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A comparison of deterministic and stochastic approaches for regional scale inverse modeling on the Mar del Plata aquifer

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SUMMARY

Inversion of the spatial variability of transmissivity (T) in groundwater models can be handled using either stochastic or deterministic (i.e., geology-based zonation) approaches. While stochastic methods predominate in scientific literature, they have never been formally compared to deterministic approaches, preferred by practitioners, for regional aquifer models. We use both approaches to model groundwater flow and solute transport in the Mar del Plata aquifer, where seawater intrusion is a major threat to freshwater resources. The relative performance of the two approaches is evaluated in terms of (i) model fits to head and concentration data (available for nearly a century), (ii) geological plausibility of the estimated *T* fields, and (iii) their ability to predict transport. We also address the impact of conditioning the estimated fields on *T* data coming from either pumping tests interpreted with the Theis method or specific capacity values from step-drawdown tests. We find that stochastic models, based upon conditional estimation and simulation techniques, identify some of the geological features (river deposit channels and low transmissivity regions associated to quartzite outcrops) and yield better fits to calibration data than the much simpler geology-based deterministic model, which cannot properly address model structure uncertainty. However, the latter demonstrates much greater robustness for predicting sea water intrusion and for incorporating concentrations as calibration data. We attribute the poor performance, and underestimated uncertainty, of the stochastic simulations to estimation bias introduced by model errors. Qualitative geological information is extremely rich in identifying large-scale variability patterns, which are identified by stochastic models only in data rich areas, and should be explicitly included in the calibration process.

1. Introduction

Groundwater model parameters are usually heterogeneous and uncertain. Fortunately, a large number of measurements of model outputs (most often heads and concentrations) are usually available, which favors formulating models in an inverse problem framework. The availability of model independent tools for inversion (Doherty et al., 1994; Poeter and Hill, 1998) has fostered its common use in hydrological practice. Still, groundwater inversion suffers from a number of problems (non-uniqueness, instability, computational cost, etc.), as illustrated by the periodic reviews of the topic (Yeh, 1986; Carrera, 1987; McLaughlin and Townley, 1996; Zimmerman et al., 1998; de Marsily et al., 1999; Carrera et al., 2005; Franssen et al., 2009; Zhou et al., 2014). Amongst them, spatial variability is likely the most difficult problem to address. This work focusses on the characterization of spatial variability of transmissivity (T).

Two sets of approaches can be identified in dealing with spatial variability and the conceptual prior information: deterministic and stochastic. Stochastic approaches rely on treating *T* as a random field and estimating its properties from prior estimates of *T* (and/or other model parameters) and available state variables (i.e., heads (h) and concentrations (ω) measurements). Initially, the problem was formulated as finding the 'best field', in the sense of minimum variance or the expected field conditioned to measurements (Clifton and Neuman, 1982; Kitanidis and Vomvoris, 1983; Rubin and Dagan, 1987b). Estimation uncertainties derived from these solutions were too optimistic (Carrera and Glorioso, 1991). This prompted the development of conditional simulation methods (Gómez-Hernández et al., 1997), and more recently moment equations approaches (Hernández et al., 2003, 2006). All these methods

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assume stationarity of the T field. That is, they all assume that, prior to measurements, nothing is known about variability patterns, so that they effectively disregard geological knowledge. Although much work has been done on geologically based geostatistics (e.g., Winter and Tartakovsky, 2002; Winter et al., 2003; Riva et al., 2006), most applications of geostatistical inversion are based on this assumption of stationarity.

The deterministic approach relies on the assumption that the patterns of spatial variability are known from geological or geophysical information, so that the whole unknown field can be expressed in terms of a limited number of uncertain parameters. The process of expressing the field as a function of parameters is called parametrization. The most widely used parametrization method is zonation, which consists of subdividing the model domain into a number of regions (zones). Zones are typically (though not necessarily) homogeneous with a single effective parameter value (e.g., Carrera and Neuman, 1986; Barlebo et al., 2004). Therefore, in contrast to stochastic methods, the spatial zonation pattern, normally inferred from the available geological information, is prescribed explicitly in the deterministic approach. The main advantage of zonation is its flexibility to incorporate geological or geophysical data available in the form of maps (sedimentary deposits, paleochannels, water conducting features, etc.). However, the identification of zones is a subjective and hard-to-systematize task. In fact, an inappropriate definition of zones is transmitted to errors in the model structure and is often a main cause of failure in actual applications (Sun et al., 1998). Some efforts have been devoted to alleviate the effect of errors in the geometry of zones (e.g., Gaganis and Smith, 2006; Roggero and Hu, 1998). However, no well-defined approach has emerged as generally accepted. Another disadvantage of the deterministic approach results from implicitly neglecting the effect of small scale heterogeneity on flow and, especially, on solute transport. Thus, the calibration process using the geostatistical approach captures the structural fine detail better than that which can be captured using a limited number of zones. However, despite of these problems, zonation remains the method of choice in hydrological practice, especially in regional or basin-scale groundwater models (e.g., Senger and Fogg, 1987; Guymon and Yen, 1990; Castro et al., 1998; Walvoord et al., 1999; Shavit and Furman, 2001; Best and Lowry, 2014; Ala-aho et al., 2015; Nocchi and Salleolini, 2013, etc.).

