resolution, mimicking heterogeneity at the smallest feasible scale. Absolute permeability at this scale is regarded as an isotropic variable. Three equally probable realizations are generated. All of them are reflecting real values from the Gardermoen delta. Based on these realizations we perform a synthetic (numerical) tracer test, which is "monitored" at the groundwater table. The residence time is visualized as breakthrough curves. Model output from these three realizations are regarded as "real observations" in the present study. In this part of the study we elucidate the stochastic nature of a breakthrough curve and apparent preferential flow in dipping layers.

The second purpose of this study is to simplify these three realizations into homogeneous flow models. In this context homogenization of flow parameters is equivalent to upscaling of parameters. Homogenization is done in terms of Bayesian inverse modeling as it is implemented in the multipurpose code iTOUGH2 (Finsterle, 1999). Estimation is conditioned on three sets of primary observations in this case study; liquid saturation, capillary pressure and pore flow velocities. Based on homogenized flow parameters we perform a new (synthetic) tracer tests and compare with the "real" breakthrough from the heterogeneous model. We also use observation data from two different infiltration conditions. Combining data from these two, however, does not yield inverse-modelled parameters that fit better. This would indicate that the homogenized parameters actually should vary with infiltration conditions.

In this study we performed inverse modelling in two steps. First we constructed homogeneous models that are consistent to the sedimentological architecture. In the heterogeneous high-resolution models (described above), there is a silty unit. This silty unit is kept intact in the first group of homogeneous models. In the second group the silty layer is simply removed,
but the estimated flow parameters are still conditioned on the same observations as previous.

The reason why we do inverse modelling in two steps is that tiny structures are difficult to detect and are therefore easily (but incorrectly) omitted in common practice. By comparing the breakthrough curves derived from models with and without the impervious silt layer, we notice an interesting feature: Travel time of water is faster if the low-pervious layer is included. Intuitively speaking this is opposite to what we might expect: A low-pervious layer (or a barrier) should increase residence time of pollutant or at best prevent pollution from arriving a target, in this case the groundwater table, but that is not true if the low-pervious layer is dipping.

**METHOD AND DATA**

The numerical flow simulator TOUGH2 (Pruess, 1991) is used to solve the forward problem. Unsaturated flow is modelled according to Richards’ equation (Richards, 1931) with the van Genuchten (1980) constitutive relations describing capillary pressure and relative permeability as a function of saturation.

The inverse problem is solved by using the Bayesian Maximum Likelihood method (Carrera and Neuman, 1986), which is implemented in the inverse modelling code iTough2 (Finsterle, 1999). The parameter set to be estimated is \( \mathbf{p} = \{ \mathbf{p}_1, \ldots, \mathbf{p}_i, \ldots, \mathbf{p}_N \} \) where \( N \) is the total number of geological units, and \( \mathbf{p}_i = \{ k_d, k_v, 1/\alpha, n \}_i \), is the vector of hydrogeologic model parameters to be estimated for each unit, \( k_d \) and \( k_v \) [m\(^2\)] are dipping and vertical permeabilities; \( 1/\alpha \) [Pa] is air entry value; and \( n [-] \) is a parameter characterizing the grain size distribution. The parameters are estimated by matching the data, which requires evaluation of the residual at each calibration point:

\[
\mathbf{r}_j = y_j^* - y_j(\mathbf{p}), \quad j = 1, \ldots, u
\]

Here, \( y_j^* \) is the observation at location \( j \) in time and space, and \( y_j \) is the corresponding value calculated with the forward model for systematic variation of the unknown parameter vector \( \mathbf{p} \). If the residual vector \( \mathbf{r} = \{ r_1, \ldots, r_j, \ldots, r_u \} \) is Gaussian, maximum likelihood estimates are obtained by minimizing an objective function that is the sum of the squared residuals weighted by the inverse of a covariance matrix \( \mathbf{C}_{yy} \):

\[
Z(\mathbf{p}) = \mathbf{r}^T \mathbf{C}_{yy}^{-1} \mathbf{r}
\]

\( \mathbf{C}_{yy} \) represents measurements error and statistical information about the \textit{a priori} information regarding \( \mathbf{p} \). If \( Z(\mathbf{p}) \) is properly conditioned, an optimal set of parameters, \( \mathbf{p}^* \), exists that minimizes (2), i.e., \( Z(\mathbf{p}^*) = \min \{ Z(\mathbf{p}) \} \). We use the Levenberg-Marquardt algorithm (Press et al., 1992) to find the minimum of the objective function.
For a reasonably small confidence region, \( y_j \) is assumed to be a linear function of \( \mathbf{p} \), in which case the covariance matrix of the estimated parameters is given by (Carrera and Neuman, 1986):

\[
\mathbf{C}_{pp} = s_0^2 \left( \mathbf{J}^T \mathbf{C}_{yy}^{-1} \mathbf{J} \right)^{-1}
\]

