WATER RESOURCES RESEARCH, VOL. 49, 3952–3977, doi:10.1002/wrcr.20145, 2013

Parameter and predictive outcomes of model simplification

Ty A. Watson,[1,2] John E. Doherty,[1,3] and Steen Christensen[4]

Received 25 May 2012; revised 23 January 2013; accepted 12 February 2013; published 8 July 2013.

[1] Simplification is an unavoidable aspect of model usage. Even complex, physically based models are simplifications of reality. More profound simplification is required to construct the "lumped parameter" models of semiphysical basis that are often employed for simulation of large-scale processes operative over one or many watersheds. Simplification can lead to model predictive error beyond that which would be expected on the basis of study-area information deficits alone. Building on a recently developed mathematical description of the model simplification process, this work employs linear subspace methods to analyze in detail the nature and ramifications of that process when applied to a 1-D, Richards equation-based unsaturated zone model used to predict recharge to a groundwater system. Two simplified versions of this model are examined. The first achieves simplification through assuming vertical parameter uniformity. The second achieves simplification through use of a lumped parameter model in place of the Richards equation-based model. Relationships between parameters employed by the complex model and those used by each of the simplified models are analyzed. The nature of predictive errors incurred through simplification is explored. Also explored is the ability of the calibration process to decrease the propensity for model error in making some predictions, while increasing the propensity for model error in the making of others (an outcome that may be considered counterintuitive from a Bayesian perspective, but which is a natural consequence of suboptimal simplification).

Citation: Watson, T. A., J. E. Doherty, and S. Christensen (2013), Parameter and predictive outcomes of model simplification, *Water Resour. Res.*, *49*, 3952–3977, doi:10.1002/wrcr.20145.

1. Introduction

[2] The issue of simplification (as well as the closely related issues of model reduction and parameter upscaling) is central to environmental simulation. This is especially the case where modeling is carried out for the purpose of environmental management. In these circumstances a model is required to make one or a number of predictions on which decisions may be based. The extent to which the process of model simplification induces errors in predictions required of the model must be assessed so that decision makers and stakeholders can thereby be aware of the credibility of such predictions.

[3] The need for a proper understanding of model simplification arises first and foremost from the fact that all models are simplifications of reality. Hence, they are imperfect simulators of the systems that they purport to represent. In addition to this, considerable simplification is often required for a model to be calibrated, for calibration uniqueness can only be attained at the cost of parameter simplification. Ideally, such simplification should achieve a status of minimized error variance for estimated parameters and for predictions which depend on them. Theoretically, this can be achieved through implementation of various types of mathematical regularization [see, for example, *Tikhonov and Arsenin*, 1977; *Menke*, 1984; *Aster et al*., 2005; *Moore and Doherty*, 2005, 2006]. Following calibration, calibration-constrained Monte Carlo methodologies such as those described by *Tonkin and Doherty* [2009] and *Herckenrath et al*. [2011] or hypothesis-testing methodologies such as that described by *Moore et al*. [2010] can be employed for analysis of the potential for error in predictions made by the simplified model. Ideally, analysis of the potential for errors in predictions made by a simplified/calibrated model is (almost) equivalent to the analysis of the inherent uncertainty of these predictions given the information available for the system under study.

[4] Theoretically, uncertainty analysis without the need for simplification as a precursor to that analysis can be undertaken in a Bayesian framework under the assumption that a model's inadequacies as a simulator of real-world environmental processes are small enough to be ignored. Examples of such analysis include the work of *Harmon and Challenor* [1997], *Kuczera and Parent* [1998], *Campbell et al*. [1999], *Campbell and Bates* [2001], *Makowski et al*. [2002], *Qian et al*. [2003], *Kanso et al*. [2003], *Vrugt*

[1]National Centre for Groundwater Research and Training, Flinders University, Adelaide, South Australia, Australia.
[2]School of the Environment, Flinders University, Adelaide, South Australia, Australia.
[3]Watermark Numerical Computing, Corinda, Queensland, Australia.
[4]Department of Geoscience, Aarhus University, Aarhus, Denmark.

Corresponding author: T. A. Watson, National Centre for Groundwater Research and Training, Flinders University, GPO Box 2100, Adelaide, SA 5001, Australia. (ty.watson@flinders.edu.au)

©2013. American Geophysical Union. All Rights Reserved.
0043-1397/13/10.1002/wrcr.20145

et al. [2009], and references cited within these studies. *Kennedy and O'Hagan* [2001] extended Bayesian analysis to include the contributions made by simplification-induced model-to-measurement misfit to inferred posterior parameter uncertainty. Their analysis, however, was applied to parameter spaces of relatively low dimension where contributions to predictive uncertainty incurred by the existence of inestimable parameters, and/or inestimable combinations of parameters, are small or nonexistent.

[5] In many cases of model design and usage, simplification is not carried out in such a mathematically controlled manner as that which is implemented through regularized inversion. Consequently, a mathematical description of the simplification process is rarely available. It is therefore difficult to account for the contribution that such simplification makes to the potential for error in predictions made by the simplified model.

[6] Recognition of the need for simplification dates back as far as modeling itself. *Meisel and Collins* [1973] discuss the need for model simplification in order to achieve (among other benefits) computational savings in an optimization context. More recently, *Ratto et al*. [2011] highlight that despite the enormous advances in computing power over recent decades, computational limitations still remain a major barrier to use of large-scale, process-based simulation models in a decision-making context. *Razavi et al*. [2012] provide a review of the growing number of documented incidences of the use of simplified or surrogate models in place of complex, physically based models in studies that demand computation of model outcomes on the basis of many different sets of what they call "explanatory variables," the nature of these depending on the nature of the study being undertaken.

[7] In response to the challenges posed by the need for model simplification, the recent literature documents a wide range of approaches to reducing the computational expense of simulating natural and man-made systems. Strategies include model emulation (or "metamodeling") [e.g., *Sivakumar*, 2008; *Young and Ratto*, 2009, 2011; *Castelletti et al*., 2011], model "reduction" [e.g., *Vermeulen et al*., 2004, 2005, 2006; *Cheng et al*., 2011], and parameter upscaling [e.g., *Farmer*, 2002; *Pachepsky et al*., 2006; *Gerritsen and Lambers*, 2008; *Mondal et al*., 2010]. Meanwhile, less formal simplification strategies involving parameter and/or process lumping have been applied as a matter of course in model design and deployment over many years. See, for example, *Lewis and Walker* [2002], *Dripps and Bradbury* [2007], *Zhu and Sun* [2009], *Francés et al*. [2010], *Martínez-Santos and Andreu* [2010], *Andreu et al*. [2011] and *Touhami et al*. [2012], all of whom modeled recharge to regional groundwater systems, this being the context of the example model discussed in the present paper.

[8] While considerable effort has been devoted to seeking simplification strategies that reduce the computational burden of environmental simulation, few studies have explored the effects of simplification on a model's predictive performance. Deleterious repercussions of simplification can include the introduction of predictive bias and a loss of ability to quantify the full range of uncertainty associated with a prediction of interest; the latter is a fundamental requirement of model usage in decision support [*Freeze et al*., 1990]. Such studies are difficult to undertake, for they often require that a simplified model be paired with a more complex one, with the latter providing metrics by which the former's performance can be judged. Nevertheless, this approach was taken by *Aanonsen* [2008] and *Scheidt et al*. [2011] in the petroleum context, by *Vrugt et al*. [2004] and *Schoups and Hopmans* [2006] in the vadose zone context, and by *Doherty and Christensen* [2011] in the groundwater context. In most modeling contexts however, while the imperfect nature of model-based simulation is recognized, little or no attempt is generally made to quantify the effects of model imperfections on model predictive performance, for time and resources typically permit no such investigation.

[9] The present paper seeks to improve our understanding of the effects of model simplification by undertaking such an investigation. It uses as its starting point theory and techniques developed by *Doherty and Christensen* [2011], who provide a generalized mathematical characterization of the model simplification process. By characterizing simplification as the omission from a model of parameters and processes that prevail in the real world, they were able to apply subspace concepts in their analysis. They then characterized simplification-induced model predictive error as arising from one or more of the following sources.

[10] 1. Failure to represent parameter/process detail to which historical measurements of system state comprising the calibration data set are sensitive.

[11] 2. Failure to represent parameter/process detail to which predictions of interest are sensitive.

[12] 3. The compensatory roles that parameters of a defective model are forced to play during the calibration process and then continue to play when the model is used to make predictions.

[13] The first of these represents a failure of the model calibration process to extract as much information from the calibration data set as is available in that data set. Because the (over)simplified model provides no receptacles for such information, the postcalibration propensity for error of some model predictions may be higher than it needs to be, given the available data set. The gap between the information content of the calibration data set and the receptacles that the model provides to hold that information is expressed as simplification-induced model-to-measurement misfit; this is commonly referred to as "structural noise." Ideally, stochastic characterization of such noise would allow the effects of simplification to be at least partially included in the quantification of model predictive error. Methods such as those described by *Kennedy and O'Hagan* [2001], *Cooley* [2004], *Cooley and Christensen* [2006], and *Cui et al*. [2011] could be used for this purpose. However, *Doherty and Welter* [2010] point out that such analysis is likely to be hampered by the fact that the covariance matrix of structural noise is generally singular.

[14] The second source of error identified by *Doherty and Christensen* [2011] represents a failure on the part of a simplified model to represent the so-called "null space" contribution to predictive uncertainty. This source of uncertainty arises from a sensitivity of model predictions to parameters and/or parameter combinations that are not inferable through the model calibration process. That is, it arises from simplifications that do not degrade a model's

ability to replicate the past but may compromise its ability to represent the future. In general, the magnitude of this term increases with the extent to which predictions of interest are different, or occur under different conditions, from those employed for model calibration.

[15] The third of the above sources of error can promote predictive bias. *Doherty and Christensen* [2011] show that adjustment of parameters of an imperfect model to achieve a good fit between model outputs and members of the calibration data set requires that some parameters assume roles that they were not necessarily designed to play. At the same time, null space parameter components are unwittingly adjusted away from their precalibration expected values, a process that *Doherty and Christensen* [2011] refer to as "null space entrainment." Predictions which are sensitive to thus-adjusted null space parameter components become biased as a result. Under certain circumstances this bias can dominate predictive error, engendering greater propensity for error in a model that has been calibrated than in a model that has not been calibrated at all. In contrast, if a prediction is entirely dependent on parameter combinations that are informed by the calibration data set (i.e., so-called "solution space" parameter combinations), its propensity for predictive error may be significantly reduced by the model calibration process, regardless of model defects and regardless of the compensatory roles played by some model parameters during the calibration process and the degree of null space entrainment endured by others. In general, this applies to predictions that are comprised of model outputs which are very similar in type and location to those used for model calibration.

[16] This paper extends the work of *Doherty and Christensen* [2011] in examining the theory and ramifications of model simplification in contexts where a model must be calibrated before being used in a predictive capacity. With some slight modification of *Doherty and Christensen*'s [2011] original theory, simplification is viewed in the present paper as parameter transformation and decomposition. The requirements of optimal transformation/decomposition are outlined, and the repercussions of suboptimal transformation/decomposition are described. The theory and concepts discussed herein are then illustrated using a relatively complex model of water movement through a heterogeneous soil profile built for the purpose of groundwater recharge estimation, together with two simplified versions of this same model.

[17] It is salient to point out that while *Vrugt et al.* [2004] and *Schoups and Hopmans* [2006] also addressed the issue of model simplification in the vadose zone context, the present study differs from these previous studies in that its particular focus is on the potential for error in simplified model parameters, and in predictions that are sensitive to them, that is incurred through the act of calibrating the simplified model. As such, it forms a useful complement to this previous work. It is also salient to point out that a significant difference between the example used in this study and that employed by *Doherty and Christensen* [2011] is that calibration of the simplified models used in the present example constitutes a well-posed inverse problem. Furthermore, one of the simplified models is oversimplified, as the fit between outputs of this model and measurements comprising the calibration data set are contaminated by structural noise. The effects of such "oversimplification" on model predictive performance are examined. In a further development of the theory presented by *Doherty and Christensen* [2011], the relationships that parameters of a simplified model have with parameters of a partnered complex model (and, by inference, to the hydraulic properties of reality itself) are examined. The degree of null space entrainment engendered through adjustment of simplified model parameters and its effects on model predictions are also examined through linear analysis.

[18] This paper is organized as follows. Section 2 provides a brief review of the theory of simplification presented by *Doherty and Christensen* [2011]. This theory is then extended to include the issue of optimal parameter transformation and the role of expert knowledge in seeking such optimality. Following that, transformations are developed through which the relationships between simplified model parameters and complex model parameters can be better understood. In section 3 we introduce a synthetic Richards equation-based model and two simplifications of it. In section 4 the paired model methodology of *Doherty and Christensen* [2011], in conjunction with theory presented in section 2, is applied to this suite of models as they are employed to make predictions of groundwater recharge. Section 5 presents a discussion of the outcomes of these analyses. Section 6 draws conclusions that are salient not only to the models that are discussed in this paper but also to environmental models in general.

2. Concepts and Theory

2.1. Introduction

[19] The theoretical analysis of simplification presented herein rests on subspace concepts, whereby a simplified model is viewed as the outcome of a parameter transformation and decomposition process. One advantage of adopting such an approach is that as we shall discuss, optimality of parameter transformation and decomposition (and hence of simplification) can, at least in principle, be defined. The success or otherwise of any particular simplification strategy can then be assessed according to this metric. It is important to point out that our analysis is not intended to constitute a mechanism for simplification and/or parameter upscaling that one would necessarily use in a real-world context. It does, however, provide a means to understand and assess the outcomes of model simplification implemented in whatever way a modeler chooses.

[20] Our analysis assumes that the relationship between model outputs and parameters employed by a model is linear and hence can be represented as a matrix. This assumption is violated by most models; however, it allows the use of subspace methods in our analysis. This, in turn, exposes outcomes of the simplification process which would be otherwise difficult or impossible to explore. These outcomes are not diminished by model nonlinearity; rather they are made more complex. Given that the intentions of our study are to expose and explore the general nature of these outcomes rather than their details in any specific modeling context, our analysis is not invalidated by the nonlinear nature of most models. Nevertheless, some numerical experiments were carried out to address this issue and to thereby ensure the integrity of the conclusions drawn in the

examples section of this paper; details are provided in section 4.6.

[21] The following subsections provide a brief review of aspects of linear analysis that are salient to our analysis of model simplification.

2.2. Linearization Concepts

2.2.1. General

[22] As stated earlier, to facilitate the application of subspace concepts and theory, a linear relationship between environmental process outputs and parameters pertaining to those processes is assumed. Reality, and any model that simulates it, are thus represented as matrices operating on parameters; the latter representing properties of a system. For ease of analysis we consider reality to be a very complex model (herein referred to as the "reality model") and numerical simulators of reality to be simpler models that strive to provide the same outputs under the same conditions. In the text that follows we therefore make repeated reference to a "reality model" as our starting point for examining the effects of simplification, the latter being a necessary accompaniment of any attempt to simulate reality. Though a "reality model" does not actually exist (for only reality itself exists), we have retained this terminology in the following text in preference to the term "complex model" to depict the starting point for our analysis in order to reinforce the concept that all models, even the most complex, are gross simplifications of reality. Hence any model, no matter how complex, is subject to the same phenomena that we discuss later when parameters of that model are adjusted in order to ensure that its outputs better match the observed behavior of the real world.

[23] For convenience in the analysis that follows, parameter values are formulated as perturbations from their expert knowledge-based expected values; model outputs are treated in the same manner. Thus, parameter values of zero give rise to model output values of zero. Adoption of this protocol reduces the complexity of the following equations. It also sets the mathematical context for optimal usage of subspace concepts in the model calibration process, namely, that parameters (or combinations of parameters) should be assigned values of zero (and hence be informed by expert knowledge alone) unless information within the data set supports estimation of these parameters (or parameter combinations).

[24] In accordance with the protocols just described, let $\mathbf{k}$ (a vector) denote the hydraulic properties of a real-world system, or equivalently the parameters used by a "reality model" which simulates that system perfectly. Let $\mathbf{Z}$ represents the action of that model under calibration conditions, and let $\mathbf{h}$ represents the calibration data set. The latter is contaminated by measurement noise $\boldsymbol{\varepsilon}$ so that

$$\mathbf{h} = \mathbf{Z}\mathbf{k} + \boldsymbol{\varepsilon}. \tag{1}$$

2.2.2. The Null Space

[25] The matrix $\mathbf{Z}$ of reality will normally have many more columns than rows, for reality is heterogeneous and complex, and its parameters are many. Unique estimation of these parameters from a calibration data set is not possible. A parallel concept to that of parameter nonuniqueness is that of the null space. By definition, a nonzero parameter set $\mathbf{k}_n$ belongs to the null space of $\mathbf{Z}$ if

$$\mathbf{0} = \mathbf{Z}\mathbf{k}_n. \tag{2}$$

[26] Suppose that a parameter set $\underline{\mathbf{k}}$ can be found that fits the calibration data set perfectly. Then,

$$\mathbf{h} = \mathbf{Z}\underline{\mathbf{k}}. \tag{3}$$

[27] By adding equation (2) to equation (3), the nonuniqueness of $\underline{\mathbf{k}}$ in the face of the existence of a null space is demonstrated.

[28] Matrices that have more rows than columns can also possess a null space. However, a matrix with more columns than rows will surely possess a null space. In many modeling contexts the purpose of model simplification is to reduce the number of parameters employed by an existing model so that the null space is eliminated, thereby promulgating uniqueness of its calibration. However, calibration uniqueness can also be achieved mathematically (and optimally, as will be explained) through the process of singular value decomposition (SVD).

2.2.3. Singular Value Decomposition

[29] Through SVD, any matrix $\mathbf{Z}$ can be decomposed as

$$\mathbf{Z} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathrm{t}}, \tag{4}$$

where $\mathbf{U}$ and $\mathbf{V}$ are orthonormal square matrices whose columns are unit vectors which span the output and parameter spaces of $\mathbf{Z}$, respectively. $\mathbf{S}$ is a matrix with diagonal elements, referred to as "singular values", ordered from highest to lowest and all of which are positive or zero. Partitioning of $\mathbf{S}$ on the basis of zero and nonzero singular values leads to concordant partitioning of $\mathbf{U}$ and $\mathbf{V}$. Applying subscripts 1 and 2 to the partitions that correspond to nonzero and zero singular values, respectively, equation (4) becomes

$$\mathbf{Z} = \mathbf{U}_1\mathbf{S}_1\mathbf{V}_1^{\mathrm{t}} + \mathbf{U}_2\mathbf{S}_2\mathbf{V}_2^{\mathrm{t}} = \mathbf{U}_1\mathbf{S}_1\mathbf{V}_1^{\mathrm{t}}. \tag{5}$$

[30] In practice, singular values that are close to zero, in addition to those that are exactly zero, are relegated to $\mathbf{S}_2$ in order to prevent "overfitting" (whereby a model is forced to reproduce characteristics of the calibration data set that are more likely to represent measurement error rather than true system behavior). The solution to the inverse problem of model calibration found through SVD is given by [see, for example, *Aster et al*., 2005]

$$\underline{\mathbf{k}} = \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^{\mathrm{t}}\mathbf{h}. \tag{6}$$

[31] The fact that this amounts to a form of parameter simplification is demonstrated by premultiplying both sides of equation (6) by $\mathbf{V}_1^t$ to yield

$$\underline{\boldsymbol{\alpha}} = \mathbf{V}_1^t\underline{\mathbf{k}} = \mathbf{S}_1^{-1}\mathbf{U}_1^{\mathrm{t}}\mathbf{h} = \mathbf{S}_1^{-1}\boldsymbol{\phi}, \tag{7a}$$

where

$$\boldsymbol{\phi} = \mathbf{U}_1^{\mathrm{t}}\mathbf{h} \tag{7b}$$

[32] $\boldsymbol{\alpha}$ is a vector comprising estimates of the scalar projections of the real-world parameter set $\mathbf{k}$ onto each of the orthogonal unit vectors $\mathbf{v}_{1i}$ comprising the columns of $\mathbf{V}_1$. Collectively, these orthogonal unit vectors span the parameter solution space; this is the orthogonal complement of the null space: orthogonal because the projection of one of these subspaces onto the other is zero or, in more colloquial terms, because there is no overlap between them. The smaller the dimensionality of the solution space, the fewer of these scalar projections that are estimated, for the dimensionality of the solution space is defined as the number of columns comprising the $\mathbf{V}_1$ matrix. Meanwhile, parameter projections onto the $\mathbf{v}_{2i}$ vectors which span the null space are not estimated. These projections therefore retain their precalibration values of zero.

[33] Projections of parameters onto the $\mathbf{v}_i$ vectors can be considered to be linear combinations of the original parameter set $\mathbf{k}$. The ratios in which these parameters are combined are given by the elements of each $\mathbf{v}_i$ vector. The calibration process thus effectively provides estimates for multipliers pertaining to some of these combinations (i.e., parameter combinations belonging to the solution space), while multipliers for other parameter combinations are assigned a value of zero as the calibration data set provides insufficient information for their estimation. At the same time, because of the diagonal status of $\mathbf{S}^{-1}{}_1$, each element of $\boldsymbol{\alpha}$ is calculated directly from its corresponding element of $\boldsymbol{\phi}$ through multiplication by the corresponding element of $\mathbf{S}_1^{-1}$. The ith element of $\boldsymbol{\phi}$ is the scalar projection of the observation data set onto the ith column of $\mathbf{U}$, the latter being denoted as $\mathbf{u}_i$. In a similar fashion to $\mathbf{v}_i$ for parameters, each $\mathbf{u}_i$ contains coefficients that combine observations in a linear manner. Equations (7a) and (7b) thus state that the ith combination of observations expressed by $\mathbf{u}_i$ is uniquely and entirely informative of the ith combination of parameters expressed by $\mathbf{v}_i$. The reader is referred to texts such as *Aster et al*. [2005] for further details.

2.2.4. Optimal Calibration

[34] Let s (a scalar) be a prediction made by the reality model. Let the vector $\mathbf{y}$ denote the sensitivity of this prediction to parameters $\mathbf{k}$ of the reality model. Then,

$$s = \mathbf{y}^t\mathbf{k}. \tag{8a}$$

[35] When the prediction is made using the calibrated model, it is calculated as

$$\underline{s} = \mathbf{y}^t\underline{\mathbf{k}}. \tag{8b}$$

[36] It can be shown [see *Moore and Doherty*, 2005] that the error variance of the prediction made by the calibrated model is

$$\sigma^2_{\underline{s}-s} = \mathbf{y}^t\mathbf{V}_2\mathbf{V}_2^t\mathbf{C}(\mathbf{k})\mathbf{V}_2\mathbf{V}_2^t\mathbf{y} + \mathbf{y}^t\mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{C}(\varepsilon)\mathbf{S}_1^{-1}\mathbf{V}_1^t\mathbf{y}, \tag{9}$$

where $\mathbf{C}(\varepsilon)$ is the covariance matrix of measurement noise, and $\mathbf{C}(\mathbf{k})$ is the covariance matrix associated with the prior probability distribution of parameters $\mathbf{k}$. As such it is an encapsulation of expert knowledge.

[37] Let us suppose that $\mathbf{C}(\mathbf{k})$ and $\mathbf{C}(\varepsilon)$ can be expressed as follows:

$$\mathbf{C}(\mathbf{k}) = \sigma^2{}_k\mathbf{I} \tag{10a}$$

$$\mathbf{C}(\varepsilon) = \sigma^2{}_\varepsilon\mathbf{I}. \tag{10b}$$

[38] The first of these equations states that in terms of expert knowledge, all parameters are independently and equally variable, with no statistical correlation between them. The second states that the errors associated with measurements comprising the calibration data set are also independent and of equal magnitude for all measurements. If the conditions given by equations (10a) and (10b) are met, then equation (9) becomes

$$\sigma^2_{\underline{s}-s} = \sigma^2{}_k\mathbf{y}^t\mathbf{V}_2\mathbf{V}_1^t\mathbf{y} + \sigma^2{}_\varepsilon\mathbf{y}^t\mathbf{V}_1\mathbf{S}_1^{-2}\mathbf{V}_1^t\mathbf{y}. \tag{11}$$

[39] The first term on the right of equation (11) falls monotonically as the number of singular values that are assigned to the solution space increases, while the second term rises monotonically at the same time. Meanwhile, the sum of these terms falls from its precalibration value (equal to precalibration predictive uncertainty) if no singular values are retained, achieves a minimum value at some number of positive singular values, and then rises, approaching infinity as the magnitude of singular values comprising the diagonal elements of $\mathbf{S}_1$ approaches zero. The minimum value of the predictive error variance curve defines the optimum number of singular values to employ in calibrating the model.

[40] Optimality of calibration can also be viewed from a parameter, as well as from a predictive, point of view. As the dimensionality of the solution space is increased, the error variance of the α_i scalars comprising the elements of the $\boldsymbol{\alpha}$ vector of equation (7a) can be computed using a slight modification of equation (11). If the error variance of an α_i is greater after calibration than before calibration (where its propensity for error is based on expert knowledge alone), it should not be estimated, and the corresponding $\mathbf{v}_i$ vector should not be included in the solution space. In other words, parameters and parameter combinations which are not estimated through the calibration process should be assigned values based on expert knowledge alone, for this endows such parameters and parameter combinations with less potential for error than that which they would accrue through the calibration process.

[41] Satisfaction of equations (10a) and (10b) is important for achieving optimality of calibration through minimization of predictive error variance through selection of the appropriate number of singular values to employ in the calibration process. Where equation (10a) in particular is not met, and especially where $\mathbf{C}(\mathbf{k})$ has off-diagonal elements, it is easy to find cases where a graph of σ^2_{s-s} versus number of singular values rises before it falls. Note also that the number of singular values used in the estimation of model parameters can be taken as a measure of calibration-induced simplification. The use of a small number of singular values implies a small dimensionality of the solution space, and hence a high degree of simplification.

2.2.5. Optimal Parameter Transformation

[42] Rarely will expert knowledge be such that equation (10a) automatically holds. However, conceptually at least, it can be achieved through appropriate parameter transformation.

[43] Let the matrices $\mathbf{F}$ and $\mathbf{E}$ (the former being orthonormal and the latter being diagonal) be defined through the following equation in which the necessarily positive definite symmetric matrix $\mathbf{C}(\mathbf{k})$ is subject to SVD:

$$\mathbf{C}(\mathbf{k}) = \mathbf{FEF}^{t}. \tag{12}$$

[44] Now let the vector $\mathbf{m}$ be defined as

$$\mathbf{m} = \mathbf{E}^{-1/2}\mathbf{F}^{t}\mathbf{k} \tag{13a}$$

so that by premultiplication of both sides of equation (16) by $\mathbf{E}^{1/2}$ and $\mathbf{F}$:

$$\mathbf{k} = \mathbf{FE}^{1/2}\mathbf{m}. \tag{13b}$$

[45] Using standard matrix relationships for propagation of covariance it is easily shown that

$$\mathbf{C}(\mathbf{m}) = \mathbf{I}. \tag{14}$$

[46] Comparing equation (14) with equation (10a), it follows that parameter estimation should take place in $\mathbf{m}$-space rather than $\mathbf{k}$-space if it is to achieve a minimum error variance status for estimated parameters and for predictions which depend on them. From equations (1) and (13b):

$$\mathbf{h} = \mathbf{Zk} + \boldsymbol{\varepsilon} = \mathbf{ZFE}^{1/2}\mathbf{m} + \boldsymbol{\varepsilon} = \mathbf{Ym} + \boldsymbol{\varepsilon}, \tag{15}$$

where

$$\mathbf{Y} = \mathbf{ZFE}^{1/2}. \tag{16}$$

2.3. Simplification and Subspaces

2.3.1. Simplification Strategies

[47] Strategies through which complex and heterogeneous natural systems are represented in a numerical model are often based on the notions of averaging and/or fixing. In a groundwater model, for example, many facies may be simulated as a single layer; parameters assigned to that single layer are hydraulic properties vertically averaged over those facies. Similarly, horizontal spatial hydraulic property averaging is required in order to assign parameters to the (possibly large) cells or elements used by a regional numerical model.

[48] The process of model structure simplification has much in common with the process of parameter simplification that is often undertaken prior to model calibration in order to achieve well-posedness of the resulting inverse problem. The latter involves the fixing of some parameters at expert knowledge-informed values and the amalgamation of others so that average properties, rather than parameterization detail, are subject to estimation. As discussed earlier, optimality of parameter simplification required for model calibration can be achieved through SVD following appropriate parameter transformation. This too can be viewed as the process of fixing certain parameters and parameter combinations at "known" values (these being parameters and parameter combinations which lie entirely within the null space) while estimating a limited number of "averaged" parameters. The "averaging coefficients" (i.e., the elements of the $\mathbf{v}_i$ vectors comprising the columns of the $\mathbf{V}_1$ matrix of equation (5)) are defined in a manner that guarantees orthogonality to null space parameter components and achieves a minimum error variance status for averaged parameters thus estimated and for predictions which depend on them.

2.3.2. Optimal Model Simplification

[49] *Doherty and Christensen* [2011] addressed the concept of optimality of model simplification through analyzing model simplification in linear subspace terms. They showed that simplification can be viewed as a kind of parameter decomposition, resulting in a set of actual and/or notional parameters which are "included" in the simplified model, together with a complimentary set of parameters which are "omitted" from this model. Under the assumption that the simplified model must be calibrated as part of its field deployment, they demonstrated that a necessary condition for achieving optimality of model simplification is that the parameter space decomposition implied by simplification is an orthogonal decomposition, and that the outcomes of this decomposition process resemble, as much as possible, that implied by transformation according to equations (13a) and (13b), followed by SVD of the resulting $\mathbf{m}$ parameter space.

[50] *Doherty and Christensen* [2011] characterized optimal model simplification as that which leads to predictions of minimized error variance. (Note that this error variance may be far from zero, as it is bounded from below by the innate uncertainty associated with model predictions given all available information pertaining to the system of interest.) They showed that where simplification is not in accordance with the transformation and decomposition process described earlier, a consequence may be inadvertent adjustment of parameter components that properly belong to the null space as the simplified model is calibrated. Predictions that are sensitive to thus entrained null space parameter components will be biased and will therefore fail to achieve minimum error variance status. Such simplification is therefore suboptimal. Simultaneously with null space entrainment, certain model parameters and/or parameter combinations assume surrogate roles as they compensate for model defects while allowing model outputs to fit the calibration data set; this further contributes to potential predictive bias. (A simple mathematical demonstration of calibration-induced null space parameter entrainment incurred through failure to comply with optimality of parameter transformation as described by equations (13a) and (13b) is provided in Appendix A.)

[51] *Doherty and Christensen* [2011] further showed that the adverse effects of a suboptimal simplification strategy are prediction specific. Where a prediction is similar in nature to data comprising the calibration data set (and therefore is sensitive solely to parameter combinations occupying the solution space), optimality of simplification

as far as that prediction is concerned requires only that a model is capable of replicating historical system behavior well; a recognizably physical basis for its parameters is of secondary importance. Alternatively, where a model is required to make predictions under different conditions, or of a different type, to the observations which comprise the calibration data set (as is often the case), its design must be such that these different conditions can indeed be simulated, and that its ability to make such predictions with minimized error variance is enhanced, rather than eroded, by the process of model calibration. The alignment of calibration and simplification subspaces discussed earlier is important in achieving this.

2.3.3. Paired Model Analysis

[52] If model simplification approaches optimality, then all predictions made by the model after it has been calibrated are of minimized error variance regardless of their degree of solution and null space dependence. However, lack of representation of real-world null space parameter components in the simplified model may preclude the possibility of exploring the error variance associated with its predictions, and hence of quantifying their uncertainties. *Doherty and Christensen* [2011] propose a methodology for model predictive uncertainty analysis that involves conjunctive use of a simplified and complex model in order to overcome this problem. At the same time, this methodology allows identification of, and correction for, calibration-induced predictive bias. Although requiring construction of a complex model for use in conjunction with the simplified model, a benefit of this approach is that the complex model does not require calibration, an undertaking which may be hampered by long run times and/or numerical instability of the model. Moreover, use of a physically based complex model provides the means through which expert knowledge pertaining to a particular study site can be best expressed.

[53] The methodology is as follows:

[54] 1. Generate many different expert knowledge-based stochastic realizations of a complex model and its parameters, with these realizations including those aspects of the system that are likely to contribute most to the uncertainty of predictions of interest. Obtain a suite of such predictions from the stochastic model realizations. Let each such prediction be referred to as s. Additionally, compute complex model outputs that correspond to observations comprising the available calibration data set.

[55] 2. For each realization of the complex model, calibrate a simplified model against those complex model outputs that correspond to members of the calibration data set. Then, make the prediction of interest using each calibrated simplified model. Let these predictions be referred to as $\underline{s}$.

[56] 3. Produce a scatterplot of s versus $\underline{s}$. A regression (best fit) line through the scatterplot can be used to correct simplified model predictions for simplification- and calibration-induced predictive bias. Meanwhile, scatter about the line of best fit quantifies predictive uncertainty (this often being dominated by the sensitivity of a prediction to null space parameter components that are not represented in the simplified model).

[57] 4. Calibrate the simplified model against the real-world data set. On the basis of information available from the s versus $\underline{s}$ plot, correct this prediction for bias and quantify its uncertainty.

[58] The described paired model analysis, while presented by *Doherty and Christensen* [2011] as a practical methodology for predictive uncertainty quantification and bias correction, also serves as a metric by which the success, in terms of predictive performance, of a given simplification approach can be judged. It is employed in the present study for this purpose.

2.4. Relationships Between Complex and Simplified Model Parameters

[59] In accordance with the approach taken by *Doherty and Christensen* [2011], we express the effects of simplification as the omission of parameters, and the processes that operate on them, from a complex "reality model" in order to derive the actual numerical model that we use in place of reality. Thus, any model that we use to simulate reality can be viewed as possessing a suite of "visible" parameters, together with a set of implied "invisible" parameters. The latter specify corrections that should be made to any aspect of the physical, numerical, and/or parameter structure of the model that would allow that model to become a perfect replica of the real world and the processes that are operative therein. This is, of course, a simplistic notion; indeed any analysis of simplification will itself be a simplification. However, as will be demonstrated later, this conceptualization of simplification allows us to gain some important insights into the effects of the simplification process that would not otherwise be so clearly visible.

[60] Let the reduced number of parameters employed by a simplified model of the study site described by $\mathbf{Z}$ be represented by the vector $\mathbf{p}$. Let the model which acts on this reduced set of parameters be designated as $\mathbf{X}$. Then, under calibration conditions, from equation (1),

$$\mathbf{h} = \mathbf{X}\mathbf{p} + (\mathbf{Z}\mathbf{k} - \mathbf{X}\mathbf{p}) + \varepsilon. \tag{17}$$

[61] The term $(\mathbf{Z}\mathbf{k} - \mathbf{X}\mathbf{p})$ can be viewed as structural error (or sometimes "structural noise" when its presence becomes apparent through attempts to calibrate the model) as it represents simplification-induced model-to-measurement misfit. As discussed earlier, analysis of this can prove difficult for a number of reasons. Furthermore, if a simplified model fits the calibration data set well, this term may be very small (or even nonexistent). Hence, it is often more fruitful to examine the ramifications of simplification on the calibration process from the point of view of its effect on parameters rather than its effects on model outputs [see, for example, *Vrugt et al.*, 2005; *Kavetski et al.*, 2006a, 2006b; *Kuczera et al.*, 2006]. Following *Doherty and Christensen* [2011] we write

$$\mathbf{Z}\mathbf{k} - \mathbf{X}\mathbf{p} = \mathbf{Z}_o\mathbf{k}_o, \tag{18}$$

where the subscript "o" stands for "omitted." $\mathbf{k}_o$ represents parameters omitted from the "reality" model in building the simplified model, while $\mathbf{Z}_o$ represents the omitted

processes which operate on them. Equation (17) therefore becomes

$$\mathbf{h} = \mathbf{X}\mathbf{p} + \mathbf{Z}_o\mathbf{k}_o + \varepsilon. \tag{19}$$

[62] The simplified model parameter set $\mathbf{p}$ can be characterized as being derived from the complex model parameter set $\mathbf{k}$ through a decomposition operation. If this is denoted by the matrix $\mathbf{L}$, then

$$\mathbf{p} = \mathbf{L}\mathbf{k} \tag{20}$$

so that from equation (17)

$$\mathbf{h} = \mathbf{X}\mathbf{L}\mathbf{k} + (\mathbf{Z} - \mathbf{X}\mathbf{L})\mathbf{k} + \varepsilon. \tag{21}$$

[63] To simplify the following analysis we will assume that the model simplification process is such that $\mathbf{X}$ is of full rank, and that estimation of $\mathbf{p}$ from the calibration data set therefore constitutes a well-posed inverse problem. If we further assume for simplicity that measurement noise is zero, and then provide all observations with the same weight, a value of $\mathbf{p}$ can be obtained for any $\mathbf{k}$ through calibrating the simplified model against a calibration data set generated by the complex model. Thus,

$$\mathbf{p} = (\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{h} = (\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z}\mathbf{k} = \mathbf{L}\mathbf{k}. \tag{22}$$

[64] Equation (22) provides the relationship between $\mathbf{p}$-space, the parameter space of the simplified representation of the real world that is the $\mathbf{X}$ model, and $\mathbf{k}$-space, the parameter space of the reality model (which we characterize as the $\mathbf{Z}$ model). Through use of this relationship, the composition of any simplified model parameter in terms of reality model parameters can be established.

[65] While simplified models are often abstractions of reality, their designers often state that their parameters can be informed by expert knowledge; in fact, they are often built specifically with this in mind. These considerations apply particularly to the lumped parameter soil moisture store models that form the basis of many regional rainfall/runoff/recharge simulators; indeed such a model is examined later in this paper. Equation (22) can be used to examine whether any particular simplified model parameter does indeed perform the function that it was designed to perform. Furthermore, the extent to which expert knowledge should be respected in terms of the degree of simplified model parameter variability allowed during calibration can be judged by computing the prior covariance matrix $\mathbf{C}(\mathbf{p})$ of the simplified model parameter set. From equation (22), this can be calculated from that of the real-world parameter set using standard relationships for propagation of covariance as:

$$\mathbf{C}(\mathbf{p}) = (\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z}\mathbf{C}(\mathbf{k})\mathbf{Z}^t\mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}. \tag{23}$$

[66] We note that this equation is similar to that derived by *Gallagher and Doherty* [2007].

[67] *Cooley and Christensen* [2006] discuss the special case where model simplification is undertaken through assuming spatial parameter uniformity in place of heterogeneity while retaining all other computational aspects of the complex model in the simplification process. (This corresponds to one of the examples presented herein.) They show that in this case the difference between estimated properties $\mathbf{p}$ and spatially averaged properties of the complex model, denoted as $\mathbf{p}_*$, is given by

$$\mathbf{p} - \mathbf{p}_* = (\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z}(\mathbf{I} - \boldsymbol{\gamma}(\boldsymbol{\gamma}^t\boldsymbol{\gamma})\boldsymbol{\gamma}^t)\mathbf{k} \tag{24a}$$

[68] The matrix $\boldsymbol{\gamma}$ is defined by the following equation:

$$E(\mathbf{k}) = \boldsymbol{\gamma}\underline{\mathbf{p}}, \tag{24b}$$

where

$$\underline{\mathbf{p}} = E(\mathbf{p}) \tag{24c}$$

with $E()$ being the expected value operator. They show for a linear model that over many realizations,

$$E(\mathbf{p} - \mathbf{p}_*) = E\left(\mathbf{p} - \underline{\mathbf{p}}\right) = 0. \tag{25}$$

[69] However, for any one realization $\mathbf{p}$ and $\mathbf{p}_*$ will generally differ, as equation (24a) shows. *Cooley and Christensen* [2006] also show that the discrepancy between $\mathbf{p}$ and $\mathbf{p}_*$ can be reduced, though not eliminated, by employing an empirically determined weighting matrix instead of measurement weights in estimating $\mathbf{p}$. This empirically determined weighting matrix is an estimate of the inverse of the total error covariance matrix, where the total error is the sum of observation error and structural error caused by the model's neglect of spatial heterogeneity.

2.5. Back Transformation to Complex Model Parameter Space

[70] To conform with nomenclature introduced earlier we will continue to employ $\mathbf{k}$ to represent a "reality" parameter set, or the parameter set employed by an equivalent complex model; $\mathbf{Z}$ represents the action of that model. We will assume, however, for the sake of simplicity in development of the theory, that equation (10a) holds (this may be either automatically or through appropriate parameter transformation) so that optimality of simplified parameterization can be achieved through SVD of $\mathbf{Z}$.

[71] As decomposition of $\mathbf{k}$ to $\mathbf{p}$ involves parameter reduction, it is not possible to find a unique back transformation from $\mathbf{p}$ to $\mathbf{k}$. However, it is possible to find a unique transformation from $\mathbf{p}$ to the solution space of $\mathbf{Z}$. This follows from the fact that for a given $\mathbf{h}$, $\mathbf{p}$ is unique and the projection of $\mathbf{k}$ onto its solution space is unique. This transformation is accomplished by seeking the $\underline{\mathbf{k}}$ (where the underscore signifies solution space occupancy) which provides the same $\mathbf{h}$ as $\mathbf{X}\mathbf{p}$. We will refer to this back-transformed parameter set as $\underline{\mathbf{k}}_p$ and define the transformation as $\mathbf{N}$. Thus, from equation (6),

$$\underline{\mathbf{k}}_p = \mathbf{N}\mathbf{p} = \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{X}\mathbf{p} \tag{26}$$

where $\mathbf{V}_1$, $\mathbf{S}_1$, and $\mathbf{U}_1$ are defined through SVD of $\mathbf{Z}$. Using the specification for $\mathbf{L}$ provided by equation (22), equation (21) can be expanded as

$$\mathbf{h} = \mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z}\mathbf{k} + \left(\mathbf{Z} - \mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z}\right)\mathbf{k} + \varepsilon. \quad (27)$$

[72] We now introduce the identity [*Aster et al.*, 2005]:

$$\mathbf{V}_1\mathbf{V}_1^t + \mathbf{V}_2\mathbf{V}^t{}_2 = \mathbf{I}, \quad (28)$$

where $\mathbf{V}_1$ and $\mathbf{V}_2$ are defined through equations (4) and (5), with partitioning taking place according to minimization of $\sigma^2{}_{s\text{-}s}$ through equation (11). Hence, from equation (1)

$$\mathbf{h} = \mathbf{Z}\mathbf{k} + \varepsilon = \mathbf{Z}\mathbf{V}_1\mathbf{V}_1^t\mathbf{k} + \mathbf{Z}\mathbf{V}_2\mathbf{V}_2^t\mathbf{k} + \varepsilon = \mathbf{Z}\underline{\mathbf{k}}_i + \mathbf{Z}\mathbf{k}_n + \varepsilon, \quad (29)$$

where we define $\underline{\mathbf{k}}_i$ as the "ideal" value of the calibrated parameter set. As such, it is the projection of the reality parameter vector $\mathbf{k}$ onto a solution space whose dimensions are those determined by minimization of predictive error variance of equation (11). It is thus calculable as

$$\underline{\mathbf{k}}_i = \mathbf{V}_1\mathbf{V}_1^t\mathbf{k}. \quad (30)$$

[73] Meanwhile, $\mathbf{k}_n$ is orthogonal to $\underline{\mathbf{k}}_i$. This includes null space components of $\mathbf{k}$, as well as components of $\mathbf{k}$ that are relegated to the null space as they are not worth estimating because their potential for error will be greater after calibration than before calibration. From equations (5) and (30) and the orthonormality of the vectors comprising $\mathbf{V}$,

$$\mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{Z}\mathbf{k} = \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{Z}\underline{\mathbf{k}}_i = \underline{\mathbf{k}}_i. \quad (31)$$

[74] If both sides of equation (29) are now premultiplied by $\mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t$ and equation (31) is substituted into the right side, we then obtain

$$\mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{h} = \underline{\mathbf{k}}_i + \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{Z}\mathbf{V}_2\mathbf{V}_2^t\mathbf{k} + \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\varepsilon. \quad (32)$$

[75] Through SVD of $\mathbf{Z}$ and using the orthonormality of $\mathbf{V}$ and $\mathbf{U}$, it is easy to show that the second term on the right of equation (32) is zero. Thus,

$$\mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{h} = \underline{\mathbf{k}}_i + \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\varepsilon. \quad (33)$$

[76] If both sides of equation (27) are now premultiplied by $\mathbf{V}_1\mathbf{S}^{-1}{}_1\mathbf{U}^t{}_1$, we obtain, with the help of equations (22) and (26),

$$\mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{h} = \underline{\mathbf{k}}_p + \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\left(\mathbf{I} - \mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\right)\mathbf{Z}\mathbf{k} + \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\varepsilon. \quad (34)$$

[77] The matrix $\mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t$ is an orthonormal matrix spanning the range space of the simplified model $\mathbf{X}$. $(\mathbf{I} - \mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t)$ spans the orthogonal complement of this. If this includes only system outputs calculated on the basis of parameter combinations corresponding to singular values that are below the singular value cutoff threshold, orthogonality of these outputs to $\mathbf{U}_1$ guarantees that the second term on the right of equation (34) is zero. However, if it includes any outputs that have a nonzero projection onto the $\mathbf{U}_1$ subspace, this term will not be zero. In other words, the second term of equation (34) describes structural noise created by an inability of the simplified model $\mathbf{X}$ to fit those aspects of the system response (encapsulated in $\mathbf{U}_1$) that are considered to be worth fitting from a parameter estimation point of view. Ideally, the design of a simplified model should be such as to reduce this term to as close to zero as possible. To the extent that this is accomplished, a comparison of equation (34) with equation (33) reveals that $\underline{\mathbf{k}}_p$ approaches $\underline{\mathbf{k}}_i$. Calibration of the simplified model thus achieves an effective real-world parameter set that has the same projection onto the real-world solution space as would have been achieved if the reality model itself were calibrated in an ideal manner.

[78] From equations (22) and (26) the relationship of $\underline{\mathbf{k}}_p$ to real-world parameters $\mathbf{k}$ is calculable as

$$\underline{\mathbf{k}}_p = \mathbf{V}_1\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z}\mathbf{k}. \quad (35)$$

[79] Equation (35) describes only the solution space projection of the effective real-world parameter set achieved through calibration of the simplified model. Let the vector $\underline{\boldsymbol{\beta}}$ contain the scalar projections of $\underline{\mathbf{k}}_p$ into each of the axes of parameter space defined through SVD of the reality model matrix $\mathbf{Z}$. Then,

$$\underline{\boldsymbol{\beta}} = \mathbf{V}_1^t\underline{\mathbf{k}}_p = \mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z}\mathbf{k}. \quad (36)$$

[80] Meanwhile, the true (reality model) set of solution space projections $\boldsymbol{\beta}$ can be calculated as

$$\boldsymbol{\beta} = \mathbf{V}_1^t\mathbf{k}. \quad (37)$$

[81] Errors in these projections are therefore calculable as

$$\underline{\boldsymbol{\beta}} - \boldsymbol{\beta} = \left(\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z} - \mathbf{V}_1^t\right)\mathbf{k}. \quad (38)$$

[82] Given the assumption that equation (10a) holds and thus the covariance matrix of $\mathbf{k}$ (i.e., $\mathbf{C}(\mathbf{k})$) is $\mathbf{I}$, the covariance matrix of solution space parameter projection error can be calculated from equation (38) as

$$\mathbf{C}\left(\underline{\boldsymbol{\beta}} - \boldsymbol{\beta}\right) = \left(\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z} - \mathbf{V}_1^t\right)\left(\mathbf{S}_1^{-1}\mathbf{U}_1^t\mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Z} - \mathbf{V}_1^t\right)^t. \quad (39)$$

[83] If a simplified model is capable of fitting a noise-free calibration data set perfectly, $\mathbf{C}(\underline{\boldsymbol{\beta}} - \boldsymbol{\beta})$ is $\mathbf{0}$, indicating achievement of correct real-world solution space parameter projections through calibration of the simplified model. However, through unavoidable, simultaneous adjustment of real-world null space parameter components as simplified model parameters are adjusted, these correct real-world solution space parameter projections may be accompanied by

nonzero (and hence biased) real-world null space parameter projections. The propensity for this to occur can be calculated using an appropriately modified version of equation (39) as

$$\mathbf{C}\left(\underline{\boldsymbol{\beta}}_{\mathrm{n}}\right) = \left(\mathbf{S}_2^{-1}\mathbf{U}_2^{\mathrm{t}}\mathbf{X}(\mathbf{X}^{\mathrm{t}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{t}}\mathbf{Z}\right)\left(\mathbf{S}_2^{-1}\mathbf{U}_2^{\mathrm{t}}\mathbf{X}(\mathbf{X}^{\mathrm{t}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{t}}\mathbf{Z}\right)^{\mathrm{t}}, \quad (40)$$

where

$$\underline{\boldsymbol{\beta}}_{\mathrm{n}} = \mathbf{V}_2^{\mathrm{t}}\underline{\mathbf{k}}_{\mathrm{p}} = \mathbf{S}_2^{-1}\mathbf{U}_2^{\mathrm{t}}\mathbf{X}(\mathbf{X}^{\mathrm{t}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{t}}\mathbf{Z}\mathbf{k}. \quad (41)$$

[84] Equivalent to equation (37), the true set of null space parameter projections $\boldsymbol{\beta}_n$ is given by

$$\boldsymbol{\beta}_{\mathrm{n}} = \mathbf{V}_2^{\mathrm{t}}\mathbf{k}. \quad (42)$$

[85] However, these can never be known.

[86] The presence of nonzero elements of $\mathbf{C}(\underline{\boldsymbol{\beta}}_{\mathrm{n}})$ represents suboptimality of the model simplification process, as it implies that parameter components that are not inferable from the calibration data set have been interjected into the effective parameter set of the reality model through calibration of the simplified model. Though such components may indeed be present in the real-world parameter set $\mathbf{k}$, their calibrated values must be zero if minimum error variance status of all model predictions is to be achieved (rather than just those that are solution space dependent). The $\mathbf{S}_2^{-1}$ term of equation (40) suggests that these unwanted terms may grow large as singular values get small. The error variance of some simplified model predictions may grow very large accordingly.

3. Synthetic Case Study: Description

[87] The theory and concepts developed earlier are now applied to a synthetic 1-D vadose zone example in which a model is to be built and calibrated for the purpose of transient groundwater recharge estimation. A "complex" model was developed, together with two different simplifications of this model. The latter differ in their degree of simplification, with one involving only parameter simplification and the other involving substantial process and structural simplification. These are now described.

3.1. Complex Model

[88] The complex model was constructed using HYDRUS-1D [*Šimůnek et al*., 2009]. HYDRUS-1D simulates variably saturated flow in porous media by solving the 1-D Richards equation:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}K\left(\frac{\partial h}{\partial z} + 1\right) - S, \quad (43)$$

where θ ($\mathrm{m^3m^{-3}}$) is the volumetric water content, t (s) is time, h (m) is the pressure head, z (m) is the vertical coordinate, S ($\mathrm{m^3m^{-3}s^{-1}}$) is the sink term, and K ($\mathrm{m\ s^{-1}}$) is the unsaturated hydraulic conductivity function. The latter is defined using the Mualem-van Genuchten model for unsaturated soil hydraulic properties [*van Genuchten*, 1980], implemented using the following equations:

$$K(S_e) = K_s S_e^l\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2, \quad (44)$$

where

$$S_e(h) = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \begin{cases} [1 + |\alpha h|^n]^{-m} & h < h_s \\ 1 & h \geq h_s \end{cases}, \quad (45)$$

and

$$m = 1 - 1/n. \quad (46)$$

[89] In equations (45) and (46), S_e is the effective water content; θ_r ($\mathrm{m^3m^{-3}}$) and θ_s ($\mathrm{m^3m^{-3}}$) are the residual and saturated water contents respectively; α ($\mathrm{m^{-1}}$) is the inverse of the air-entry pressure head h_s (m); n is a pore-size distribution index; K_s ($\mathrm{m\ s^{-1}}$) is the saturated hydraulic conductivity; and l is a pore-connectivity parameter.

[90] The complex HYDRUS-1D model used in our study simulates water movement within a 10-layer vertical soil column of 500 cm depth. The top of the column is defined by an atmospheric boundary condition. This switches between prescribed head and prescribed flux depending on the pressure head at the soil surface; meanwhile, any excess water on the soil surface is immediately removed as surface runoff. A seepage face condition comprises the lower boundary. Root water uptake is simulated using the *Feddes et al*. [1978] model of water uptake reduction. This model enforces cessation of root water uptake below wilting point and close to saturation, with a linear transition to a constant, optimal uptake between these two extremes. Daily time series of precipitation and potential evapotranspiration over a period of 522 weeks spanning 1 January 1990 to 31 December 1999 serve as inputs to the model. These time series were measured at the World Meteorological Organization (WMO) 06072 weather observation station in Ødum, Denmark. The first 285 weeks of these data were used during the calibration and predictive phases of model deployment. The entirety of this data set was employed during a 522 week model warm-up period (see later). Only transpiration, with no evaporation, is assumed to occur in the simulated soil column.

[91] One thousand stochastic realizations of soil column hydraulic properties were generated based on synthetic expert knowledge encapsulated in prior parameter probability distributions. Two levels of variability were employed in assigning values to different parts of the 1-D model domain. First, for each soil column, random values were generated for θ_s and θ_r based on normal distributions, and for K_s, α and n based on log-normal distributions. The means μ and standard deviations σ_1 of these distributions appear in the first two columns of Table 1. A random set of each parameter type was then generated and assigned to the 10 layers comprising the model domain, each layer being of 50 cm thickness. (Log-)Normal distributions were once again employed, with the mean of each distribution being the previously generated random value for each parameter type; standard deviations σ_2 for these secondary distributions appear in the third column of Table 1. This stochastic parameter generation process was repeated for each of the 1000 realizations. A single value of 100 cm for root depth was employed in all realizations. (Lack of numerical

Table 1. Statistical Parameters Used in Generation of Stochastic Realizations of Soil Hydraulic Properties Employed by the HYDRUS-1D Complex Model[a]

Parameter	μ	σ_1	σ_2
$\log(K_s)$ (cm d^{-1})	2.03	0.5	0.1
θ_s	0.41	0.05	0.01
θ_r	0.065	0.02	0.004
$\log(\alpha)$	−1.12	0.5	0.1
$\log(n)$	0.28	0.1	0.02

[a] μ and σ_1 are the mean and standard deviation, respectively, for the first level of random parameter value generation, while σ_2 represents the standard deviation defining interlayer parameter variability within one particular soil column.

differentiability of model outputs with respect to this parameter precluded its inclusion in the linear analysis documented later.)

[92] For all parameter set realizations, HYDRUS-1D was run in order to generate a calibration data set, as well as three different predictions. Unfortunately, HYDRUS-1D did not converge for 2 of the 1000 parameter set realizations; thus, the nonlinear analysis presented later is based on 998 realizations. In all cases the model was run for a 522 week warm-up period driven by the precipitation and potential evapotranspiration time series described earlier. The calibration data set was assumed to consist of observations of total weekly drainage through the bottom boundary of the column for the next 230 weeks (i.e., weeks 523–752 of the simulation). Predictions were then made over weeks 753–807 of the simulation. The three different predictions considered in this study are (1) the total recharge summed over all of the 55 weeks comprising the prediction period, (2) the maximum recharge occurring during any 4 week interval within the prediction period, and (3) the maximum recharge occurring during any 1 week interval within the prediction period.

[93] For ease of reference, the above model is referred to as "complex HYDRUS" hereafter.

3.2. Simplified Models

[94] As mentioned earlier, two simplified models were employed in conjunction with complex HYDRUS. Both of these were driven by the same precipitation and evapotranspiration time series as complex HYDRUS. In obtaining the first simplified model, herein referred to as "simplified HYDRUS", only parameterization simplification was undertaken; the 10 layer heterogeneous soil column of complex HYDRUS was simply replaced by a column that is homogeneous in all parameters.

[95] A lumped parameter "bucket" recharge model (herein referred to as LUMPREM, i.e., "LUMped Parameter REcharge Model") was employed as the second simplified model. Like the two HYDRUS models, LUMPREM works on a daily time step. Evapotranspirational losses E (m) from the soil moisture store are calculated using the equation:

$$E = f\,E_p \frac{1 - e^{-\gamma v'}}{1 - 2e^{-\gamma} + e^{-\gamma v'}}, \tag{47}$$

where f is a crop factor, E_p (m) is the potential evapotranspiration, γ is a shape parameter, and v' is the relative volume of water in the bucket, i.e., V/V_{max}, where V (m^3) is the current volume of water in the bucket, and V_{max} (m^3) is the total bucket volume.

[96] Water lost as recharge to the groundwater domain (i.e., R (m s^{-1})) is calculated as

$$R = K_s \left[v'\right]^l \left[1 - \left(1 - \left[v'\right]^{1/m}\right)^m\right]^2, \tag{48}$$

where m is a shape parameter. An additional parameter *rdelay* (s) defines the delay between water draining from the soil moisture store and the same water appearing as recharge to the groundwater system.

[97] In conducting the numerical experiments discussed later, LUMPREM was run over the same time periods as were the HYDRUS models (including the 522 week warm-up period) and generated the equivalent calibration and predictive outputs.

3.3. Calibration and Prediction

[98] For each of the 998 realizations of the 50 stochastic parameters comprising the complex HYDRUS parameter set, both the simplified HYDRUS and LUMPREM models were calibrated against the 230 weekly recharge observations comprising the calibration data set as generated by the complex HYDRUS model. Equal weights were assigned to all recharge observations. For each of the simplified HYDRUS and LUMPREM models, five parameters were estimated using this calibration data set. For simplified HYDRUS, these were θ_s, θ_r, and the logs of K_s, α, and n, while for LUMPREM the logs of $V_{\max}$, *rdelay*, K_s, m, and f were estimated. (The logarithms, rather than native values, of most parameters were estimated in order to improve model linearity and also to provide a degree of parameter normalization; this being implicit in the estimation of the logs of parameters.)

[99] Calibration of each of these simplified models against the 230 week recharge data set constitutes a well-posed inverse problem. No random noise was added to the complex HYDRUS outputs in generating each calibration data set; hence failure to achieve a perfect fit during the calibration of each simplified model is an outcome of model simplification alone. Calibration of LUMPREM was effected using PEST [*Doherty*, 2011], while calibration of the simplified HYDRUS model was accomplished using the adaptation of the covariance matrix adaptation evolution strategy (CMA-ES) algorithm of *Hansen and Ostermeier* [2001] and *Hansen et al*. [2003] available through the PEST suite. While use of CMA-ES requires more model runs than that of PEST, it affords better protection against model output numerical granularity and entrapment in local optima.

[100] Estimation of a set of LUMPREM parameters required approximately 20 s on a 3.07 GHz Intel Core i7 CPU. In contrast, calibration of a simplified HYDRUS model required several hours. It is also pertinent to note that attempts were made to calibrate the complex HYDRUS model (using regularized inversion to estimate its 50 adjustable parameters) against complex HYDRUS-generated

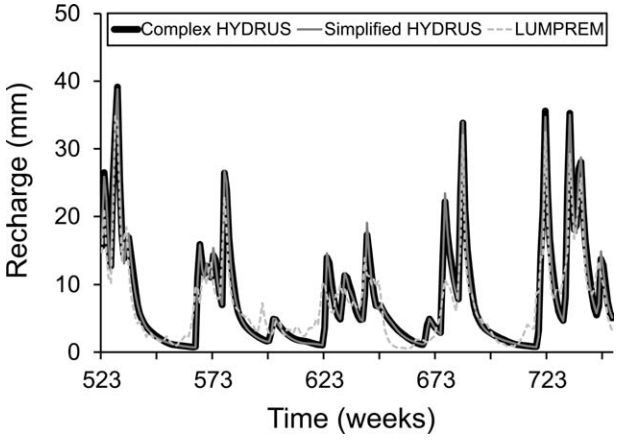

Figure 1. Example of the fits attained through calibration of both the simplified HYDRUS and LUMPREM models against complex HYDRUS weekly recharge outputs.

observation data sets. However, this could not be achieved because HYDRUS numerical instability resulted in frequent model run failures during these attempted calibration processes. This exemplifies the difficulties that are often encountered in calibrating complex models and therefore illustrates the attractiveness of using a relatively simple model in the calibration process.

[101] As stated earlier, the simplified HYDRUS and LUMPREM models were calibrated against all of the 998 data sets generated by the complex HYDRUS model, each calculated using a different stochastic parameter field. The outcomes of these 1996 calibration exercises were 998 simplified HYDRUS and LUMPREM counterparts to the 998 complex HYDRUS model realizations. The same predictions as those that were made with the complex HYDRUS models were then made using each of the calibrated simplified models.

3.4. Calculation of Sensitivities

[102] The linear analysis discussed later employs sensitivities of the 230 weekly recharge model outputs used for calibration purposes and the three outputs used for predictive purposes, to the adjustable parameters of the complex HYDRUS, simplified HYDRUS, and LUMPREM models. Complex HYDRUS and simplified HYDRUS sensitivities were evaluated using finite differences, with all parameters slightly perturbed from their expected values (see Table 1). For LUMPREM, a parameter set obtained through calibration of this model against a data set generated using the expected values of complex HYDRUS model parameters was employed in finite difference sensitivity calculation.

4. Results

[103] Outcomes of all analyses are now presented. They are discussed as they are presented. A more general discussion follows in section 5.

4.1. Quality of Calibration

[104] Figure 1 shows the fits attained between simplified and complex model outputs for one particular realization of the complex HYDRUS parameter set. These are representative of the average fits of both simplified HYDRUS and LUMPREM across the 998 complex HYDRUS realizations. Figure 1 demonstrates that weekly recharge values generated using a complex HYDRUS parameter field can be matched in nearly every detail by an appropriately parameterized simplified HYDRUS model. Given that the latter has only five parameters and that the former employs 50 parameters, if an attempt were made to calibrate a complex HYDRUS model against a calibration data set of this type, the dimensionality of the null space would be about 45, indicating nonidentifiability of about 45 combinations of parameters on the basis of this data set.

[105] Like the simplified HYDRUS model, the LUMPREM model also employs five parameters. However, while adjustment of these five parameters allows a reasonable fit to be obtained between its outputs and those of the complex HYDRUS model, the fit is far from perfect. This indicates that its parameters do not span the full solution space of the complex HYDRUS model when calibration is undertaken against this particular data set. Nevertheless, as is evident from Figure 1, the salient features of the recharge time series are generally reproduced. Such a fit may be considered acceptable in many real-world modeling contexts where measurement noise would contribute significantly to misfit.

4.2. Quality of Predictions

[106] As discussed earlier, predictions of three types were made on the basis of each complex HYDRUS parameter set realization, and then using the two calibrated simplified model counterparts to each such realization. The predictive abilities of the latter were assessed using s versus $\underline{s}$ scatterplots as described in section 2.3.3. These plots for the three predictions are shown in Figure 2. Note that, to enhance the linearity of these scatterplots, the logs of each predicted recharge quantity are employed in lieu of their native values. Regression lines through the scatterplots are calculated as

$$s = a + b\underline{s}, \tag{49}$$

where a and b are the regression intercept and slope, respectively. Ninety-five percent prediction intervals are also displayed in Figure 2 (see, for example, *Draper and Smith* [1998, equation (1.4.12)] for details of prediction interval calculations). Table 2 lists regression parameters and statistics for the s versus $\underline{s}$ scatterplots of Figure 2.

[107] Equations describing the relationship between predictions made by a complex model and those made by a simplified model calibrated against a data set generated by the former are derived in *Doherty and Christensen* [2011]. These equations show that where a simplified model fits the calibration data set well, vertical scatter of complex model predictions about the line of best fit appearing in plots such as those shown in Figure 2 records the null space contribution to predictive uncertainty. Horizontal scatter of simplified model predictions about this same line represents the contribution of measurement noise to predictive uncertainty. A regression line slope of less than unity indicates predictive bias incurred by calibration-induced null space entrainment. Where a simplified model provides a less-than-perfect fit to complex model outputs, vertical scatter is

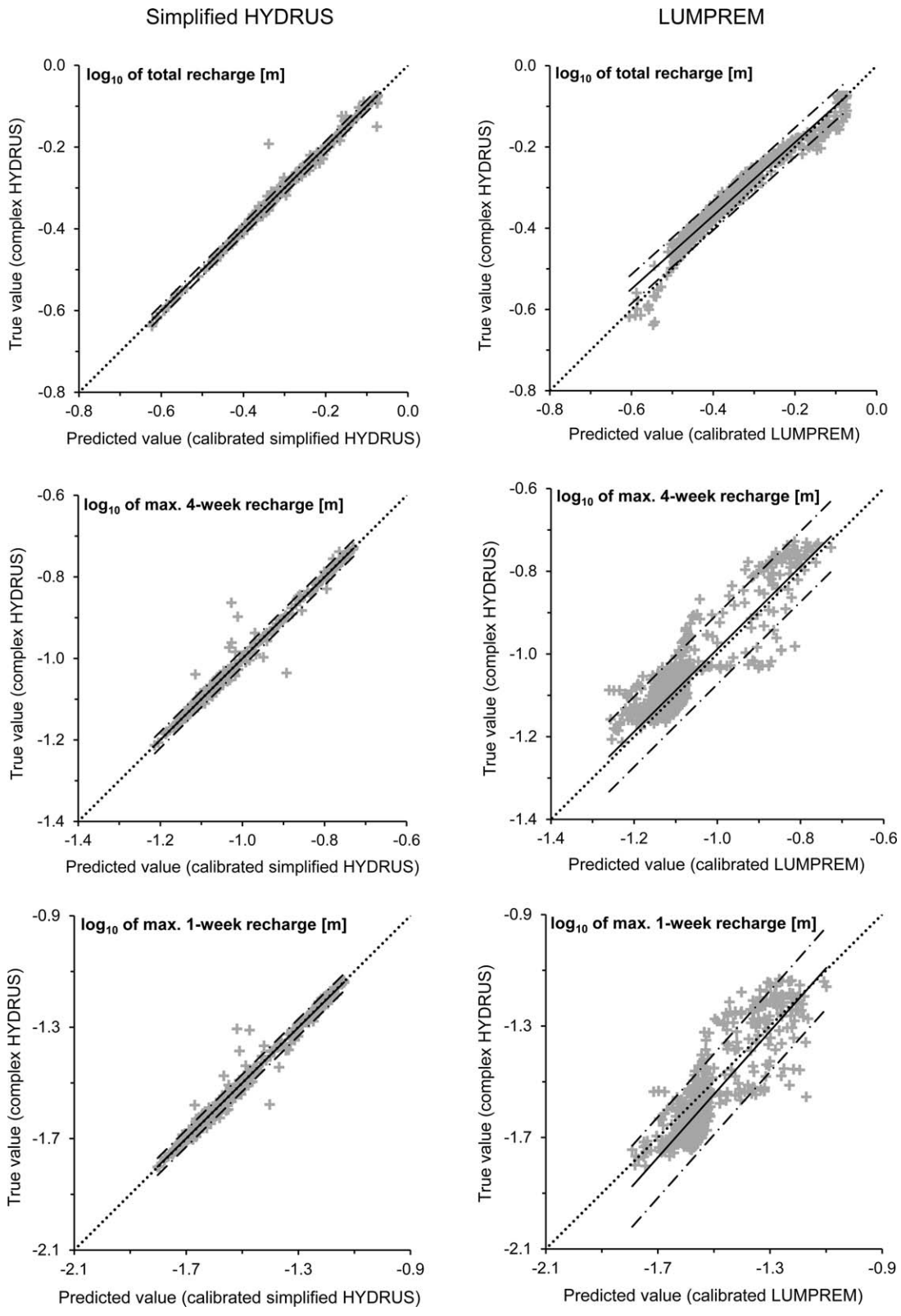

Figure 2. s versus $\underline{s}$ scatterplots for (left) simplified HYDRUS and for (right) LUMPREM. The dotted line is the 1:1 line.

increased through an artificially expanded null space, while horizontal scatter is increased because of the addition of structural noise to any measurement noise present in the calibration data set. The extra null space dimensions comprise the solution space components that are missing from the simplified model.

Table 2. Regression Coefficients and Statistics Pertaining to the s Versus $\underline{s}$ Scatterplots Depicted in Figure 2[a]

	Simplified HYDRUS				LUMPREM			
Prediction	a	b	r^2	σ	a	b	r^2	σ
Total recharge	0.001	1.003	0.995	0.007	−0.008	0.902	0.967	0.018
Maximum 4-week recharge	−0.002	0.998	0.989	0.010	0.010	0.998	0.793	0.043
Maximum 1-week recharge	−0.009	0.994	0.988	0.016	0.152	1.131	0.724	0.074

[a] a and b are the regression coefficients of equation (49), r^2 is the coefficient of determination, and σ is the standard deviation.

[108] The following features of the scatterplots of Figure 2 are salient.

[109] 1. The limited vertical scatter in the simplified HYDRUS plots indicates limited null space contribution to the predictions which are the subject of the current study.

[110] 2. The slopes of the s versus $\underline{s}$ lines of best fit for all simplified HYDRUS predictions are very close to unity. This is also a reflection of the predominant solution space dependency of the predictions considered in this study. (As will be shown later, it does not indicate the absence of null space parameter entrainment. However, such entrainment is invisible in these plots as the predictions of interest are not sensitive to entrained parameters.)

[111] 3. The failure of LUMPREM parameters to span the full solution space of the complex HYDRUS model (highlighted by the less-than-perfect fit of LUMPREM to complex HYDRUS outputs demonstrated in Figure 1) results in an expanded null space and considerable scatter about the s versus $\underline{s}$ lines of best fit. This scatter is fairly mild for the long-term recharge prediction but much more pronounced for the short-term recharge predictions.

[112] 4. The predictive performance of LUMPREM varies with prediction values, this being expressed through variability of scatter about the s versus $\underline{s}$ line of best fit. This suggests that LUMPREM's performance as a recharge predictor is parameter dependent.

[113] If the complex model is made to include more hydraulic processes, while the complexities of its simplified counterparts are maintained at their present levels, the propensity for bias in simplified model predictions is likely to increase. This results from the need for simplified model parameters to adopt surrogate roles in fitting data sets generated on the basis of more complex processes than they are capable of simulating. This was tested by repeating the above analyses with variability of root depth included in the complex HYDRUS realizations. (As stated earlier, root depth was fixed at 100 cm in the preceding analyses.) Root depth was varied randomly between realizations using a normal distribution with a mean value of 100 cm and a standard deviation of 25.5 cm. The s versus $\underline{s}$ regression outcomes for these analyses are provided in Table 3. The s versus $\underline{s}$ scatterplots are not shown for the sake of brevity.

[114] It was found that the ability of simplified HYDRUS to fit the calibration data set is only marginally degraded with the addition of root depth variability to complex HYDRUS parameter realizations. At the same time, the level of scatter in the corresponding s versus $\underline{s}$ plots increases (compare Tables 2 and 3). Similar considerations apply to LUMPREM.

[115] Comparison of Tables 2 and 3 demonstrates that the enhanced complexity of the complex model increases the propensity for bias in all predictions made by both simplified models. For simplified HYDRUS, the slopes b of the s versus $\underline{s}$ regression lines fall below unity. From this it can be inferred that the simplified HYDRUS parameter space is misaligned with the solution space of the complex HYDRUS model. Calibration of simplified HYDRUS against a data set generated by the process-enhanced complex HYDRUS therefore induces null space parameter entrainment and the concomitant need for some estimated parameters to adopt compensatory roles to a greater extent. Because the predictions of interest are somewhat sensitive to null space parameter components (predominantly plant root depth) they thus inherit this bias.

[116] The increase in the s versus $\underline{s}$ slopes for the LUMPREM maximum 4-week and 1-week recharge predictions indicates that LUMPREM does not possess the parameter and process sophistication that would enable some of its parameters to adopt surrogate roles when undergoing calibration against the process-enhanced HYDRUS model. Furthermore, complex HYDRUS null space parameter components that reflect root depth variability are effectively hard-wired at erroneous values in the LUMPREM model. Thus, it cannot replicate the increased predictive variability that variability of plant root depth promulgates; an s versus $\underline{s}$ slope of greater than unity is the inevitable result.

[117] We now turn to linear analysis. Due to lack of differentiability of HYDRUS-1D model outputs with respect to root depth variability, the latter remains fixed at 100 cm for all subsequent analyses.

Table 3. Regression Coefficients and Statistics Pertaining to s Versus $\underline{s}$ Scatterplots Equivalent to Figure 2 but With Variable Root Depth in Complex HYDRUS Realizations

	Simplified HYDRUS				LUMPREM			
Prediction	a	b	r^2	σ	a	b	r^2	σ
Total recharge	0.003	0.957	0.978	0.015	0.007	0.861	0.956	0.021
Maximum 4-week recharge	−0.024	0.967	0.960	0.019	0.15	1.10	0.74	0.048
Maximum 1-week recharge	−0.057	0.953	0.959	0.029	0.406	1.267	0.622	0.086

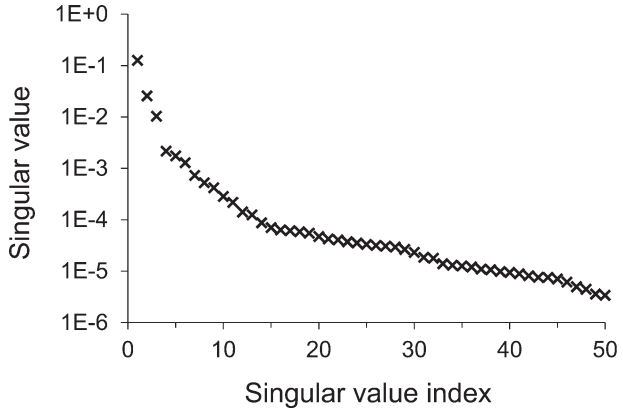

Figure 3. Singular values calculated for the complex HYDRUS **Y** matrix.

4.3. Optimal Simplification

[118] It was proposed in section 2 that model simplification can be considered optimal when it is undertaken using SVD following transformation of reality model parameters to a parameter space where equation (10a) holds. In this section we demonstrate such simplification as applied to the complex HYDRUS model.

[119] Ranked singular values calculated for the **Y** matrix of equation (16) are plotted in Figure 3. All 50 singular values are nonzero, this indicating a 0-D null space for a calibration data set comprising the 230 weekly recharge values discussed earlier. However, singular values beyond approximately the fifth are very small, this implying that adjustment of only five parameter combinations (at most) is required for attainment of a very good fit with the calibration data set. This notion is supported by the fact that the simplified HYDRUS model, with only five parameters, is capable of fitting complex HYDRUS calibration outputs very well, as Figure 1 demonstrates.

[120] In practice, a field calibration data set would be contaminated by measurement noise. As discussed earlier, this would limit the number of singular values employed in the calibration process. Equation (11) can be used to determine the number of singular values at which predictive error variance is minimized in the presence of measurement noise, and to quantify this variance. This is achieved by plotting a curve such as that shown in Figure 4a, which pertains to the log maximum 1 week recharge prediction. In order to construct Figure 4a a measurement noise standard deviation of 1.5 mm, with no temporal correlation between measurements, was assumed. Similar curves emerge for the other predictions considered in this study. The vertical scale of Figure 4a is truncated to clearly show the minimum of the curve and the contributions to total predictive error variance made individually by the first (null space) and second (solution space) terms of equation (11). Note that the total predictive error variance for zero singular values is 5.21E−3, this corresponding to the prior uncertainty variance of this prediction. Figure 4b reproduces the total error variance curve of Figure 4a for a further four hypothetical magnitudes of measurement noise standard deviation.

[121] It is apparent from Figure 4 that the minimum of the predictive error variance curve occurs between three and six singular values; it is also apparent that this does not vary greatly over a range of realistic values of measurement noise standard deviation. The curve is essentially flat in this area. Hence, with these amounts of measurement noise, a properly designed simplified model need possess as few as three adjustable parameters to attain an acceptable fit with the calibration data set. The dominant contribution to the uncertainty of this particular prediction is made by the solution space term. The small contribution to predictive error variance made by null space parameter components is supported by the small degree of scatter in Figure 2 *s* versus $\underline{s}$ plots pertaining to simplified HYDRUS.

[122] The right column of Figure 5 depicts the estimable combinations of parameters that emerge from optimal simplification (i.e., from SVD of the matrix representing the model after parameters have been appropriately transformed). Denoted as $\mathbf{v}_{1y}$ through $\mathbf{v}_{5y}$, these are the first five columns of the matrix $\mathbf{FE}^{1/2}\mathbf{V}_y$. $\mathbf{V}_y$ is equivalent to **V** of equation (4) but arises from SVD of **Y** instead of **Z**. $\mathbf{V}_y$ is premultiplied by $\mathbf{FE}^{1/2}$ (see equation (13b)) so that these estimable combinations of parameters can be presented in **k**-space (and thus in terms of recognizable complex HYDRUS parameters) rather than **m**-space. The left column of Figure 5 depicts combinations of observations that are uniquely and directly informative of these parameter combinations. These are the columns of $\mathbf{U}_y$ which are

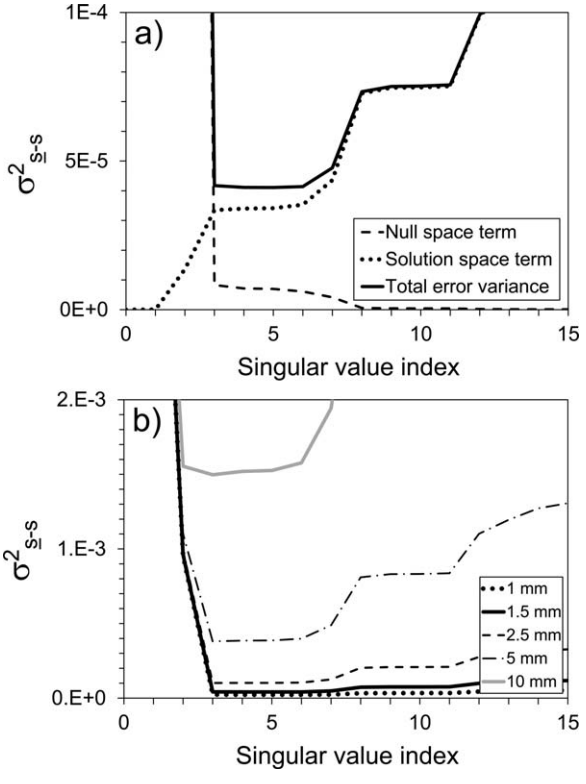

Figure 4. (a) Predictive error variance, including contributions from solution space and null space terms, versus number of singular values for the log maximum 1 week recharge prediction; measurement noise standard deviation is 1.5 mm. (b) Total predictive error variance curve reproduced for four additional measurement noise standard deviations.

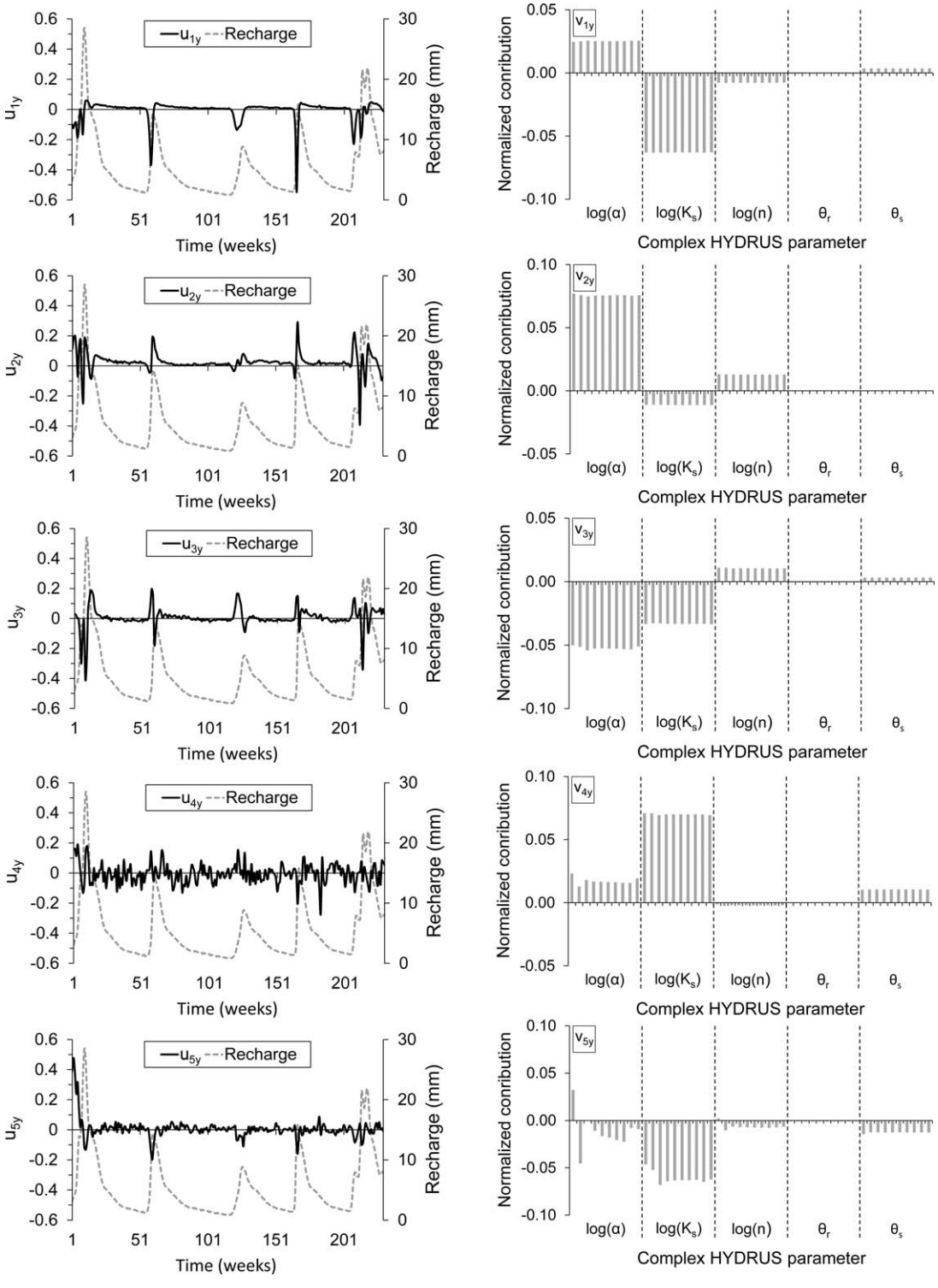

Figure 5. (right) Estimable combinations of parameters emerging from optimal simplification of complex HYDRUS (i.e., columns of the $\mathbf{V}_y$ matrix ($\mathbf{v}_{1y}$ through $\mathbf{v}_{5y}$) calculated through SVD of the $\mathbf{Y}$ matrix of equation (16), after transformation to complex HYDRUS model parameter space. (left) Corresponding combinations of calibration observations comprising the first five columns of the $\mathbf{U}_y$ matrix ($\mathbf{u}_{1y}$ through $\mathbf{u}_{5y}$). The 10 columns for each complex HYDRUS parameter type represent the different model layers (increasing with depth from left to right).

partnered to the columns of $\mathbf{V}_y$ (see equations (7a) and (7b) together with text following that equation for further details). The elements of these columns of $\mathbf{U}_y$ (with columns being denoted as $\mathbf{u}_{1y}$ through $\mathbf{u}_{5y}$) are plotted against time as the recharge observations to which they pertain (also shown in this plot) are time dependent.

[123] Salient features of Figure 5 are as follows:

[124] 1. The most estimable parameter combination (i.e., the parameter combination corresponding to the largest singular value) is dominated by the ratio of $\log(\alpha)$ to $\log(K_s)$. The information which furnishes this estimate resides in peak recharges and in the recharge decays which follow them.

[125] 2. Information within the calibration data set appears to be much more informative of α, K_s, and n than it is of volumetric parameters. The former parameters affect the timing and sharpness of recharge events. Attempts at model simplification in this context should therefore result in a model that exposes these controls to adjustment.

[126] 3. No one parameter type dominates any parameter eigencomponent (i.e., column of $\mathbf{V}_y$), with the possible exception of $\mathbf{v}_{2y}$ which features the α parameter prominently. The information on α appears to reside in the steepness of recharge peaks.

[127] 4. As the singular value number increases, the amount of detail represented in $\mathbf{u}_{iy}$ increases. Such detail is of high-frequency content and may be difficult to distinguish from measurement noise in a real-world situation. The information contained in these combinations of observations is therefore easily lost; the parameter combinations which they inform are therefore likely to be uncertain.

4.4. Simplified Model Parameter Composition

4.4.1. Complex Model Parameter Contributions

[128] Equation (22) can be used to characterize the composition of each simplified model parameter in terms of complex model parameters, thereby elucidating the parameter decomposition implied by model simplification. Figure 6 shows the composition of each simplified HYDRUS and LUMPREM parameter in terms of complex HYDRUS parameters as calculated using equation (22). Recall that simplified HYDRUS is generally able to achieve a near-perfect fit with calibration data generated by complex HYDRUS (see Figure 1) through adjustment of its five parameters. Because these parameters have the compositions illustrated in Figure 6, it follows that it is possible to replicate this particular calibration data set by mainly adjusting volumetric and drainage response parameters that pertain to only a small part (namely, the shallowest layers) of the subsurface, rather than drainage response parameters pertaining to the whole model domain.

[129] The parameter compositions depicted in Figure 6 differ markedly from the compositions of optimal parameter components presented in Figure 5. Thus, both simplified HYDRUS and LUMPREM constitute substantially suboptimal simplifications of the complex HYDRUS model. It follows that unless these models are used to make predictions which are predominantly solution space dependent (which are normally predictions that are very similar in character to those comprising the calibration data set), predictions made by either of these models may be subject to a high degree of calibration-induced bias. It has been demonstrated that the predictions required of these models in the present case do, in fact, have a high solution space dependency and therefore are not as prone to bias as other predictions made by these models may be. In this sense, despite their suboptimal simplification, the simplified HYDRUS and LUMPREM models are "fit for purpose."

[130] It is pertinent to examine the extent to which the compositions of simplified model parameters are consistent with the complex model parameters that they purport to represent. Ideally, from a parameter estimation perspective, parameter values achieved through calibration of the simplified HYDRUS model should equate to averages over the entire soil column of their complex model counterparts. Equation (24a) demonstrates that to the extent to which they can be considered to be estimates of averaged layer properties, these estimates are in error. Figure 6 reveals part of the reason for this error. At best, a given simplified HYDRUS parameter has a dominant contribution from the same complex HYDRUS parameter type over only a part of the overall soil column. At worst it almost entirely represents parameters other than that after which it is named. For example, complex HYDRUS parameters α and K_s are essentially absent from the compositions of simplified HYDRUS parameters of the same name.

[131] The situation is a little better for the LUMPREM model. The LUMPREM V_{max} parameter does indeed appear to chiefly reflect complex HYDRUS θ_s-θ_r for the whole soil column. Nonetheless, similar to simplified HYDRUS, shallow complex HYDRUS parameters are generally better represented in LUMPREM parameters than are those associated with deeper parts of the soil column.

4.4.2. Simplified Model Parameter Variability

[132] Equation (23) allows calculation of the propensity for variability of simplified model parameters from that of complex model parameters. Presumably, the latter are forthcoming from the expert knowledge of the modeler. In practice, expert knowledge may be supplied to the calibration process as a covariance matrix associated with prior information on model parameter values. It can also be used in the setting of parameter bounds in order to limit parameter variability to a level that is considered realistic as parameters are adjusted during the calibration process. In the present synthetic case the covariance matrix of "reality" is known (i.e., the covariance matrix $\mathbf{C}(\mathbf{k})$ describing the parameter variability that was employed in generating the random complex HYDRUS parameter sets discussed in section 3.1). The $\mathbf{C}(\mathbf{p})$ matrix computed through equation (23), on the other hand, is the expression of "expert knowledge" as it pertains to a simplified model. It is thus the covariance matrix that must be associated with the precalibration probability distribution of simplified model parameters. Failure to use this matrix (in particular, if a matrix that expresses a smaller degree of parameter variability is used in its place) may restrict the ability of the calibration process to assign values to simplified model parameters that allow that model to fit any data set generated by the complex model that is feasible based on the precalibration probability distributions of complex model parameters (i.e., true expert knowledge).

[133] Tables 4 and 5 provide the $\mathbf{C}(\mathbf{p})$ matrix for simplified HYDRUS and LUMPREM parameters calculated using equation (23).

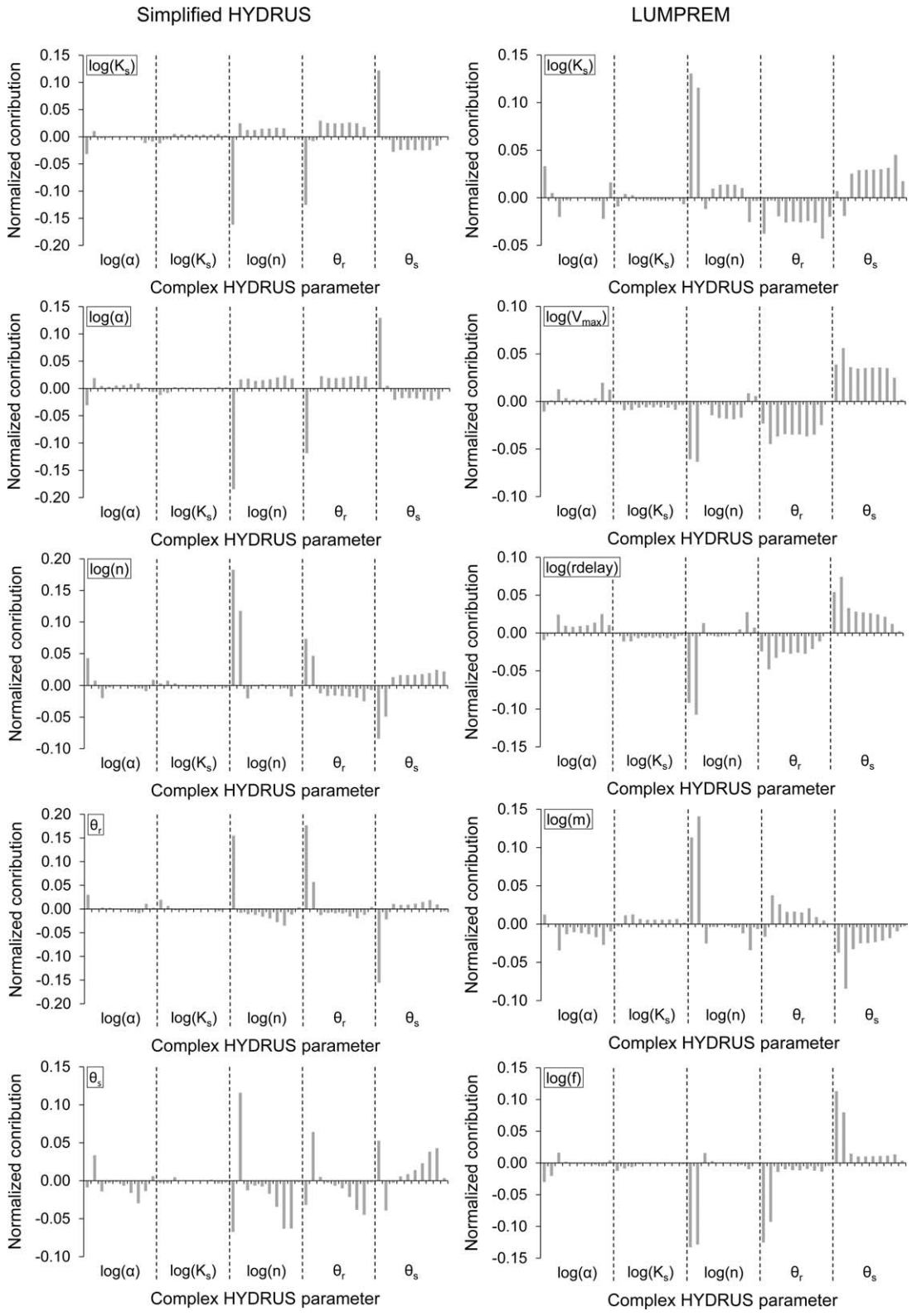

Figure 6. Normalized composition of (left) each simplified HYDRUS and (right) each LUMPREM parameter in terms of complex HYDRUS parameters (i.e., each row vector, normalized by its total length, comprising the matrix **L** of equation (22)). The 10 columns for each complex HYDRUS parameter type represent the different model layers (increasing with depth from left to right).

Table 4. Prior Covariance Matrix of Simplified HYDRUS Parameters Calculated Using Equation (23)

	$\log(\alpha)$	$\log(K_s)$	$\log(n)$	θ_r	θ_s
$\log(\alpha)$	0.0326	−0.1062	−0.0026	0.0065	−0.0044
$\log(K_s)$	−0.1062	1.0056	−0.0609	−0.0536	0.0426
$\log(n)$	−0.0026	−0.0609	0.0130	0.0036	−0.0044
θ_r	0.0065	−0.0536	0.0036	0.0055	−0.0034
θ_s	−0.0044	0.0426	−0.0044	−0.0034	0.0030

[134] The size of the off-diagonal terms of both of these matrices indicates a high degree of correlation between parameters. Such interparameter statistical correlation does not exist for complex HYDRUS parameters. The square root of each diagonal element of the prior covariance matrix is the prior standard deviation of the corresponding parameter (or its log, as indicated). In the case of simplified HYDRUS, prior parameter standard deviations can be directly compared with the true standard deviations of their complex HYDRUS counterparts. Figure 7 shows the ratios of simplified HYDRUS parameter standard deviations to corresponding complex HYDRUS parameter standard deviations. It is apparent that the prior standard deviations of some simplified HYDRUS parameters are significantly inflated compared to their complex HYDRUS counterparts. This suggests that the role that true (real-world) expert knowledge can play in parameterization of a simplified model is, at best, unclear. Consider, for example, the question of what bounds a modeler should place on simplified model parameters during the calibration process, and/or what prior probability distribution he/she should award to these parameters in establishing posterior predictive probability distributions through Bayesian analysis.

4.5. Back Transformation to Complex Model Parameter Space

[135] Equations (39) and (40) allow us to explore the hypothetical propensity for error in a complex model incurred by its notional calibration through use of a surrogate simplified model. (Note that because equation (10a) does not automatically hold for complex HYDRUS, this analysis required the replacement of **Z** in equations (39) and (40) with **Y** of equation (16), and the replacement of **S**, **U**, and **V** with $\mathbf{S}_y$, $\mathbf{U}_y$, and $\mathbf{V}_y$, respectively.) Ideally, $\mathbf{C}(\underline{\boldsymbol{\beta}} - \boldsymbol{\beta})$ of equation (39) should be **0**, indicating perfect de facto estimation of complex model solution space parameter components through simplified model calibration. $\mathbf{C}(\underline{\boldsymbol{\beta}}_n)$ of equation (40) should also be **0**, indicating the absence of complex model parameter null space entrainment incurred through simplified model calibration. Figure 8 shows the square root of the first five diagonal elements of $\mathbf{C}(\underline{\boldsymbol{\beta}} - \boldsymbol{\beta})$ for both simplified HYDRUS and LUMPREM. It thus shows the standard error of estimation of each of the elements of $\boldsymbol{\beta}$ that define the values of solution space parameter projections of the complex HYDRUS model. (Note that both $\mathbf{C}(\underline{\boldsymbol{\beta}} - \boldsymbol{\beta})$ and $\mathbf{C}(\underline{\boldsymbol{\beta}}_n)$ are effectively normalized as $\mathbf{C}(\boldsymbol{\beta})$ is equal to $\mathbf{I}$. This follows from equation (37) with $\mathbf{m}$ in place of $\mathbf{k}$, and the orthonormality of $\mathbf{V}_1$.)

Table 5. Prior Covariance Matrix of LUMPREM Parameters Calculated Using Equation (23)

	log (V_{max})	log (*rdelay*)	$\log(K_s)$	$\log(m)$	$\log(f)$
$\log(V_{max})$	0.2913	0.0082	0.0019	−0.0316	0.0158
$\log(rdelay)$	0.0082	0.0003	0.0001	−0.0011	0.0001
$\log(K_s)$	0.0019	0.0001	0.0071	−0.0003	−0.0016
$\log(m)$	−0.0316	−0.0011	−0.0003	0.0045	0.0001
$\log(f)$	0.0158	0.0001	−0.0016	0.0001	0.0042

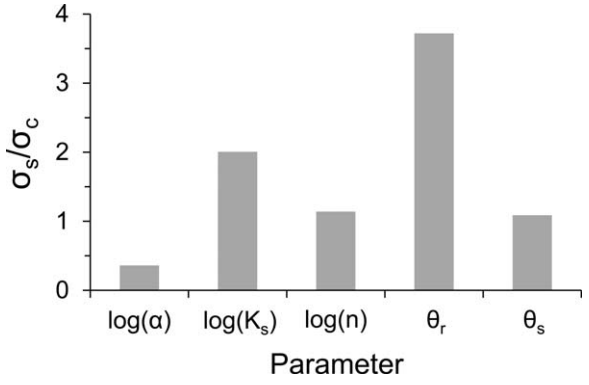

Figure 7. Ratio of each simplified HYDRUS model parameter standard deviation (σ_s) to corresponding complex HYDRUS model parameter standard deviation (σ_c).

[136] It is apparent from Figure 8 that implicit estimation of complex HYDRUS model parameter solution space components is better achieved through the parameter transformation and decomposition implied by the use of simplified HYDRUS than through that implied by the use of LUMPREM. This is hardly surprising given the fact that calibration of simplified HYDRUS leads to a better fit with a calibration data set generated by the complex HYDRUS model than does calibration of LUMPREM. What is surprising, however, is the rapidity with which these errors rise after the third singular value. This suggests (as does Figure 4) that a properly constructed model that uses as few as three parameters would be just as suitable for replicating a recharge time series as a model with five parameters, especially where the necessity for a good fit is relaxed through the presence of measurement noise in the calibration data set.

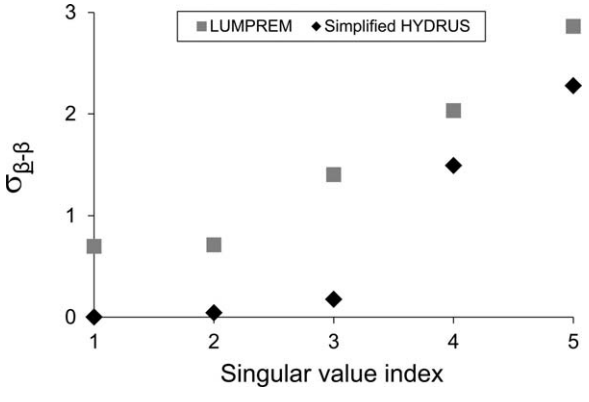

Figure 8. Standard deviations of error, incurred by simplification, in estimation of projections of optimal complex HYDRUS model parameters onto parameter solution space axes.

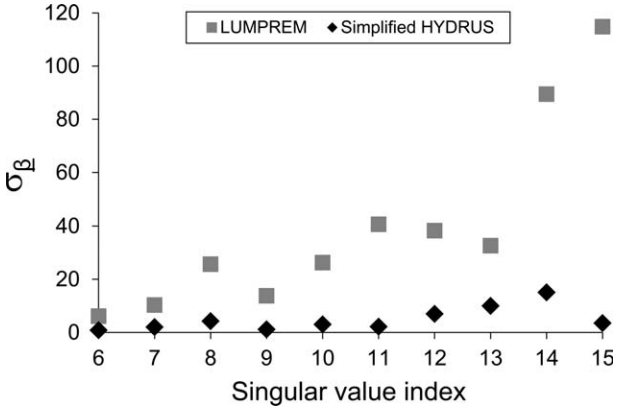

Figure 9. Standard deviations of error, incurred by simplification, in estimation of projections of optimal complex HYDRUS parameters onto parameter null space axes.

[137] Figure 9 shows the square root of the diagonal elements of $\mathbf{C}(\underline{\boldsymbol{\beta}}_n)$ for singular value indices of 6–15 (i.e., the first 10 components of the complex HYDRUS null space). Ideally, parameter transformation and decomposition implied in the calibration of the simplified HYDRUS and LUMPREM models should bestow values of zero on complex model parameter components that correspond to singular values beyond the fifth. Failure to achieve this implies entrainment of complex HYDRUS null space parameter components through calibration of a replacement simplified model. Figure 9 indicates that the risk of calibration-induced parameter bias is relatively high for both the LUMPREM and simplified HYDRUS models. As previously discussed, the degree to which this promulgates predictive bias is prediction specific, for it expresses itself only to the extent that a prediction is sensitive to entrained null space parameter components.

4.6. Linearity Assumption

[138] As is explained earlier in this paper, although an assumption of model linearity underpins the theoretical and experimental work documented herein, conclusions pertaining to optimality of simplification, and to the repercussions of calibrating a suboptimally simplified model, are not affected by this assumption. This is because the phenomena exposed by our analyses are not related to the linearity (or otherwise) of a model. However, these phenomena are more easily exposed and described where local linearity is assumed. Nevertheless, in order to demonstrate the validity of the outcomes of the preceding analysis, we undertook a number of additional numerical experiments in order to assess the extent to which these outcomes are affected by nonlinearity of the models that we employed. Details are as follows; figures are not presented in the interests of brevity.

[139] 1. Figure 7 was replotted based on the statistics inferred from actual parameter values estimated through the calibration of simplified HYDRUS against complex HYDRUS outputs (see section 3.3). The heights of the bars pertaining to different parameters are comparable. Relativity of these heights is preserved.

[140] 2. Figures 5 and 6 were replotted following calculations based on the **Z** matrices computed using a number of different realizations of complex HYDRUS parameters. The plots differ only in minor details.

[141] 3. Equation (22) was used to calculate a simplified HYDRUS parameter set **p** from each of the 998 stochastic realizations of complex HYDRUS parameter sets **k**. Calibration objective functions computed on the basis of these parameter sets were all acceptably low, demonstrating their ability to fit corresponding complex HYDRUS-generated calibration data sets.

[142] 4. Figure 8 was replotted using sensitivities pertaining to a number of different complex HYDRUS parameter realizations together with those pertaining to corresponding best fit simplified model parameters. The points corresponding to the fourth and fifth singular value indices showed some variability between realizations, particularly for the simplified HYDRUS model. However, relativity of these values was preserved.

[143] 5. The above analysis was also undertaken for Figure 9, with similar outcomes.

5. Discussion

[144] The present study advances the theory and concepts that were introduced in a previous work (namely, *Doherty and Christensen* [2011]) and applies them to a different kind of model from that which was investigated in that work. The theoretical work of *Doherty and Christensen* [2011] explores both optimality of simplification and the consequences of suboptimal simplification in contexts wherein a model must be calibrated before being employed in a predictive capacity. The present study employs linear analysis to demonstrate and explore these concepts as they apply to a vadose zone model constructed for the purpose of providing time-varying recharge to a groundwater model. The intention of this paper is therefore twofold: (1) to extend the theoretical basis of model simplification from a subspace perspective, thus providing a foundation for further theoretical and numerical research into the confounding but pervasive issue of model simplification; and (2) to contribute to current understanding of the parameter and associated predictive outcomes of typical simplification practice, through the application of this theory, together with other analyses, to some representative synthetic examples.

[145] Model simplification can be considered optimal when calibration of a thus simplified model allows implicit estimation of reality model solution space parameter components without concomitant assignment of nonzero values to reality model null space parameter components. Or, to put it another way, simplification is optimal when calibration of a simplified model leads to the same predictive outcomes that would be achieved if the reality model itself were calibrated using truncated SVD in estimation of parameters that have been transformed in accordance with their prior variability. All predictions made by a reality model calibrated in this way would possess minimal bias.

[146] Calibration of a suboptimally simplified model awards nonzero values to at least some reality model null space components; in doing this it implicitly alters at least some reality model parameter values that are not supported by the data. However, if calibration of the simplified model achieves a good fit with field data, reality model solution

space components are nevertheless implicitly well estimated. Hence, predictions made by the calibrated simplified model that are solely dependent on reality model solution space parameter components will be made with as much accuracy as if the reality model itself were calibrated and then used to make these same predictions. In fact, if there was no measurement noise associated with the calibration data set, such predictions would be made without error by the simplified model. If a simplified model has been built and calibrated to make only these kinds of predictions, then suboptimality of simplification matters little, for the model that is entirely fit for purpose. (This is not expected to be a common phenomenon, however. Models are usually built to make predictions of system behavior under conditions that are at least partially different from those that prevailed during its calibration. These predictions are therefore likely to be sensitive to at least some parameters, or combinations of parameters, that are not informed by the calibration data set, and hence belong to the null space.)

[147] In carefully considering the processes simulated by a model, model simplification strategies often attempt to separate those processes that are either salient to a prediction or informed by a calibration data set, from those processes which are not. The former are then represented in a form whereby, through averaging or appropriate definition of lumped process elements, inestimable parameters and/or parameter relationships (these often pertaining to system detail) are eliminated from the model. Such physically based simplification implicitly attempts to follow the precepts of optimal simplification outlined herein, in that it attempts to separate system components which can be informed by the measurement data set from those which cannot be thus informed. Such separation takes place under an implied assumption that the two components are indeed separable and hence are orthogonal from a parameter estimation point of view. Rarely will such separation be completely orthogonal however, as is suggested by the examples analyzed in the present study. Hence, while careful physically based simplification can attain much in terms of the metrics presented herein, it is unlikely that the possibility of calibration-induced bias for at least some predictions will be completely eliminated.

[148] Through linear analysis of a complex vadose zone model, together with two simplifications of this model, we have attempted to illustrate the consequences of suboptimal simplification by demonstrating the implicit and unavoidable transformation of reality model parameters that occurs when a simplified model is calibrated in its place. We have shown that despite this transformation, if a simplified model can fit the calibration data set well, the legitimacy of estimation of the projection of reality model parameters onto the calibration solution space is maintained. In contrast, where simplification is such as to compromise the ability of a simplified model to fit the calibration data set well, implicit estimates of reality model solution space parameter projections are demonstrably in error.

[149] The unintended adjustment of reality model null space parameter components from their preferred values of zero through calibration of a substitute simplified model has also been demonstrated. Should a prediction required by a simplified model be sensitive to these aspects of reality, the simplified model would incur significant error in making that prediction as a consequence of this.

[150] The present study has demonstrated that even comparatively mild simplification, in the present case applied through replacing hydraulic property heterogeneity with hydraulic property homogeneity, can lead to significant entrainment of reality model null space parameter components. At the same time, the homogeneous parameters that are estimated through calibration of the simplified model have a complicated relationship with the parameters of the reality model that they replace. As estimates of the average values of equivalent reality model parameters they are thus significantly in error. Though beyond the scope of the present paper, this has repercussions for interpretation of experimental data gathered at field sites (such as lysimeter sites) where experiments are designed explicitly to allow estimation, through calibration, of "field-scale" hydraulic properties. It also has repercussions for the role of expert knowledge in calibrating a simplified model. The variability of most simplified HYDRUS parameters required to reproduce complex HYDRUS data is greater than the true variability of the complex HYDRUS reality model parameters that they purport to represent. Thus, if expert knowledge is applied in defining parameter bounds employed in calibrating a simplified HYDRUS model, its application would compromise the ability of this model to fit the calibration data set. This would, in turn, compromise the ability of the calibration process to implicitly estimate reality model solution space parameter components and would therefore degrade the accuracy of simplified model predictions which depend solely on these parameter components. On the other hand, it would lessen the degree of null space entrainment, through reducing the degree of parameter surrogacy that is allowed to occur during calibration; in doing so it would reduce the propensity for error in predictions which are sensitive to such entrained components.

[151] It appears, therefore, that an important outcome of suboptimal simplification is the creation of a tension between expert knowledge on the one hand and information contained in a calibration data set on the other hand. This tension extends beyond the often-encountered situation whereby expert knowledge and historical measurements of system state may suggest different values for certain parameters. This tension is more fundamental, in that it reflects an inability on the part of a model to adequately respond to information originating from both of these sources simultaneously, for response to one of these sources compromises its ability to respond to the other. It follows that the goodness of fit sought between simplified model outputs and historical measurements of system state should be prediction specific. Where a prediction required of a model is entirely solution space dependent (i.e., is entirely informed by past system behavior), a modeler is entitled to fit historical data to a level that is commensurate with measurement noise. On the other hand, where a prediction depends on null space parameter components that are subject to entrainment through the simplified model calibration process, a modeler should seek a reduced level of fit between model outputs and field measurements in calibrating the model, thus allowing expert knowledge to hold greater sway in the model parameterization process. Unfortunately however, a modeler cannot know the extent

to which he/she should "fail to fit" field data to accommodate this imperative and minimize potential predictive error. If simplification were optimal in the way defined earlier, this would not be an issue, for application of expert knowledge (soft data) would not compromise assimilation of hard data. The tension (bordering on incompatibility) between the two kinds of information required for the reduction of predictive error is an outcome of the fact that less-than-optimal model simplification provides receptacles that cannot hold both types of information simultaneously.

6. Conclusions

[152] All models are simplifications of reality. Some are made very simple by design. Others are specifically designed to include as much real-world complexity as possible but are nevertheless simple when compared with reality. Most models employed for environmental management are calibrated against historical behavior of the system which they simulate. This serves a number of purposes. One of these is to verify that the model can indeed replicate the behavior of that system. Another is to extract information from the historical record that informs parameters and thereby reduces the propensity for error associated with predictions of future system behavior made by the model.

[153] Simplification comes at a cost. Informed model-based decision making requires that this cost be understood and accommodated. In this paper we have cast model simplification as a form of parameter transformation and decomposition. This has allowed us to define optimal simplification as a standard against which other forms of simplification can be judged. Simplification is considered to be optimal when its outcomes are identical to those that would have been achieved through transformation of real-world parameters in accordance with the nature of their variability, followed by orthogonal decomposition of these transformed parameters into solution and null subspaces defined on the basis of the available calibration data set.

[154] If a simplified model can reproduce a historical calibration data set well, then a prediction which is entirely solution space dependent (and is thereby completely informed by this data set) will be made with little error, regardless of the physical basis (or lack thereof) of the simplified model. However, where a prediction is less than totally informed by the calibration data set, the history-matching process may detract from the credibility of that prediction by introducing distortions into the components of that prediction which must be informed by expert knowledge. Simplification is suboptimal when it allows this to occur. Mathematically, this happens when the decomposition of real-world parameter space implied by simplification is not aligned with that provided by the idealized simplification process described earlier.

[155] Bayesian analysis informs us that if a model is a perfect simulator of environmental behavior, its predictive performance can only be enhanced by imposing constraints on parameter values through the history-matching process. The same cannot be said for a simplified model unless simplification is optimal in the sense described earlier (which will rarely, if ever, be the case). Where a model's simulation of real-world processes is defective, the benefits of calibration become prediction specific. When a simplified model extracts information from an historical observation data set, it may place that information into incorrect receptacles. For certain types of predictions (namely, those bearing greatest similarity to observations comprising the calibration data set), this may be of no consequence, for extraction of information from the calibration data set is all that matters; all information receptacles are therefore "good receptacles." For other types of predictions, namely, those that require that information from both the calibration data set and expert knowledge be combined, the "pushing aside" of expert knowledge that occurs when calibration information is placed into suboptimal parameter receptacles, which cannot hold both of these types of information simultaneously, can engender bias in those predictions. Without a complementary complex model through which the performance of a simplified model can be assessed, this (possibly very substantial) bias cannot be quantified.

[156] In the present paper we have studied a complex model of a type that finds common usage in everyday modeling practice, together with two simplified counterparts of that model. Through linear analysis we have attempted to formulate the transformations that are implied in simplification of the complex model and to then understand the extent to which simplification has, or has not, compromised the performance of the simplified models. To the extent that lessons learned from the analyses documented herein have broader implications, we now state conclusions from this work that can be extended to other modeling contexts.

[157] 1. Even where the model simplification process is such that a simplified model tries to be faithful to the physics of the processes that it simulates, and employs parameters that attempt to replicate measurable physical properties of the system, what each such parameter actually represents in the calibrated model may be very different from the system property after which it is named.

[158] 2. As a result, attempts to infer local system properties through calibration of even a highly complex physically based model may lead to highly erroneous estimates of these properties.

[159] 3. When even a highly complex physically based model is calibrated against a real-world data set, attainment of a good fit with that data set may require a greater range of parameter variability than that which would be allowed on the basis of expert knowledge alone.

[160] 4. Where a model is intended to make predictions that are similar in character to the observations against which it is calibrated, obtaining a good fit with the calibration data set is more important than adherence to user-informed parameter bounds. In fact, a correct physical basis for the model may matter less than whether its parameters collectively span the solution space of the reality model of which it is a simplification.

[161] 5. Where a model is built to make predictions of many different types (as many models are), the benefits of constraining parameters in order to ensure replication of past system behavior become difficult to assess. Even a relatively small amount of nonoptimal simplification can force parameters to play roles that compensate for model inadequacies and thereby entrain reality model null space parameter components as they are adjusted. Any prediction that is sensitive to these null space parameter components will be biased as a result. It is possible that calibration of

the model for the making of those particular types of predictions will do more harm than good.

[162] The conclusions from this study are far from satisfying and in some ways pose more questions than they answer. These include the following:

[163] 1. Should the accepted notion (which underpins a great deal of commercial and research-based model usage) that calibration and prediction are entirely separate aspects of model construction and deployment be abandoned (together with the sense of finality that the word "calibration" implies)?

[164] 2. Should a model be calibrated not once, but many times according to different fitting metrics, in order to thereby optimize its ability to make different types of predictions?

[165] 3. Where predictions can be demonstrated to be predominantly solution space dependent, should reliance be placed more on lumped parameter models that are easily calibrated than on complex physically based models that are difficult to calibrate?

[166] 4. Where predictions have a moderate to high degree of null space dependency, should a model that is complex enough to express this null space be calibrated only mildly, or perhaps not at all?

Appendix A: Inappropriate Parameter Transformation and Null Space Entrainment

[167] This appendix provides a simple demonstration of failure to take account of prior parameter uncertainty when simplification is effected through combining complex model parameters into a smaller number of parameters in order to achieve well-posedness of an inverse problem. It demonstrates that, like other forms of suboptimal simplification, this can lead to null space parameter entrainment as the simplified model is calibrated. A linear model is employed in this example; hence, the analysis that follows is exact.

[168] Figure A1 depicts a section through an aquifer. Let r_1 and r_2 define the resistances of the two hydrogeological units represented in Figure A1. We define resistance to groundwater flow through the equation:

$$r = \Delta h/q, \tag{A1}$$

where q is the flow through the permeable unit, and Δh is the drop in potential across it incurred by this flow. Let us suppose that the only data available for estimation of these resistances is a single upgradient head measurement. The inverse problem of estimating r_1 and r_2 is obviously ill-posed. Let the action of the model on these two parameters be represented by the matrix $\mathbf{Z}$; let the vector $\mathbf{r}$ represent both of these parameters together. Then (ignoring measurement noise for the sake of simplicity of the analysis),

$$\mathbf{h} = \mathbf{Z}\mathbf{r}, \tag{A2}$$

where

$$\mathbf{Z} = q[1 \quad 1], \tag{A3}$$

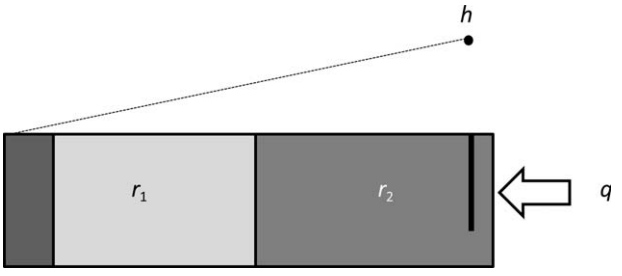

Figure A1. Conceptual model for estimation of two resistances using a single head measurement. The head is fixed at zero at the left of the model domain; inflow into the right is known.

$$\mathbf{r} = \begin{bmatrix} r_1 \\ r_2 \end{bmatrix}, \tag{A4}$$

and

$$\mathbf{h} = [h]. \tag{A5}$$

q in equation (A3) is inflow into the right of the model domain, while h in equation (A5) is the head measured in the well at the right of the domain. For convenience we assume that the head at the left boundary of the model domain is fixed at zero.

[169] Suppose that geological considerations suggest that r_2 has a greater propensity for variability than r_1. Its prior uncertainty is therefore greater than that of r_1. For illustrative purposes, let us assume that it is, in fact, twice as uncertain. If $\mathbf{C}(\mathbf{r})$ is the covariance matrix of $\mathbf{r}$, then

$$\mathrm{C}(\mathbf{r}) = \alpha \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix}, \tag{A6}$$

where α is a constant of proportionality. Suppose that in an attempt to solve this inverse problem, we use SVD without normalizing parameters with respect to their innate variability. This is equivalent to estimating the average value of r_1 and r_2 and assigning it to the whole model domain (a common calibration strategy). The $\mathbf{V}$ matrix achieved through SVD of $\mathbf{Z}$ is

$$\mathbf{V} = \frac{q}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{A7}$$

[170] Because the calibration data set is comprised of only one observation, the solution subspace of parameter space contains only one dimension. From equation (A7), it is defined by the vector $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$; meanwhile, the null space is defined by the vector $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$. As discussed in the body of this paper, the solution to the inverse problem of model calibration is obtained as the projection of the real (and unknown) parameter vector onto the solution space. We thus seek a value for the sum of r_1 and r_2 while insisting that the difference between r_1 and r_2 be zero. That is, we seek a value for the average r, with "average" defined as $(r_1 + r_2)/2$. Parameter space is depicted in Figure A2.

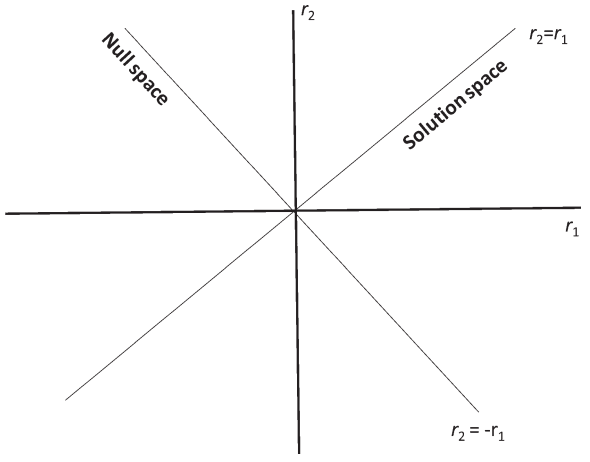

Figure A2. 2-D parameter space showing the 1-D solution and null spaces arising from the inverse problem depicted in Figure A1.

[171] Figure A3 depicts a "reality" vector **r**, as well as its projection onto the solution space. A prior probability contour of **r** is also shown; let it be assumed that this is a contour of low probability so that the shaded area defines the area of parameter space in which **r** is most likely to lie. It is apparent that the calibration process endows r_1 with a greater postcalibration potential for error than it had prior to calibration. The same will apply to any model prediction that is heavily dependent on r_1.

[172] The fact that calibration increases, rather than decreases, the potential for error of some model predictions arises because parameters were not normalized with respect to their propensity for variability before being estimated. As a consequence of this, null space parameter components are entrained as the model is calibrated, as will now be demonstrated. A solution to the inverse problem of model calibration, which conforms to expert knowledge as reflected in the **C**(**r**) prior parameter covariance matrix, should ensure that r_1 is varied from its precalibration expected value less than

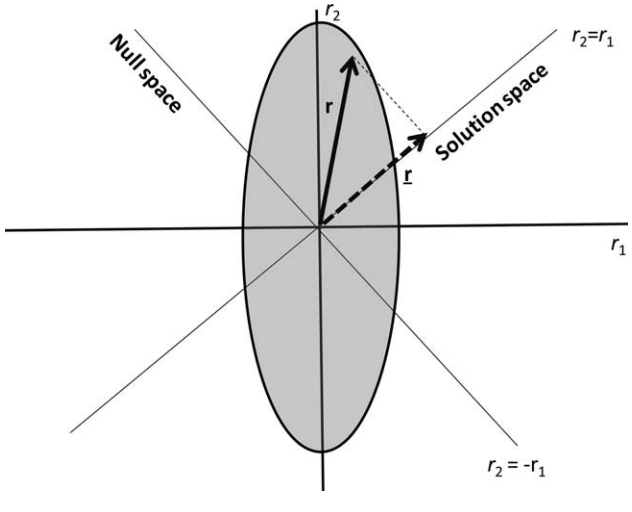

Figure A3. Solution of the inverse problem is obtained as the projection of the true parameter vector onto the solution space. The region of high prior probability of **r** is shown shaded.

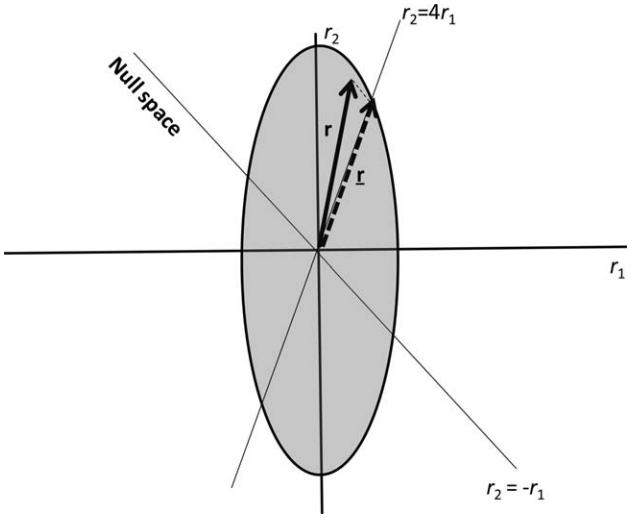

Figure A4. Solution of the inverse problem in **t**-space after back transformation to **r**-space.

r_2 is varied from its precalibration expected value. In fact, to the extent that such variation is required in order to fit the single head observation h, r_2 should be encouraged to vary twice as much as r_1. This can be achieved through the estimation of two transformed parameters t_1 and t_2, with the transformation **T** defined as

$$\begin{bmatrix} t_1 \\ t_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} = \mathbf{Tr}. \tag{A8}$$

[173] The covariance matrix of **t** is then given by

$$\mathbf{C}(\mathbf{t}) = \mathbf{T}\mathbf{C}(\mathbf{r})\mathbf{T}^{\mathrm{t}} = \alpha \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{A9}$$

[174] The model equation then becomes

$$\mathbf{h} = \mathbf{Z}\mathbf{r} = \mathbf{Z}\mathbf{T}^{-1}\mathbf{t} = \mathbf{Y}\mathbf{t}, \tag{A10}$$

where **Y**, the model used for parameter estimation purposes, is defined as

$$\mathbf{Y} = q[1 \quad 2]. \tag{A11}$$

[175] The null space of **Y** is defined by the unit vector $\frac{q}{\sqrt{5}}\begin{bmatrix} -2 \\ 1 \end{bmatrix}$, while its solution space is defined by the vector $\frac{q}{\sqrt{5}}\begin{bmatrix} 1 \\ 2 \end{bmatrix}$. Obviously, these spaces are orthogonal to each other in **t**-space. However, back transformation of these to **r**-space using the $\mathbf{T}^{-1}$ transformation leads to the nonorthogonal spaces $\frac{2q}{\sqrt{5}}\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ and $\frac{q}{\sqrt{5}}\begin{bmatrix} 1 \\ 4 \end{bmatrix}$, respectively. Unsurprisingly, the former is aligned with the previous null space. The latter is depicted in Figure A4, together with the projection onto this space implied by calibration of the **Y**-based model. The fact that the solution to the inverse problem is more in harmony with expert knowledge is obvious.

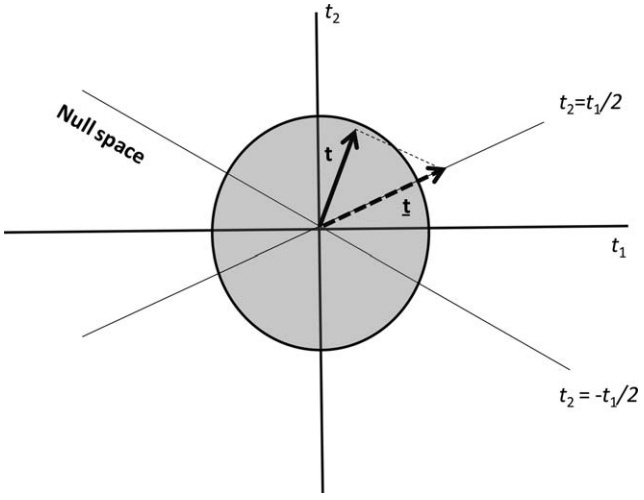

Figure A5. Solution of the inverse problem in **r**-space after transformation to **t**-space. The **r**-space solution to the inverse problem has a nonzero projection onto the **t**-space null space.

[176] In contrast, the 1-D solution space found through SVD undertaken in **r**-space **T**-transforms to the vector $\underline{\mathbf{t}}$ shown in Figure A5, which depicts **t**-space. Null space entrainment of the **r**-space solution in this space is obvious.

[177] The importance of taking expert knowledge into account during simplification is thus obvious. This applies irrespective of the simplification methodology adopted. For example, suppose that a modeler decides to fix one of the resistances in Figure A1 and estimate the other, rather than implicitly or explicitly estimating an average resistance. Obviously he/she should fix r_1 and estimate r_2 as r_1 has less innate variability than r_2; the potential for wrongness in fixing the chosen parameter at its expected value is therefore smaller.

[178] **Acknowledgments.** We gratefully acknowledge the funding and support for this work provided by the National Centre for Groundwater Research and Training, a collaborative initiative of the Australian Research Council and the National Water Commission. We thank James Craig and two anonymous reviewers for reviewing this manuscript.

References

Aanonsen, S. I. (2008), Efficient history matching using a multiscale technique, *SPE Reservoir Eval. Eng.*, *11*(1), 154–164.

Andreu, J. M., F. J. Alcalá, A. Vallejos, and A. Pulido-Bosch (2011), Recharge to mountainous carbonated aquifers in SE Spain: Different approaches and new challenges, *J. Arid Environ.*, *75*, 1262–1270.

Aster, R. C., B. Borchers, and C. H. Thurber (2005), *Parameter Estimation and Inverse Problems*, 301 pp. Elsevier, Amsterdam, Netherlands.

Campbell, E. P., and B. C. Bates (2001), Regionalization of rainfall-runoff model parameters using Markov chain Monte Carlo samples, *Water Resour. Res.*, *37*(3), 731–739.

Campbell, E. P., D. R. Fox, and B. C. Bates (1999), A Bayesian approach to parameter estimation and pooling in nonlinear flood event models, *Water Resour. Res.*, *35*(1), 211–220.

Castelletti, A., S. Galelli, M. Restelli, and R. Soncini-Sessa (2011), Data-driven dynamic emulation modeling for the optimal management of environmental systems, *Environ. Model. Software*, *34*, 30–43, doi:10.1016/j.envsoft.2011.09.003.

Cheng, W.-C., M. Putti, D. R. Kendall, and W. W.-G. Yeh (2011), A real-time groundwater management model using data assimilation, *Water Resour. Res.*, *47*, W06528, doi:10.1029/2010WR009770.

Cooley, R. L. (2004), A theory for modeling ground-water flow in heterogeneous media, *U.S. Geol. Surv. Prof. Pap. 1679*, 220 pp.

Cooley, R. L., and S. Christensen (2006), Bias and uncertainty in regression-calibrated models of groundwater flow in heterogeneous media, *Adv. Water Resour.*, *29*, 639–656, doi:10.1016/j.advwatres.2005.07.012.

Cui, T., C. Fox, and M. J. O'Sullivan (2011), Bayesian calibration of a large scale geothermal reservoir model by a new adaptive delayed acceptance Metropolis Hastings algorithm, *Water Resour. Res.*, *47*, W10521, doi:10.1029/2010WR010352.

Doherty, J., and S. Christensen (2011), Use of paired simple and complex models to reduce predictive bias and quantify uncertainty, *Water Resour. Res.*, *47*, W12534, doi:10.1029/2011WR010763.

Doherty, J., and D. Welter (2010), A short exploration of structural noise, *Water Resour. Res.*, *46*, W05525, doi:10.1029/2009WR008377.

Doherty, J. (2011), PEST: Model-Independent Parameter Estimation, User Manual, Watermark Numer. Comput. [Available at http://www.pesthomepage.org/Downloads.php.].

Draper, N. R., and H. Smith (1998), *Applied Regression Analysis*, 3rd ed., 706 pp., John Wiley, New York.

Dripps, W. R., and K. R. Bradbury (2007), A simple daily soilwater balance model for estimating the spatial and temporal distribution of groundwater recharge in temperate humid areas, *Hydrogeol. J.*, *15*(3), 433–444, doi:10.1007/s10040-007-0160-6.

Farmer, C. L. (2002), Upscaling: A review, *Int. J. Numer. Methods Fluids*, *40*, 63–78, doi:10.1002/fld.267.

Freeze, R. A., J. Massman, L. Smith, T. Sperling, and B. James (1990), Hydrological decision analysis: 1. A framework, *Ground Water*, *28*(5), 738–766.

Feddes, R. A., P. J. Kowalik, and H. Zaradny (1978), *Simulation of Field Water Use and Crop Yield*, John Wiley, Hoboken, N. J.

Francés, A. P., E. Berhe, and M. Lubczynski (2010), Spatio-temporal groundwater recharge assessment using a lumped-parameter distributed model of the unsaturated zone (pyEARTH-2D), *Geophys. Res. Abst.*, *12*, EGU2010–6627-2.

Gallagher, M. R., and J. Doherty (2007), Parameter interdependence and uncertainty induced by lumping in a hydrologic model, *Water Resour. Res.*, *43*, W05421, doi:10.1029/2006WR005347.

Gerritsen, M., and J. V. Lambers (2008), Integration of local-global upscaling and grid adaptivity for simulation of subsurface flow in heterogeneous formations, *Comput. Geosci.*, *12*, 193–208.

Hansen, N., and A. Ostermeier (2001), Completely derandomized self-adaptation in evolution strategies, *Evol. Comput.*, *9*, 159–195.

Hansen, N., S. D. Muller, and P. Koumoutsakos (2003), Reducing the time complexity of the derandomized evolution strategy with covariance matrix adaptation (CMA-ES), *Evol. Comput.*, *11*, 1–18.

Harmon, R., and P. Challenor (1997), A Markov chain Monte Carlo method for estimation and assimilation into models, *Ecol. Model.*, *101*, 41–59.

Herckenrath, D., C. D. Langevin, and J. Doherty (2011), Predictive uncertainty analysis of a salt water intrusion model using null space Monte Carlo, *Water Resour. Res.*, *47*, W05504. doi:10.1029/2010WR009342.

Kanso, A., M. C. Gromaire, E. Gaume, B. Tassin, and G. Ghebbo (2003), Bayesian approach for the calibration of models: Application to an urban stormwater pollution model, *Water Sci. Technol.*, *47*(4), 77–84.

Kavetski, D., G. Kuczera, and S. W. Franks (2006a), Bayesian analysis of input uncertainty in hydrological modeling: 1. Theory, *Water Resour. Res.*, *42*, W03407, doi:10.1029/2005WR004368.

Kavetski, D., G. Kuczera, and S. W. Franks (2006b), Bayesian analysis of input uncertainty in hydrological modeling: 2. Application, *Water Resour. Res.*, *42*, W03408, doi:10.1029/2005WR004376.

Kennedy, M. C., and A. O'Hagan (2001), Bayesian calibration of computer models, *J. R. Stat. Soc. Ser. B Stat. Methodol.*, *63*, 425–464, doi:10.1111/1467–9868.00294.

Kuczera, G., D. Kavetski, S. Franks, and M. Thyer (2006), Towards a Bayesian total error analysis of conceptual rainfall-runoff models: Characterising model error using storm-dependent parameters. *J. Hydrol.*, *331*, 161–177, doi:10.1016/j.jhydrol.2006.05.010.

Kuczera, G., and E. Parent (1998), Monte Carlo assessment of parameter uncertainty in conceptual catchment models: The Metropolis algorithm, *J. Hydrol.*, *211*, 69–85.

Lewis, M. F., and G. R. Walker (2002), Assessing the potential for episodic recharge in south-western Australia using rainfall data, *Hydrogeol. J.*, *10*, 229–237.

Makowski, D., D. Wallach, and M. Tremblay (2002), Using a Bayesian approach to parameter estimation; comparison of the GLUE and MCMC methods, *Agronomie*, *22*, 191–203.

Martínez-Santos, P., and J. M. Andreu (2010), Lumped and distributed approaches to model natural recharge in semiarid karst aquifers, *J. Hydrol.*, *388*, 389–398. doi:10.1016/j.jhydrol.2010.05.018.

Meisel, W. S., and D. C. Collins (1973), Repromodeling: An approach to efficient model utilization and interpretation, *IEEE Trans. Syst. Man Cybern., SMC-3*, 349–358.

Menke, W. (1984), *Geophysical Data Analysis: Discrete Inverse Theory*, 289 pp., Academic, New York.

Mondal, A., Y. Efendiev, B. Mallick, and A. Datta-Gupta (2010), Bayesian uncertainty quantification for flows in heterogeneous porous media using reversible jump Markov chain Monte Carlo methods, *Adv. Water Resour.*, *33*(3), 241–256.

Moore, C., and J. Doherty (2005), The role of the calibration process in reducing model predictive error, *Water Resour. Res.*, *41*, W05020, doi:10.1029/2004WR003501.

Moore, C., and J. Doherty (2006), The cost of uniqueness in groundwater model calibration, *Adv. Water Resour.*, *29*(4), 605–623, doi:10.1016/j.advwatres.2005.07.003.

Moore, C., T. Wöhling, T., and J. Doherty (2010), Efficient regularization and uncertainty analysis using a global optimization methodology, *Water Resour. Res.*, *46*, W08527, doi:10.1029/2009WR008627.

Pachepsky, Y. A., A. K. Guber, M. Th. van Genuchten, T. J. Nicholson, R. E. Cady, J. Simunek, and M. G. Schaap (2006), Model abstraction techniques for soil-water flow and transport, prepared for Division of Fuels, Engineering and Radiological Research, Office of Nuclear Regulatory Research, *U.S. Nuclear Regulatory Commission, Rep. NUREG/CR-6884*, 135 pp.

Qian, S. S., C. A. Stow, and M. E. Borsuk (2003), On Monte Carlo methods for Bayesian inference, *Ecol. Model.*, *159*, 269–277.

Ratto, M., A. Castelletti, and A. Pagano (2011), Emulation techniques for the reduction and sensitivity analysis of complex environmental models, *Environ. Model. Software*, *34*, 1–4, doi:10.1016/j.envsoft.2011.11.003.

Razavi, S., B. A. Tolson, and D. H. Burn (2012), Review of surrogate modeling in water resources. *Water Resour. Res.*, *48*, W07401, doi:10.1029/2011WR011527.

Scheidt, C., J. Caers, Y. Chen, and L. J. Durlofsky (2011), A multi-resolution workflow to generate high-resolution models constrained to dynamic data, *Comput. Geosci.*, *15*(3), 545–563, doi:10.1007/s10596-011-9223-9.

Schoups, G., and J. W. Hopmans (2006), Vadose Zone Journal Special Issue. Evaluation of model complexity and input uncertainty of field-scale water flow and salt transport, *Vadose Zone J.*, *5*, 951–962.

Šimůnek, J., M. Šejna, H. Saito, M. Sakai, and M. Th. van Genuchten (2009), *The HYDRUS-1D Software Package for Simulating the One-Dimensional Movement of Water, Head, and Multiple Solutes in Variably-Saturated Media*, Dep. of Environ. Sci., Univ. of Calif. Riverside, Riverside.

Sivakumar, B. (2008), Dominant processes concept, model simplification and classification framework in catchment hydrology, *Stochastic Environ. Res. Risk. Assess.*, *22*, 737–748.

Tikhonov, A. N., and V. Y. Arsenin (1977), *Solution of Ill-Posed Problems*, Winston, Washington, D. C.

Tonkin M., and J. Doherty (2009), Calibration-constrained Monte Carlo analysis of highly parameterized models using subspace techniques, *Water Resour. Res.*, *45*, W00B10, doi:10.1029/2007WR006678.

Touhami, I., J. M. Andreu, E. Chirino, J. R. Sánchez, H. Moutahir, A. