RELATING GEOPHYSICAL AND HYDROLOGIC PROPERTIES USING FIELD-SCALE ROCK PHYSICS

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ABSTRACT

Understanding how geophysical and hydrologic properties are related is a key problem in hydrogeophysical data fusion. Traditionally this link has been made by rock physics investigations that define how pore-scale variations in properties like mineralogy, fluid content, and grain geometry affect the geophysical response of a rock or sediment. As the scale of investigation increases from the lab to the field, an individual geophysical measurement averages over different types of rocks and sediments in addition to local pore-scale variations. As a result, spatial heterogeneity and preferential sampling at the field-scale can cause a shift in the rock physics relationship away from that determined in the lab. In a typical field survey, multiple large-scale measurements are combined through inversion to estimate the geophysical properties of the subsurface. In this case, additional factors, e.g., the spatially varying resolution of geophysical surveys, may also affect the rock physics relationship. As a result, there is a need for methods that integrate variations in pore-scale rock properties with an understanding of geophysical sampling at the field-scale. In this paper we consider the role of rock physics in general hydrogeophysical data fusion problems and review the spectrum of approaches to rock physics currently available, which ranges from traditional pore-scale approaches to emerging field-scale methods.

1. INTRODUCTION: DATA FUSION & ROCK PHYSICS

A critical problem often faced in hydrologic investigations is a lack of data necessary to constrain alternative hypotheses or conceptual models for groundwater flow and transport. By providing minimally invasive, high-resolution measurements over large extents of the subsurface, geophysical data hold the promise to reduce the severity of this issue. The problem of how to best incorporate geophysical data into the framework of a hydrologic investigation remains, however, a standing question. A fundamental aspect of the data fusion problem involves understanding how spatial and temporal variations of hydrologic properties (e.g., water content and solute concentration) are related to the responses observed during a geophysical survey.

The data fusion problem can be tackled in either a sequential or integrated manner (Figure 1). The sequential approach treats data fusion as a consecutive series of processing steps: first, the geophysical survey data are inverted to estimate the distribution of geophysical properties of the subsurface; next, the estimated geophysical properties are converted to hydrologic properties; finally, the geophysical estimates of the hydrologic properties are used to address the hydrologic problem. In contrast, the integrated approach directly assimilates the geophysical data within the context of the hydrologic problem (e.g., Kowalsky et al., 2005). This can be achieved by perturbing the parameters of a coupled hydrologic and geophysical model until an acceptable match to the geophysical field data is obtained.

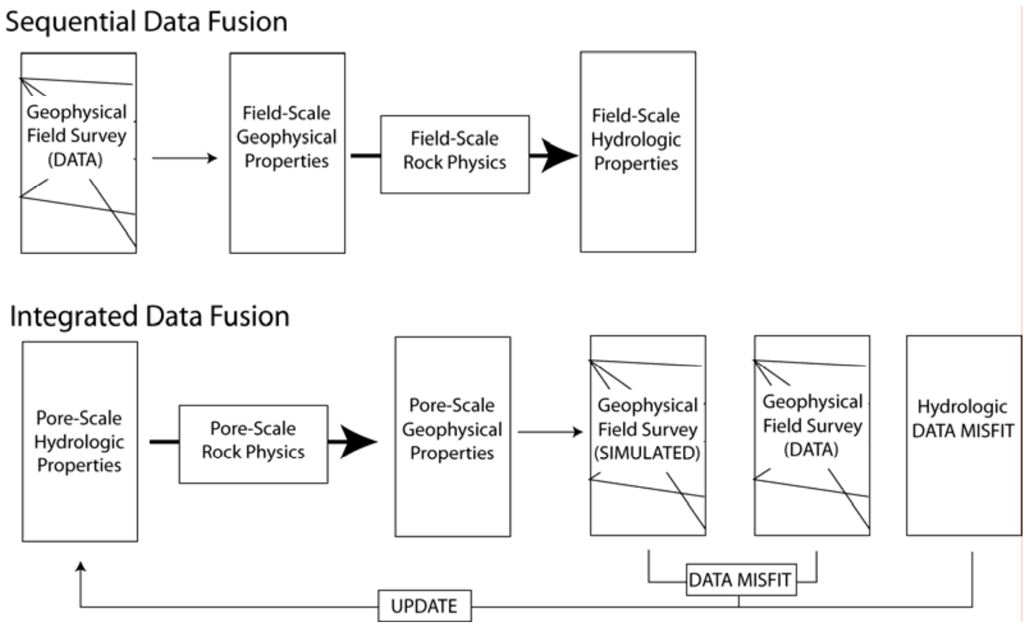

FIGURE 1: The role of rock physics in sequential and integrated data fusion.