(3)

where \( \mathbf{J} \) is the Jacobian or sensitivity matrix evaluated at \( \mathbf{p}^* \):

\[
\mathbf{J}_{ij} = - \frac{\partial r_i}{\partial p_j} = \frac{\partial y_i}{\partial p_j}
\]

(4)

The estimated error variance serves as a goodness-of-fit measure:

\[
\hat{s}_0^2 = \frac{Z(\mathbf{p})}{u-v} = \frac{\mathbf{r}^T \mathbf{C}_{yy}^{-1} \mathbf{r}}{u-v}
\]

(5)

where \( u \) is the number of observations, and \( v \) is the number of parameters.

In this study, observations were taken from the results of numerical simulations (forward run). The matrix architecture model and its parameters are however based on an extensive data material from the Gardermoen research site. GPR profiles (Fig.1) and borehole logs have identified a heterogeneous delta layer structure beneath c. 2 m, which also includes silty layers with high water content. Grain size distribution curves from 1875 soil samples were used to estimate hydraulic conductivity (Fig.2), and statistical moments for different clusters were derived. These values are discussed and applied by Kitterød (2001) and Alfnes et al. (2002). The statistical moments for the sandy foreset layers were used in this study to generate stochastic parameters for 24 different sandy layers. Although the parameters \( k \), \( \alpha \) and \( n \) are correlated, there was no information available so as to take account of that fact, and they were thus generated independently. \( \alpha \) and \( n \) moments had to be altered somewhat in order to get physical values in all parameter sets; also, the \( k \) mean value had to be increased a bit to avoid convergence problems following too many low-permeable layers. Parameter values applied are listed in Tab.1 just beneath.

<table>
<thead>
<tr>
<th></th>
<th>( k )</th>
<th>( 1/\alpha )</th>
<th>( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>mean</td>
<td>-24</td>
<td>6.9</td>
<td>3</td>
</tr>
<tr>
<td>std.dev</td>
<td>0.97</td>
<td>0.4</td>
<td>0.4</td>
</tr>
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Table 1. Normal distribution for \( n \), lognormal for the other parameters.
Determining the shape of the model grid elements is important. As for the TOUGH2 code, anisotropy can only be set by applying different interelemental conductivities; hence the implementation of an anisotropy following the dipping angle of a layered soil structure requires that the elements be arranged in that same structure. Also, when modelling structure-dependent flow, element structure should be arranged in a way that respects the dominant flow features.

For dipping layer structures, funnelling flow can be expected as a result of hydraulic or capillary barriers. Holm (1998) has shown that in continuum hydraulics solving Richards’ equation, this phenomenon is explained by the parameter differences in the pressure – hydraulic conductivity – water content relationship model (pK and pF curves) applied. A study of a single dipping finer layer interbedded in a coarser material (Holm, 1998) illustrates the mechanism: If water percolates at a rate equivalent to the hydraulic conductivity value of the crossing point of the two pK curves of the respective materials (Fig.3), pressure is uniform in both, and water flows straight down. If however percolation is at another rate, pressure in the two materials will differ, and is un-uniformly adjusted so as to be continuous throughout. This un-
uniform pressure field, when imposed over a *dipping* layer interface, triggers funnelled flow (Fig.4).

Figure 4. Flow direction patterns. (a) corresponds to 2 mm/d infiltration, and (b) to 200 mm/d, as shown in Fig.3.

The grid was thus made with rectangular elements in the top 1.8 m, and with dipping elements beneath (Fig.5). The dip was \( \tan^{-1}(5/20)=14.0^\circ \). To the silty layer was ascribed a thickness of 4 grid layers of dipping elements, whereas the 24 sandy layers encompassed only a single grid layer each; the same cycle of different sandy layers was repeated about four times, though.

Figure 5. An essential excerpt from the grid.

Independent parameter sets of \( k, \alpha, n \) were generated for three cases: \( a, b \) and \( c \). Each case was a forward simulation run with a starting steady-state infiltration of 2.5 mm/d followed by 16 days of 42 mm/d infiltration. Simulated values of saturation, pressure and water flow at both the starting and the ending point of time were excerpted to serve as observation data for the inverse simulations, in different combinations.

The model set-up to be used in the inverse modelling differed from the forward cases only in that the 24 sandy dipping layers were exchanged with one single soil type, the parameters \( k_d, k_v, \alpha, n \) of which were to be estimated (\( k_d \) is permeability in the dipping direction, \( k_v \) in the vertical). This means that whereas the observation data came from a *heterogeneous* and *isotropic* case, the inversely estimated parameters were supposed to apply for a *homogeneous* and *anisotropic* case. Some inverse runs were also performed without the silty dipping layer, i.e. homogenizing the whole foreset.

