Four Decades of Progress in Monitoring and Modeling of Processes in the Soil-Plant-Atmosphere System: Applications and Challenges

The Impact Of Field Data Acquisition Methodology Upon Prediction Of Transport In The Made Aquifer

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Abstract

The hydraulic conductivity $K$ of the aquifer of the MADE transport experiment, was measured in the past at a dense three-dimensional network of sampling stations. Two methodologies were employed: initially, the flowmeter (using numerous piezometers) and recently the DPIL (direct push injection logger) method. The results for the statistical moments of the lognormal $K$ distribution were similar for the horizontal and vertical integral scales, but quite different for the geometric mean and the variance. By using our recently developed model of transport in highly heterogeneous formations we were able to predict the observed longitudinal mass distribution spreading and to compare with measurements. We found that prediction based on DPIL parameters led to agreement, while flowmeter data resulted in discrepancy. Using our transport model, we explore here in a systematic manner the impact of the different statistical parameters upon the breakthrough curve at different distances from the injection zone.

1. Introduction and background.

Spreading of solutes in the subsurface is a topic of great interest due to its relevance to pollution of soil and aquifers. Laboratory experiments carried out in soil-packed columns have shown that spreading can be described with the aid of a advection-dispersion equation with a constant dispersivity coefficient, which is of the order of the pore scale. However, field tests have demonstrated that spreading is of much larger extent, and the corresponding macrodispersivity is larger than the laboratory one by orders of...
magnitude. This increase was attributed to the omnipresent heterogeneity of the hydraulic conductivity $K$, which may vary in space by orders of magnitude in natural formations. The intuitive reasoning is that portions of the solute plume advected by the fluid move quicker in zones of high permeability than in those of low one and the subsequent spreading is characterized by the length scale of $K$ spatial variations rather than the pore scale.

Various theoretical models and field experiments were carried out in order to investigate field scale transport and quantify it (see e.g. the monographs [5, 8, 14]). The use of models for prediction is vital, as pollutant plumes spread slowly, over periods of tens to hundreds of years. Due to the seemingly erratic variation of $K(x)$ and scarcity of data, it is common to model it as a stationary lognormal random space function of axisymmetric two-point covariance, such that $Y=\ln K$ is characterized by 4 parameters: the geometric mean $K_G$, the variance $\sigma_G^2$, and the horizontal and vertical scales $I$ and $I_v$, respectively. Furthermore, flow and transport were analyzed mostly for mean uniform flow corresponding to natural gradient, i.e. for a constant horizontal mean head gradient $J$ and a mean velocity $U=K_{eh} J$, where $K_{eh}$ is the horizontal effective conductivity of the heterogeneous formation. A solute plume is injected at $t=0$ in the plane $x=0$, and it spreads subsequently primarily due to advection by the fluid velocity. Longitudinal spreading is quantified by $M(x,t)$, the breakthrough curve (BTC), defined as the mass of solute (relative to the initial mass) which has moved past the control plane at $x$ at time $t$; in particular $m(x,t)=-\partial M/\partial x$ describes the longitudinal mass distribution at time $t$. Various models have been developed in order to determine the dependence of $m$ on the structural $Y$ parameters and the mean gradient $J$. Most of them assumed weak heterogeneity, i.e. $\sigma_G^2 \ll 1$, in which case $m$ is Gaussian and can be characterized by the longitudinal macrodispersion coefficient $D_I=\alpha_v U$, with $\alpha_v$ the macrodispersivity.

A few elaborate transport field experiments were conducted in the past in order to validate the theoretical models. Thus, the ones at Borden Site [12] and Cape Cod [10], were characterized by the aquifer weak heterogeneity ($\sigma_G^2 \approx 0.3$). In these two cases measured and predicted $m$ agreed satisfactorily. More recently the field experiment known as MADE [3] was carried out in a highly heterogeneous aquifer ($\sigma_G^2 \approx 7$) for which $m$ was found to be skewed and far from Gaussian.