In the course of either data fusion approach, geophysical properties must be converted to hydrologic properties (or vice versa) using a rock physics relationship. The issues and scales important for determining the rock physics relationship are considerably different for the two approaches. In Figure 1 we illustrate how the integrated data fusion approach converts hydrologic properties to geophysical properties at the scale of the forward model used to simulate the geophysical survey. In contrast, the sequential approach transforms properties estimated by a field-scale geophysical survey to hydrologic properties at the scale of the inverse model. In the integrated approach, the rock physics relationship can often be adequately determined empirically using laboratory experiments or theoretically based on pore-scale considerations. In comparison, the rock physics relationship for sequential data fusion must additionally account for the greater range and complexity of heterogeneity present at the field scale compared to the lab scale, the sampling physics of individual measurements at the field scale, the complex averaging of heterogeneity resulting from the collection of multiple measurements in a geophysical survey, and artifacts that may be introduced during data inversion. We therefore use the terms ‘pore-scale’ and ‘field-scale’ to *conceptually* differentiate between the two different sets of information captured by a rock physics relationship in each data fusion approach.

In this paper, we review the differences in information captured by pore-scale and field-scale rock physics relationships. We then provide an overview of some of the new approaches that have recently been developed to improve the prediction of field-scale rock physics relationships, including: random-field averaging, full-inverse statistical calibration, and statistical rock physics.

2. THE SPECTRUM OF ROCK PHYSICS: FROM PORE-SCALE TO FIELD-SCALE

Pore-scale rock physics relationships fundamentally consider a rock (or sediment) to be defined as a composite medium built from individual components, such as mineral grains, pore spaces (air), and fluids, each with well-defined physical properties. The properties of the composite rock can then be defined in terms of the (i) physical properties, (ii) volume fractions, and (iii) geometry of the components as well as (iv) interactions between the components. A rock physics relationship describes how the bulk geophysical properties change as a function of the composition of the rock.

In theoretical studies, effective medium theory is often used to predict the macroscopic properties of the composite rock as a function of the individual components. A well-known example of this approach to rock physics was developed by Hashin and Shtrikman (1963) for defining the bounds on geophysical properties. Inclusion-based and differential effective medium theories are another approach to relating the properties of a composite to its components (e.g., Berryman; 1995). The importance of capturing the connectivity between pores is seen in the work of Hunt (2004) and Hautot and Tarits (2002) who provide examples where percolation theory is used to evaluate the dependence of electrical conductivity on porosity and water content. Universal to these kinds of theoretical studies is the upscaling of the properties of the individual components to obtain the effective property of a rock, though the upscaling method may vary.

Empirical investigations provide a more direct way to obtain a relationship between hydrologic and geophysical variables of interest for a composite medium. Topp et al. (1980) provide a classic example where lab measurements made on four sets of soils were used to fit a polynomial relationship between the dielectric constant and water content of a soil. The "Topp equation" is still used extensively in lab and field studies today. Han et al. (1986) give another good example where measurements on core samples were used to develop a set of empirical relations describing the dependence of seismic velocity on the porosity and clay content of sandstones. Adler et al. (1992) bridged the gap between theory and empiricism by demonstrating that the pore-scale rock physics relationships found by simulating current flow (i.e., solving the Laplace equation) in pore networks constructed from thin section data were in agreement with those determined empirically using laboratory measurements.

A composite medium approach can also be applied at the scale of a field study. In this case, the composite medium is viewed as a heterogeneous region of the subsurface consisting of component volumes with varying lithologies, porosities, or pore fluids. Following this idea, Backus (1962) produced a seminal paper in seismology that described an averaging technique to estimate the elastic constants for a set of layered geologic units. Today, the Backus average is regularly applied in the petroleum industry to upscale well-logs that are used to determine rock physics relationships applicable to normal-incidence seismic reflection data (Wang, 2001). Archie (1942) provides another example where field-scale measurements (i.e., well-log data) were used to determine a relationship between bulk electrical conductivity and porosity. What has come to be known as Archie's law is now often applied at all scales of investigation and many studies have attempted to use theory to validate the relationship (e.g., Hunt, 2004).

