AGU PUBLICATIONS

Water Resources Research

INTRODUCTION TO A SPECIAL SECTION

10.1002/2017WR020774

Special Section:
Modeling Highly Heterogeneous Aquifers: Lessons Learned in the Last 30 years From the MADE Experiments and Others

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Citation:
Gómez-Hernández, J. J., J. J. Butler, A. Fiori, D. Bolster, V. Cvetkovic, G. Dagan, and D. Hyndman (2017), Introduction to special section on Modeling highly heterogeneous aquifers: Lessons learned in the last 30 years from the MADE experiments and others, *Water Resour. Res.*, *53*, 2581–2584, doi:10.1002/2017WR020774.

Received 16 MAR 2017
Accepted 26 MAR 2017
Accepted article online 31 MAR 2017
Published online 19 APR 2017

Introduction to special section on Modeling highly heterogeneous aquifers: Lessons learned in the last 30 years from the MADE experiments and others

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1. Introduction

During the sessions of the AGU Chapman Conference “The MADE Challenge for Groundwater Transport in Highly Heterogeneous Aquifers: Insights from 30 Years of Modeling and Characterization at the Field Scale and Promising Future Directions” held in Valencia (Spain) on 5–8 October 2015 [*Gómez-Hernández et al.*, 2016], there was a heated debate on how heterogeneous an aquifer must be to be called “highly” heterogeneous. Is the heterogeneity within a hydrofacies what matters, or is it that across different hydrofacies? For many years, there was general agreement that if the variance of the logarithm of hydraulic conductivity (henceforth, log conductivity) is below one, the aquifer is, at most, mildly heterogeneous, whereas when it is above that level—especially when it is above two— the aquifer is highly heterogeneous. But this variance limit was related to the restrictions imposed by approximations invoked for the analytical solution of the stochastic flow and transport equations, and not what is observed in natural systems. Thus, when dealing with natural systems, do we need to redefine what is meant by “highly” heterogeneous?

More than 25 years ago, field experiments began at the MAcroDispersion Experiment (MADE) site in Columbus, Mississippi, a site with an initially reported log conductivity variance above 4. The objective was to improve understanding of solute transport in highly heterogeneous natural systems. As a result of the MADE experiments and related work, it is now generally accepted that heterogeneity has a large impact on subsurface flow and transport processes. Moreover, we now recognize that the variance of log conductivity will be seldom below 1, and we should not be surprised by variances greater than 10. Although our understanding of the role of heterogeneity on flow and transport processes continues to improve, our ability to address practical issues, such as remediation of sites of groundwater contamination, continues to be stymied by heterogeneity. How can we translate our improved understanding of the impact of heterogeneity to address societal expectations for our discipline? These and related questions were discussed at length in the Valencia Chapman conference and prompted the preparation of this special issue on characterization and modeling of highly heterogeneous aquifers.

The section is composed of seven papers, some of them corresponding to presentations at the conference and some contributed by authors whose interests parallel those of conference attendees. The range of topics covered by the papers is broad and only reflects a small portion of those covered at the Chapman conference; yet, they demonstrate the high level of interest that the MADE experiments continue to generate in the hydrological community.

2. Summary of Papers

Two of the papers are focused on field characterization, how to take measurements in heterogeneous systems and how to interpret those measurements. Three of the papers can be grouped under the heading of characterization by inverse modeling. One paper addresses the impact of heterogeneity on the estimation of the health risk associated with an aquifer contamination event, while an additional paper discusses the insights that can be gleaned from application of percolation-based theories of solute transport in porous media.

Field characterization, a mainstay of hydrogeologic investigations is confronted by many challenges in heterogeneous systems, which can be amplified in fractured settings. The paper by *Klammler et al*. [2016] describes a new device to measure flow and transport in fractured media; the device is a fractured rock passive flux meter capable of providing information about locations and orientations of fracture open to flow, and estimates of groundwater flow direction and magnitude in these fractures. In addition, estimates of the cumulative magnitudes of groundwater and contaminant fluxes can be determined over time for individual fractures. The major innovation of this extension of the passive flux meter to fractured systems is that active fractures and the fluxes through them can be identified and quantified, respectively. Existing borehole imaging technology, at most, can provide fracture locations, but not information on fluxes.

All scales of heterogeneity are relevant for proper transport modeling, particularly small-scale heterogeneity, associated with small support volumes around the location where the measurements are being made. However, characterization of small-scale heterogeneity has been difficult in all settings. Over the last decade, high-resolution vertical profiles of hydraulic conductivities have been obtained in granular aquifers using direct-push technology. *Bohling et al*. [2016] describes the application of the direct-push injection logger (DPIL) and the direct-push permeameter (DPP) at the MADE site to obtain estimates of hydraulic conductivity at a vertical spacing of 1.5 cm. This work, which refines an approach developed earlier, focusses on how to transform the high-resolution injection rates and injection-induced pressure changes recorded by the DPIL into hydraulic conductivity estimates using data from hydraulic tests performed with the DPP. The result is a description of vertical variations in hydraulic conductivity at a resolution that has not previously been possible for practical applications.

We all know that the conditions under which Theis' solution of the transient groundwater flow equation, which allows the determination of transmissivity and storativity estimates in confined aquifers, are never strictly met in reality. Aquifers are not homogeneous, neither in transmissivity nor in storativity, and the result of an interpreted pumping test in natural systems has always been understood to be a large-scale volumetric average of the heterogeneous hydraulic properties of the portions of the aquifer affected by the pumping test. The paper by *Zech et al*. [2016] starts from the premise that the aquifer is heterogeneous and derives type curves, not to estimate the transmissivity of the aquifer, but to derive the parameters that characterize the heterogeneity of transmissivity, more specifically, assuming that the transmissivity follows a multi-Gaussian distribution of given mean, variance, and isotropic Gaussian (or double exponential) covariance, the authors provide means to estimate the mean, variance, and covariance correlation length from a pumping test. (The storativity, assumed constant, is also estimated.) The authors conclude that the assumption of multi-Gaussianity could be strong, but that their approach can be considered as a first step towards the characterization of more complex heterogeneity models.

The paper by *Xu and Gómez-Hernández* [2016a] also focuses on the characterization of heterogeneous fields using state variable observations but with a more ambitious goal: that of characterizing the spatial variability of both hydraulic conductivity and porosity in heterogeneous settings dominated by lengthy curvilinear elements (i.e., channeling), something difficult to handle with a multi-Gaussian model. For this purpose, they use the normal-score ensemble Kalman filter, an algorithm that has already shown its strengths for the characterization of non-Gaussian fields. The main contribution of this paper is the addition of temperature observations, as an easily observable state variable, to observations of piezometric head and solute concentration. The authors produce an extensive analysis showing the trade-offs between the different state variables, reaching the conclusion that the amount of information carried by each state variable for the purpose of characterizing the aquifer parameters is time-dependent. For instance, for the specific example analyzed in the paper, it is best to assimilate piezometric heads early and then switch to temperature data.

Xu and Gómez-Hernández [2016b] propose another application of the ensemble Kalman filter in heterogeneous aquifers, but, in this case, for the purpose of identifying the parameters describing a contaminant source, that is, its location, the initial release time, and the amount of contaminant released into the aquifer. The novelty of their approach is that it is the first time that contaminant source identification is performed using the ensemble Kalman filter, and, considering the successful application to inverse modeling in many other areas, it opens a new avenue of research for contaminant source identification. The results presented in this paper are demonstrative of the technique only, since they assume that the aquifer heterogeneity is completely known. The authors recognize that the challenge lies in the joint identification of the contaminant source and the aquifer heterogeneity.

Assessing the threat of human exposure to contaminated groundwater is typically a difficult task, involving several sources of uncertainty, related to both the contaminant and the geological environment, as well as the human physiology. *de Barros et al*. [2016] analyze the impact of the aquifer heterogeneity on the risk assessment of adverse health effects. By employing a semianalytical model, suitable for highly heterogeneous formations such as at the MADE site, the authors developed the concept of the hazard attenuation factor, which is a random variable that depends on the solute travel time, from the source to the target, and a decay parameter that models processes like anaerobic biodegradation or radioactive decay. Hence, the factor combines both flow heterogeneity and contaminant-related processes. The authors show the strong impact of heterogeneity on the human health risk, and, in particular, the reduction of the hazard due to the presence of zones of low hydraulic conductivity that cause a considerable increase in the travel time and consequently a larger decay. The opposite effect, the increased hazard produced by solute moving along preferential "fast" pathways, is also significant. The above effects are proportional to the degree of heterogeneity of the subsurface system.

Solute transport theories should be able to inform the understanding of chemical weathering and soil production, particularly in cases where such processes are transport limited. Correlations between chemical weathering and soil formation observed in the past suggest indeed that soil formation may also be limited by solute transport. *Hunt and Ghanbarian* [2016] propose a theoretical analysis aiming at providing a unified view of soil weathering, soil production, and carbon storage, employing a solute transport scaling derived from percolation theory, an alternative to the classic advection-dispersion modeling approach. The authors show that attributing the spatiotemporal scaling of a variety of soil biogeochemical processes over wide ranges of timescales to the limitations set by non-Gaussian solute transport in highly heterogeneous media greatly simplifies the interpretation of diverse data, including soil production and chemical weathering rates as functions of time/space and moisture fluxes, among others. Verification of both the scaling functions and the fundamental time scales for solute transport as calculated using percolation theory is reported in the paper.

3. Concluding Remarks

That aquifers are heterogeneous is a fact that cannot be dismissed without acknowledging its implications for flow and transport modeling. Despite decades of research, we still are challenged by how best to characterize heterogeneous systems, to incorporate the heterogeneity into a modeling framework, and to simulate transport processes in such systems. This special section, which grew out of a Chapman conference focussed on the lessons learned from 30 years of studying the highly heterogeneous—and, at one time, highly instrumented—aquifer at the MADE site, includes papers that range across the spectrum of current theoretical and experimental research on groundwater flow and transport in highly heterogeneous systems. We hope these contributions will give the reader a sense of the excitement we all felt during the conference in Valencia.

Acknowledgment
The authors gratefully acknowledge financial support from the United States National Science Foundation, via grant EAR 1542320, to organize the Chapman meeting.

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