Breakthrough curves were not produced by the TOUGH2 code itself, but by combining the flow field with a pure advective algorithm with no dispersion.
RESULTS
The results can be grouped in two, the first group being the three forward cases. Case \textit{a} (Fig.6) was the medial of these concerning the stochastic parameters generated, case \textit{b} showing less, and case \textit{c} more flow diversion, which may also be suggested by their breakthrough curves (Fig.7).

Figure 6. Flow paths and water saturation. Darker shadow indicates higher saturation.

Figure 7. Cases \textit{a,b,c}. The breakthrough is at the area between 0.3 and 1.5 m at groundwater table, cfr. Fig.6.
The second group is the inverse modelling results. Some of these simulations did not converge for the 16 days 42 mm/d infiltration run. As will be discussed later, the set-up turned out not to be ideal for quantitative comparison of the breakthrough curves. However, some qualitative inspection may be done (Fig.8,9). Breakthrough curves are based on the number of particles arriving at the foot of the silty layer, i.e. between the lateral positions of 0.3 and 1.5 m at the groundwater table.

Figure 8. Breakthrough curves (case a) at the 0.3-1.5 m silty layer foot. The thick line is the heterogene forward case. Whole lines are several inverse cases based on different data types at 42 mm/d infiltration, or both 42 and 2.5 mm/d. Dotted lines are based on 2.5 mm/d inf., whereas dashed lines are inversely modelled without the silty layer.

Figure 9. The spatial breakthrough curves (case a) demonstrate how the heterogeneous case (circles) differ from the homogenized cases by its dispersion. The whole lines denotes breakthrough at the 0.3-1.5 m silty layer foot.
DISCUSSION

A main purpose of this study was to generate synthetic models with geometry and heterogeneity constructed as close as possible to what is observed in a real aquifer, in this case that of Gardermoen. The three realizations show that flow paths and residence time of water in the unsaturated zone do not only depend on the magnitude of heterogeneity, but also on the internal arrangement of it. In our opinion this explains apparent preferential flow in apparently homogenous dipping sand layers. Anisotropy at a greater scale may thus be decomposed into a funnelled flow component deriving from a smaller scale heterogeneity, as well as an anisotropy intrinsic to the smaller scale. It is also clearly demonstrated that deflection of travel paths depend on degree of saturation. The higher saturation, the more vertical are the travel paths.

An important objective for modelling flow in the subsurface is to make forecasts of residence time. Sometimes it may also be of interest to predict flowpaths. In order to validate forecast modelling, it is necessary to perform a tracer test. However, to be able to utilize tracer tests as conditional observations for inverse modelling, the mass of tracers has to be monitored. The mass balance has to be controlled. In principle this is only possible in carefully controlled laboratory experiments where boundary conditions are possible to control. A field tracer test is performed in an open system where boundary conditions are affected by uncertainties and very difficult to control. Valuable tracer tests are performed in unsaturated zone at Gardermoen, but mass balance was not possible to control. In that case, sensors for extraction of soil water was located above the silty layer (Søvik et al., 2002). The three stochastic realizations (Fig.7) clearly demonstrate the uncertainty of travel paths in the unsaturated zone, thus in our opinion extraction probes in the unsaturated zone can only be considered as additional information. The amount of tracer has to be collected in one or more extraction wells in the saturated zone in order to control mass balance.

The second purpose of this study was to evaluate the possibility of reproducing real breakthrough curves by homogenized (upcaled) parameters. We did estimation in terms of inverse modelling which ensure consistent reproduction of primary observations. In our opinion the results are promising in terms of qualitative prediction of travel time. Simulation of advective travel time by homogenized flow parameters envelop the "observed" breakthrough curve. Note that in this case the breakthrough curve is independent data. However, to draw quantitative conclusions we have to make a minor improvement of the heterogeneous grid. Due to random heterogeneities, flow paths will reach the groundwater table differently from case to case. Because of this ambiguity we are unable to make consistent comparison between any two breakthrough curves. That's the reason why the breakthrough curves (Fig.7,8) sum up to different numbers of particles. This ambiguity can be avoided by
introducing a second silt layer parallel to the first, and in addition repeat the heterogeneity between the two dipping silt layers on both sides of the confining silt layers. I.e. the flow field has to be repetitive, thus making random flow diversion irrelevant. If not, consistent comparison between different cases is impossible. Instead of camouflaging this annoying ambiguity we think it important to emphasize such problems in order to encourage others to make improvements. The ambiguity illustrates in addition the difficulties of introducing heterogeneity in dipping structures. Often imperfection is more food for thought than perfection!

REFERENCES