Moysey and Knight (2004) recently investigated the relationship between dielectric constant and water content in heterogeneous environments where geologic variations are represented using spatially correlated random fields. These authors found that when an individual geophysical measurement (in their case an electromagnetic wave produced by ground-penetrating radar) averages over small-scale heterogeneities, the rock physics relationship at the measurement scale will be different from that defined at the scale of the property variations. These authors suggested that the rock physics relationship is independent of measurement scale only when a medium is self-similar.

Although these studies approach rock physics at a scale relevant to field studies, they do not necessarily produce a true 'field-scale rock physics relationship' that is generally applicable to sequential data fusion problems. This is because composite medium methods address only one aspect of the field-scale problem, i.e., averaging of heterogeneity below the measurement scale. In some cases, such as for normal-incidence seismic reflection surveys, using the composite medium approach to derive an empirical relationship is adequate because the way that a geophysical measurement averages the subsurface is approximately constant. However, in geophysical surveys where complex averages of the subsurface are obtained, such as in tomographic imaging, the composite medium approach is insufficient because the geophysical properties estimated and, therefore, the rock physics relationship depends on *how* the subsurface is sampled.

Day-Lewis and Lane (2004) presented a theoretical study illustrating that the spatially variable resolution of a tomographic survey causes the relationship between a hydrologic and geophysical variable to change as a function of spatial position. This is an effect not predicted by traditional composite medium approaches and that would be difficult to capture empirically. Singha and Gorelick (2006) have shown the same effect in field data by demonstrating that Archie's law fails to accurately reproduce solute concentrations estimated using ERT surveys. These studies indicate that a true field-scale rock physics relationship must account for both the heterogeneous composition of the subsurface and the complex averaging of these components that leads to the property estimates obtained from a geophysical survey.

3. NEW APPROACHES TO FIELD-SCALE ROCK PHYSICS

Two approaches have recently emerged to account for the many factors that affect field-scale rock physics relationships: random field averaging (RFA) (Day-Lewis and Lane, 2004; Day-Lewis et al., 2005) and full-inverse statistical (FISt) calibration (Moysey and Knight, 2003; Moysey et al., 2005). These methods parallel traditional rock physics approaches in that they use a mathematical (or numerical) model to describe how a geophysical measurement samples the subsurface. In contrast to traditional approaches, however, these methods also account for how the set of measurements collected in a geophysical survey contribute to the estimate of a geophysical property rather than focusing on how a single measurement averages the subsurface.

Both the RFA approach and FISt calibration determine the rock physics relationship between a geophysical and hydrologic variable as a statistical association, captured by a joint probability density function (PDF), rather than a deterministic functional dependence. It is important to note that in both methods this PDF is explicitly dependent on spatial location, thereby inherently accounting for the spatially varying resolution of geophysical surveys. The main difference between the two approaches is that the RFA approach is a parametric (i.e., relies on a specific functional form for the PDF), semi-analytical approach whereas FISt calibration is primarily a non-parametric, numerical approach.

3.1 Random Field Averaging (RFA)

In the RFA approach developed by Day-Lewis and Lane (2004) and Day-Lewis et al. (2005) the hydrologic variable of interest, *h,* is related to the geophysical property estimated by a field survey, $\hat{m}$, through the joint PDF $f_{h,\hat{m}}$. The inference of $f_{h,\hat{m}}$ is accomplished in two steps. First, the joint PDF, $f_{m_i,\hat{m}_i}$, is established between the true geophysical property of the subsurface, m_i, and the value estimated by a geophysical survey, $\hat{m}_i$, for location *i*. Second, the geophysical PDF is transformed to $f_{h_i,\hat{m}_i}$ using the reciprocal of the 'pore-scale' rock physics relationship, i.e., $h = \tilde{g}(m)$.

$$f_{h_i,\hat{m}_i} = f_{m_i,\hat{m}_i} \frac{(m_i + \Delta m_i) - m_i}{\tilde{g}(m_i + \Delta m_i) - \tilde{g}(m_i)} \qquad (1)$$

Based on Bayes theorem, the joint distribution is given by the product of the conditional and marginal distribution: $f_{m,\hat{m}} = f_{\hat{m}|m} \cdot f_m$. The RFA approach assumes that all of these PDFs can be represented using Gaussian distributions, which leads to the result:

$$f_{m_i,\hat{m}_i} = \frac{1}{2\pi\sigma_m\sigma_{\hat{m}_i|m_i}} \exp\left\{ \frac{-(m-\mu_m)^2}{2\sigma_m^2} - \frac{(\hat{m}-\mu_{\hat{m}_i|m_i})^2}{2\sigma_{\hat{m}_i|m_i}^2} \right\} \qquad (2)$$

where μ_m and σ_m are the mean and standard deviation of the true geophysical property of the subsurface, which is assumed to be stationary, and $\mu_{\hat{m}_i|m_i}$ and $\sigma_{\hat{m}_i|m_i}$ are the conditional mean and standard deviation of the estimated geophysical property.

The conditional distribution $f_{\hat{m}_i|m_i}$ captures the upscaling from true properties in the subsurface, *m*, to the estimates obtained by the geophysical survey, $\hat{m}$. The key to the RFA approach is in how this upscaling is performed. Day-Lewis and Lane (2004) and Day-Lewis et al. (2005) approach the problem from the perspective of linear inverse theory, where the estimated properties are related to the true values by the model resolution matrix, R (e.g., Menke, 1989):

$$\hat{m}_i = \sum_{j=1}^{N} R_{ij} m_j \,. \qquad (3)$$

The model resolution matrix, R, contains all the relevant information about the sampling physics for a measurement, the design of a geophysical survey, and the influence of regularization during inversion. Though the concept of R is built from linear inverse theory, the approach is fully applicable to non-linear problems that have been linearized. In this case, R is determined during the final iteration of the inversion.

The essence of Eq.3 is that $\hat{m}$ is a weighted volumetric average of *m*, and thus the RFA approach effectively represents a compositional approach to rock physics analogous to all the 'pore-scale' methods described earlier. However, in the RFA approach the weights contained by R incorporate the field-scale nature of the problem. Building on results from the theory of random fields, which captures patterns of subsurface heterogeneity using spatial covariance functions, Day-Lewis et al. (2005) were then able to use Eq.3 to derive analytical expressions for $\mu_{\hat{m}|m}$ and $\sigma_{\hat{m}|m}$ for use in Eq.2.

The RFA approach provides an efficient method for building field-scale rock physics relationships that account for the resolution of a geophysical survey while allowing for spatial variability due to subsurface heterogeneity, therefore making it applicable to a variety of practical problems. The main drawback of the method is that it applies only to situations where heterogeneity can be represented by a stationary, Gaussian random field. The importance of this constraint is currently uncertain, however, given that the RFA approach accounts for site-specific (i.e., non-stationary) heterogeneity at a site by conditioning to data through inversion. Also, though the method relies on linearization about the final solution of an inverse problem, it is unlikely that this restriction will be an important limitation for most problems since the inversion itself can be performed using any non-linear optimization method, (assuming that a global minimum is reached during the optimization).

3.2 Full-Inverse Statistical (FISt) Calibration

Moysey and Knight (2003) and Moysey et al. (2005) approached the field-scale problem from a similar perspective, but used a numerical rather than analytical methodology. These authors proposed that the effects of geophysical averaging of heterogeneity and other factors affecting field-scale rock physics relationships could be inferred by studying numerical analogs to a field site. In general, the method is more flexible than the RFA approach, but can also be much more computationally demanding. FISt calibration follows five basic steps: (i) hydrologic property simulation (h), (ii) pore-scale rock physics (m=g(h)), (iii) geophysical property upscaling ($m \rightarrow \hat{m}$), (iv) hydrologic property upscaling ($h \rightarrow \hat{h}$), and (v) inference of a field scale-rock physics relationship ($\hat{h} = \hat{g}(\hat{m})$). Steps 1-4 are repeated for many realizations. As a result, many pairs of points ($\hat{h}, \hat{m}$) are generated, one pair for each realization at each location in the subsurface. This set of points is used to infer the field-scale rock physics relationship in step 5, which ideally takes the form of a non-parametric joint PDF for $\hat{h}$ and $\hat{m}$, though practically the points could also be used to fit any deterministic expression (e.g., a linear relationship).

A good example of FISt calibration was recently given by Singha and Moysey (2006). In this study, the authors used flow and transport simulations through a conditional hydraulic conductivity realization to generate a realistic solute plume in the subsurface (Step 1). The solute concentration at each point in the subsurface was then transformed to bulk resistivity using Archie's law (Step 2). Using the resulting resistivity realization, an electrical resistivity tomography (ERT) experiment was simulated and the data inverted using the same parameters as used in the base case in the study (i.e., the case representing the "true" field experiment) (Step 3). The inversion was performed using the same grid as ERT simulation, thus there was no need for upscaling of the hydrologic properties (concentrations) for the realizations in this example (Step 4). Following steps 1-4, 50 different realizations were generated and then used to determine a field-scale rock physics relationship between solute concentration and ERT estimated resistivity for each cell in the model (Step 5). Figure 2 shows that the estimate of solute concentrations obtained using the field-scale rock physics relationship determined by FISt calibration far outperforms Archie's law – even though Archie's law was explicitly used to define this relationship at the small scale.

The benefits of FISt calibration are that it is conceptually straightforward, can account for complex types of geologic heterogeneity, and easily integrates multiple types of data in the geologic simulation phase (i.e., Step 1). A significant disadvantage of the approach is that it can be very computationally intensive, especially for 3-D, transient problems. An implicit advantage of the RFA approach was that the resolution matrix is dependent on the geophysical data from the field experiment, making it less sensitive to the geologic conceptual model for a site. A similar geophysical data dependence could be achieved in FISt calibration if for each realization the $(\hat{h}, \hat{m})$ points used to infer the PDF were weighted by the global data misfit between the true and simulated field experiment. Both FISt calibration and the RFA approach are promising practical tools for solving data fusion problems in hydrogeophysics.

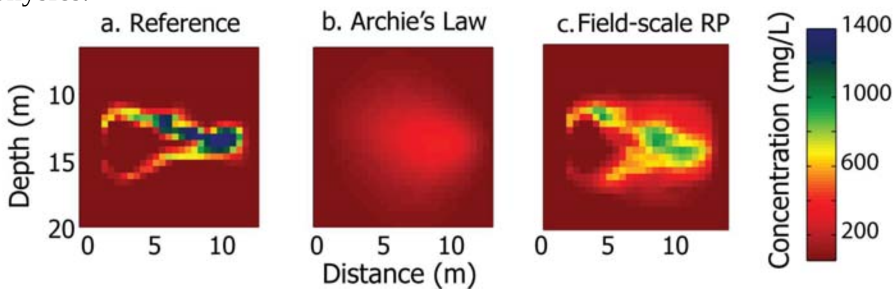

FIGURE 2: Comparison of (a) true solute concentrations to those obtained using (b) Archie's law and (c) FISt calibration in a synthetic ERT experiment (Singha and Moysey, 2006).

4. OTHER NEW APPROACHES TO ROCK PHYSICS

4.1 Rock Physics Relationships Estimated by Inversion

Coming from the perspective of the integrated approach to data fusion, Kowalsky et al. (2005) provide an interesting example where one of the parameters in a volumetric mixing model was used as a fitting parameter in the joint hydrologic-geophysical inverse problem. While this semi-empirical approach is highly promising, a great deal more research is needed to evaluate issues like sensitivity of the method to geologic heterogeneity and the uniqueness of the inverse problem when spatially variable rock physics relationships are considered.

4.2 Statistical Rock Physics

One critical problem in rock physics that is independent of measurement scale occurs when geologic conditions in the subsurface are not represented by calibration data (e.g., well-logs). Mukerji et al. (2001) address this problem using statistical rock physics where basic rock physics concepts and geostatistical simulation are used to expand the calibration database to include possible conditions not yet observed in the data. In the example of Mukerji et al. (2001), the effects of different pore fluids on the rock physics relationship was determined. This approach is complementary to the RFA approach or FISt calibration and should be used in conjunction with these methods whenever appropriate.

5. SUMMARY

Rock physics relationships play a central role in hydrogeophysical data fusion problems. As a result, these relationships must capture a range of processes applicable at different scales.

Understanding pore-scale processes is critical for understanding the basic physics that affects rock behavior. As one moves to larger scales of investigation, however, geologic heterogeneity, sampling physics, and geophysical resolution change and must be accounted for. New methods such as the random field averaging (RFA) approach and full-inverse statistical (FISt) calibration are promising new approaches to account for these effects.

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