The geostatistical approach has been applied successfully to cases where geological information is not strong enough to allow predefining patterns of spatial variability. This is certainly the case in synthetic aquifers (e.g., Yeh and Liu, 2000; Kowalsky et al., 2004; Zhu and Yeh, 2005, 2006; Alcolea et al., 2006b; Hao et al., 2008; Franssen et al., 2009; Riva et al., 2010, 2011) and laboratory sandboxes (e.g., Liu et al., 2002, 2007; Illman et al., 2007, 2009). Field applications are restricted to relatively small scale problems, where geology is not very binding, with well defined stresses and responses. These include hydraulic test interpretation (e.g., Meier et al., 2001; Vesselinov and Neuman, 2001; Li et al., 2005; Hernández et al., 2006; Rubin et al., 2010; Murakami et al., 2010; Janetti et al., 2010; Bianchi Janetti et al., 2010; Berg and Illman, 2011, 2013, 2015), well capture zone delineation (e.g., Vassolo et al., 1998; Kunstmann et al., 2002; Harrar et al., 2003; Riva et al., 2006), river-aquifer interaction (e.g., Rötting et al., 2006), or coastal aquifers (Alcolea et al., 2007, 2009) and others (Barlebo et al., 2004; Franssen and Kinzelbach, 2008; Vesselinov et al., 2001a,b; Chen et al., 2012).

Few stochastic studies have been carried out for large-scale problems. Clifton and Neuman (1982) and Rubin and Dagan (1987a,b) used a stochastic inversion approach to model the Avra Valley aquifers under steady-state conditions. Rubin and Dagan (1988) and Rubin et al. (1990) demonstrated the applicability of the geostatistical approach in the Israeli Coastal Aquifer and the Rio Maior aquifer, respectively. These examples proved useful in advancing the method during its early stages. However, they did not really demonstrate its validity, which is usually the case in real-word large scale applications because little data are available to test independently the model. In fact, to date, there is a very important lack of real-world applications of stochastic theories and approaches at large scale (Dagan, 2002; Neuman, 2004; Renard, 2007). Recent exceptions include the works of Jardani et al. (2012) and Dausman et al. (2015). This lack is much more marked when it comes to stochastic inversion of flow and transport data. We argue that the problem lies in ignoring geological information, which is much richer at large than at small scale. That is, patterns of geological variability (and, therefore, hydraulic variability) are usually well known at regional scale. Ignoring them would be poor practice. Thus, when facing a regional-scale model, professionals find that the easily accessible stochastic approaches fail to incorporate the geological information and prefer deterministic approaches. Instead, geological information at the local scale ($<$1 km) is usually much less specific, and patterns of variability cannot be stated a priori. In such cases, parsimony justifies stationarity as the prior model, which explains the broad use and success of small scale stochastic models.

Much effort has been dedicated to overcome this limitation of stochastic approaches. Perhaps, the most successful attempts are based on categorizing heterogeneity in terms of hydrogeological facies. Models of transition probabilities based on Markov chains (TPMC) analyze spatial variability and generate equally-likely realizations of geological units or facies. TPMC methods are a powerful geostatistical approach to estimate the spatial distribution of geological units using categorical indicator variables (e.g., Carle and Fogg, 1996, 1997; Fogg et al., 1998; Ritzi, 2000; Elfeki and Dekking, 2001; Park et al., 2004; Ritzi et al., 2004; Zhang et al., 2006; Li, 2007a,b; Dai et al., 2007; Zhang and Li, 2008; Ye and Khaleel, 2008; Khaninezhad et al., 2012a,b). These approaches have been generalized using multiple-point geostatistics and connectivity concepts (see Renard and Allard (2013) for a recent review). In practice, these approaches involve generating a large number of lithofacies distributions and/or hydraulic conductivity fields and rejecting those that fail to honor observed heads (e.g., Sakaki et al., 2009; Zhou et al., 2012; Alcolea and Renard, 2010; Berg and Illman, 2011; Khodabakhshi and Jafarpour, 2013). Other approaches aimed at reproducing actual variability patterns are based on geophysical data to compensate for the scarcity of in situ hydrological measurements and to improve the accuracy of spatial heterogeneity characterization (e.g., Rubin et al., 1992; Copty et al., 1993; Hyndman et al., 1994; Hubbard et al., 1997; Ezzedine et al., 1999; Hubbard and Rubin, 2000; Chen et al., 2001; Doro et al., 2013). Although all these techniques look promising, their application to real regional systems is still in developmental stages.

In light of the above considerations, the first relevant question is whether the geostatistical approach is suitable for modeling real regional aquifers or whether in these cases the inverse problem is best handled in a deterministic framework.

A complementary key question when using geostatistical inversion approaches is the source of T data. These are generally obtained from long-term pumping tests, which are expensive (and thus scarce). Alternatively, additional T data can be derived from specific capacity (pumping rate, Q, divided by drawdown, s). Specific capacity (SC) is the parameter most often provided by drillers from step-drawdown tests to characterize the performance of a well. Hence, SC data are often much more abundant than T data. Clifton and Neuman (1982) and Ahmed and Marsily (1987) argued that the estimation of a T field is improved by using both pumping test and specific capacity data. On the other hand, Meier et al. (1999) demonstrated that these two types of