One of the key issues in field experiments and in prediction is the measurement of $K$ at a large number of points in order to characterize its statistical structure. This is a costly operation, which poses problems of accuracy, of duration as well as of development of appropriate technologies. This is a topic of intensive research and new methods, hydraulic or geophysical, are under development. At the aforementioned older experiments at Borden and Cape Cod, a large number of boreholes were drilled and numerous soil samples were extracted and used for laboratory determination of $K$; this is a costly and tedious procedure and the measurements are affected by the disturbance of the soil. In contrast, at the MADE experiment the initial methodology was primarily the flowmeter one, in which the vertical variation of the discharge along pumping wells is determined in situ (see next Section) and translated into $K$ values. The data from numerous boreholes served in order to characterize the logconductivity statistics. Recently the Direct Push technology, was applied to the same aquifer (see next Section) and a thorough comparison of the data obtained by the two methods was carried out by Bohling et al [4]. The direct push method has the advantage of a much quicker and less costly data acquisition than the flowmeter. The main outcome of the comparison was that while the identified $Y$ spatial structures were similar with close values of $I$ and $I_v$, major differences affected $K_G$ and at a lesser extent $\sigma_G^2$. Though Bohling et al [4] provide arguments in favor of the DP determined values, the salient question of the impact of the differences upon transport prediction was investigated only recently [7]. This has become possible due to a model of flow and transport in highly heterogeneous formations we have developed in the last decade (coined as MIM, the multi-indicator model; see e.g. [6]). The application of the model to the MADE transport data led to the conclusion that indeed the DP technology yields an identified $Y$ statistical structure which predicts much better the observed plume than the flowmeter data. However this was a side topic and the comparison was
carried out only for one snapshot of the plume out the available six ones. The aim of the present study is to expand and elaborate the comparison of the two technologies.

The plan of the paper is as follows: in the following Section we recapitulate briefly the MADE site description, the two methodologies and the model. Subsequently, in Section 3 we present the application of MIM with the two sets of data. The last Section summarizes and concludes the study.

2. Recapitulation of MADE site data and the MIM

2.1. The MADE site

The MADE (macrodispersion experiment) site located in the Columbus Air Force base in USA was described in a series of papers, summarized by the recent one [15]. The formation consists of an alluvial terrace of poorly sorted to to well-sorted sandy gravel and gravely sand with significant amounts of silt and clay, with an average thickness of about 10 meters. It is underlain by a continuous clay layer.

The hydraulic conductivity distribution was initially determined by using 58 fully penetrating wells [13], which were supplemented by additional wells in the following years. The values of \( K \) were determined by the borehole flowmeter technology. The procedure consists in steadily pumping the well and measuring the vertical flow through the borehole with the aid of an impeller flowmeter, which is moved vertically by steps of 15 cm. The difference between steps provides the discharge pertaining to the layer. Subsequently, assuming that the aquifer behaves like a stratified one, with each layer being homogeneous, the conductivity \( K \) was determined by using the solution of steady flow. This way, 2483 estimates of hydraulic conductivity at different locations were obtained initially, to be augmented to 3925 subsequently. While this is an in-situ procedure, it may be affected by a few errors stemming for instance from soil disturbance near the well, measurement errors and idealized flow model. One of the limitations which is particularly relevant to MADE is the presence of a lower threshold of flow measurement by the impeller which translates into a lower limit of \( K \approx 10^{-6} \text{ m/sec} \).

A more recent campaign was conducted at the MADE site [11] by using two DP (direct push) methods: DPIL (direct push injection logger) and DPP (direct push permeameter). In both cases a small diameter rod is pushed continuously into the soil by a percussion machine. Water is injected continuously through a short screened section near the tip. The rod is advanced by 1.5 cm steps and at each step the discharge \( Q \) (maintained constant during the profiling) and the injection pressure \( P \), are measured (these are the only measurements taken in the DPIL mode). The permeability of the zone adjacent to the screen is assumed to obey the relationship \( \ln(K) = a \ln(Q/P) + b \), where the constants \( a, b \) pertaining to the formation have to be calibrated. The DPP consists of the same rod, equipped additionally with two pressure transducers, at 15 cm and 40 cm above the screen, respectively. By measuring the pressure and by using a numerical solution of the flow around the rod induced by the water injected through the screen, the integrated permeability over the interval between the transducers can be determined. It can be also used in order to calibrate the above DPIL constants. At the MADE site the two tools were combined in a high resolution tool which is described in [4]. Thus, the 31123 DPIL measurements were supplemented by 95 DPP ones. Bohling et al [4] provide a comprehensive analysis of the \( K \) data obtained by the flowmeter and direct push methodologies and a comparison between them (the reader is sent to the paper for details).

Both methods indicate that the univariate \( Y = \ln K \) at MADE site is normal and characterized by \( \mu_G \) and \( \sigma^2_Y \). Furthermore, identified vertical and horizontal variograms have sills (though the vertical one displays a possible nonstationary effects at lags larger than 6 m) and horizontal and vertical integral scales could be identified. The final result is summarized in Table 1 of [4]: the mean values are \( \mu_G = 4.3 \times 10^{-5} \text{ m/s} \) and \( \sigma^2_Y = 4.4 \) for the flowmeter while \( \mu_G = 8.9 \times 10^{-6} \text{ m/s} \) and \( \sigma^2_Y = 6.6 \) for the DPIL. Similarly, Table 2 reveals
that the average integral scales values are $I_v = 1.5\, \text{m}$ for both methods while $I = 12.3\, \text{m}$ and $I = 10.2\, \text{m}$, for the flowmeter and DPIL, respectively. It is seen that there is a great disparity, of one order of magnitude between the identified $K_G$, which is explained by Bohling et al [4] primarily by the inability of the flowmeter to capture low $K$ values.

Fig. 1. Illustration sketch of the conceptual model.

2.2. The MADE transport experiment

In the first natural gradient transport experiment (1986-1988) conservative tracers were injected into a linear array of 5 wells at 1 m spacing in a plane normal to the mean gradient over a 48h period [3]. The gradient $J$ of the water table fluctuated somewhat seasonally around the mean value of 0.0036, which is the steady value adopted here. The bromide concentration was measured by a large number of multilevel samplers, in arrays parallel to the injection one, at a large density in the input zone, and decreasing downstream. By using the data collected at different times from the injection, snapshots of the longitudinal distribution $m(x,t)$ of the plume at different fixed times $t = 49, 126, 202, 279, 370, 503$ days were determined by integration over vertical planes and interpolation along $x$ (they are reproduced in Fig. 7 of [1]). The striking feature is the skewed, far from Gaussian, shape of the distribution. It is emphasized that the initial plume has expanded (primarily in the vertical direction) during the injection period reaching a vertical size of approximately 8 m (Fig. 6 of [1]). The mass recovery of the plume, as determined by integration of $m$ over $x$, was incomplete with a value decreasing from 200% at first sampling at $t = 49$ d to 43% at the last one at $t = 503$ d. Various explanations were forwarded for this finding (see e.g. [1] and [7]) and the issue is not yet elucidated. We tend to believe that the problem stemmed from the formation of plume “fingers” along paths of preferential flow in zones of high permeability, which were not captured by the samplers. Similar features were present at the much more homogeneous aquifers at the Borden and Cape Cod sites.

2.3. Modeling transport at MADE

The non-Gaussian transport in the highly heterogeneous aquifer, which cannot be modeled with the aid of a macrodispersivity, has motivated derivation of models like CTRW [2] and the dual domain mass transfer [9]. These models contain parameters which could be fitted such as to capture the behavior of the
observed MADE plume. However, the parameters are not directly related to the K measurements so that they cannot be used in order to assess the impact of the data acquisition methodology upon transport.

In contrast, we have advanced in the last decade (see, e.g., [6]) a model of flow and transport which was coined as MIM. The model regards the formation as a collection of rectangular blocks which tessellate continuously the space (an illustration sketch is depicted in Figure 1). The elements of volume \( \omega^{(i)} \) and centroid coordinates \( \bar{x}^{(i)} \), have constant and random conductivity \( K^{(i)} \), such that the structure is described by

\[
K(x) = \sum_{i=1}^{M} K^{(i)} I(x - \bar{x}^{(i)}) \quad ; \quad Y(x) = \sum_{i=1}^{M} Y^{(i)} I(x - \bar{x}^{(i)})
\]

where the indicator function \( I(x-\bar{x}^{(i)})=1 \) for \( x \in \omega^{(i)} \) and \( I(x-\bar{x}^{(i)})=0 \) for \( x \notin \omega^{(i)} \). In spite of the seemingly idealized structure, it can model any formation of given \( K_G \) and \( \sigma^2 \), by generating \( Y^{(i)} \) correspondingly, and of any horizontal and vertical scales \( l \) and \( l_v \), by selecting the block sizes. By a series of approximations, which were validated by accurate numerical simulations, we were able to develop a simple model of flow and transport, based on this model. Skipping the details (see e.g. [7]), in essence the travel time of a solute parcel injected at \( t=0 \) at \( x=0 \), is the mean \( x/U \), supplemented by the sum of the independent and random travel times residuals \( \tau^{(j)} \) pertaining to the blocks \( j=1,..M \) (\( M \geq 1 \)), covered by the parcel. The latter have analytical expressions, such that \( \tau_R = \sum_{j=1}^{M} \tau^{(j)} \) is a random variable which depends on \( K^{(i)} \). Its pdf can be computed numerically either by a convolution of Fourier Transforms or by a Monte Carlo simulation with \( K^{(i)} \) drawn at random from the lognormal distribution. By assuming an ergodic plume, the BTC \( M(x,t) \) is simply related to the travel time pdf and so is \( m(x,t) \), the longitudinal mass distribution. Thus, by using the parameters \( K_G, \sigma^2 \) and \( l \) (\( l_v \) was found to be immaterial), as well as the mean head gradient \( J \), the model can be employed in order to determine \( m(x,t) \) pertinent to the given formation. The model is not limited by the value of \( \tau^2 \), and it was applied to simulations with \( \sigma^2 \leq 8 \) [6]. Indeed, for highly heterogeneous formations the resulting \( m \) is non-Gaussian and skewed.

3. Application of the MIM to the MADE transport experiment.

In [7] the MIM was applied to MADE to determine the longitudinal mass distribution \( m(x,t) \) by using the two sets of parameters: the ones determined by the flowmeter (\( K_G = 4.3 \times 10^{-5} \text{m/s}, \sigma^2 = 4.4, l = 12.3 \text{ m} \)) and those arrived at by DPIL (\( K_G = 8.9 \times 10^{-6} \text{m/s}, \sigma^2 = 6.6, l = 10.2 \text{ m} \)). The outcomes have been compared with the experimental plume snapshot at \( t = 279 \text{ d} \) (Fig. 3 of [7]). The result was that while the DPIL based parameters led to a satisfactory agreement with experiment (op cit Fig. 2d), \( m \) based on the flowmeter parameters was largely different. Furthermore, the difference stemmed primarily from the large gap in the \( K_G \) values, whereas those of \( \sigma^2 \) and \( l \) had a much lesser impact.

As already stated the aim of the present paper is to further elucidate the matter by carrying out the comparison for the entire set of six snapshots at different times. The computations were carried out as stated above and in Figures 2a-f we represent the experimental and the two modeled distributions. It is seen indeed that at all times the same finding is evident: the DPIL determined parameters lead to a much better agreement between model and field measurements than the flowmeter ones.

It is worthwhile to recall here two features discussed in [7]. First, the rugged appearance of the experimental mass distribution is due to the fit to measurements at a discrete number of cross-sections. More significant is the difference in the total mass, the area beneath the \( m \) graph. As already mentioned the experimental mass recovery was incomplete, whereas the theoretical \( m \) is of unit area as no retention mechanism is present in the model. According to our interpretation the mass deficiency is due to the
insufficient sampling of the concentration in the wake of the plume, which is determined mainly by solute which has moved along connective paths of high permeability. It was gratifying, therefore, to find out that the theoretical mass distribution based on the DPIL parameters agrees quite well with measurements for the leading part and in particular with the entire plume for the only time for which recovery was complete ($t=126$ days).

Fig. 2. MADE experiment: Relative mass distribution as function of longitudinal distance for 6 snapshots (a-f). Comparison between experimental, theoretical with flowmeter and DPIL data.

4. Summary, discussion and conclusions.

Characterization of permeability spatial distribution in aquifers is an essential step toward modeling spreading of pollutants. Various field methodologies were used in the past and new ones are under development, aiming at reducing cost and duration and improving accuracy.
The two methodologies used in the characterization of the highly heterogeneous MADE site were the flowmeter and the DPIL (direct push). The analysis of the numerous data led to similar lognormal univariate distributions, with parameters which were of relatively close values, except the geometric mean $K_G$. The latter was larger by roughly an order of magnitude for flowmeter than for DPIL. To illustrate the difference between the two distributions we represent them in Fig. 3. A direct comparison of the two methodologies [4] suggested that the difference stems primarily from the inability of the flowmeter to identify low permeability values.

In the present study we investigate the impact of the differences between the two sets of parameters upon prediction of the longitudinal mass distribution of the MADE plume by using our model of transport MIM [6, 7]. The result of prediction is compared with field measurements [3] in Fig. 2. To focus the discussion we concentrate on the snapshot of $m(x,t)$ at $t=126$ days, for which there was full mass recovery. Inspection of Fig. 2b shows that prediction based on the DPIL data reproduces quite accurately the observed skewed distribution and particularly the concentration of the mass in the injection zone. This finding was discussed in [7]: the MIM captures the nonlinear behavior of the travel time distribution, with much larger delay in zones of low permeability than advance in those of high permeability. In contrast, the prediction based on the flowmeter data leads to a plume which has moved downstream of the observed one, with a wider mass distribution. This behavior stems from two features of the logconductivity distribution (Fig. 3). First, the mean velocity $U=K_{ef} J$ is larger as $K_{ef}=10.8$ m/d, as compared to the value 2.8 m/d corresponding to the DPIL data. Secondly, due to the shift of the distribution of Fig. 3 the probability of encounter of low permeability zones is lower for the prediction based on DPIL. Conversely, the probability of covering high permeability zones is enhanced, leading to lack of agreement for the large $x$ tail as well. Thus, it is demonstrated that a much better agreement could be attained with the DPIL data rather than the flowmeter ones.

Two conclusions which can be drawn at present are: (i) previous studies which used the flowmeter data in order to model the MADE plume may need reconsideration of the data basis and (ii) field methodologies which are able to identify more accurately low conductivity aquifer zones, like DPIL, are to be preferred as a basis for prediction.

We emphasize that the present results and conclusions have been based after the analysis of longitudinal mass distribution $m$. Our MIM methodology is unable at present to model local quantities,
like e.g. the local concentration statistics, and we therefore are unable to extend our conclusions to other transport measures. Still, we believe that a detailed characterization of the conductivity field, like the one provided by DPIL, is a necessary prerequisite to any transport model.

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References

[1] Adams EE, Gelhar LW. Field study of dispersion in a heterogeneous aquifer: 2. Spatial moments analysis. Water Resour Res 1992;28(12):3293-3307, doi:10.1029/92WR01757.
[2] Berkowitz B, Scher H. Theory of anomalous chemical transport in random fracture networks. Phys Rev E 1998;57(5):5858-5869.
[3] Boggs JM, Young SC, Beard LM, Gelhar LW, Rehfeldt KR, Adams EE. Field study of dispersion in a heterogeneous aquifer: 1. Overview and site description. Water Resour Res 1992;28(12):3281-3291, doi:10.1029/92WR01756.
[4] Bohling GC, Liu G, Knobbe SJ, Reboulet EC, Hyndman DW, Dietrich P, Butler JJ. Geostatistical analysis of centimeter-scale hydraulic conductivity variations at the MADE site. Water Resour Res 2012;48:W02525, doi:10.1029/2011WR010791.
[5] Dagan G. Flow and Transport in Porous Formations, Springer, New York, 1989.
[6] Fiori A, Janković I, Dagan G. Modeling flow and transport in highly heterogeneous three-dimensional aquifers: Ergodicity, Gaussianity, and anomalous behavior; 2. Approximate semianalytical solution: Water Resour Res 2006;42:W06D13, doi:10.1029/2005WR004752.
[7] Fiori A, Dagan G, Jankovic I, Zarlenga A. The plume spreading in the MADE transport experiment: Could it be predicted by stochastic models? Water Resour Res submitted.
[8] Gelhar LW. Stochastic Subsurface Hydrology. Prentice-Hall, Upper Saddle River, NY, 1993.
[9] Harvey C, Gorelick SM. Rate-limited mass transfer or macrodispersion: Which dominates plume evolution at the macrodispersion experiment (MADE) site? Water Resour Res 2000;36(3):637-650, doi:10.1029/1999WR900247.
[10] LeBlanc DR, Garabedian SP, Hess KM, Gelhar LW, Quadri RD, Stollenwerk KG, Wood WW. Large-scale natural gradient tracer test in sand and gravel, Cape Cod, Massachusetts: 1. Experimental design and observed tracer movement, Water Resour Res 1991;27(5):895-910, doi:10.1029/91WR00241.
[11] Liu G, Butler JJ, Bohling GC, Reboulet E, Knobbe S, Hyndman DW. A new method for high-resolution characterization of hydraulic conductivity. Water Resour Res 2009;45:W08202, doi:10.1029/2009WR008319.
[12] Mackay DM, Freyberg DL, Roberts PV, Cherry JA. A natural gradient experiment on solute transport in a sand aquifer: 1. Approach and overview of plume movement: Water Resour Res 1986;22(13):2017-2029, doi:10.1029/WR022i013p02017.
[13] Rehfeldt KR, Boggs JM, Gelhar LW. Field study of dispersion in a heterogeneous aquifer: 3. Geostatistical analysis of hydraulic conductivity. Water Resour Res 1992;28(12):3309-3324, doi:10.1029/92WR01758.
[14] Rubin Y. Applied Stochastic Hydrology. Oxford Univ. Press, New York, 2003.
[15] Zheng C, Bianchi M, Gorelick SM. Lessons Learned from 25 Years of Research at the MADE Site. Ground Water 2011;49:649-662. doi:10.1111/j.1745-6584.2010.00753.x.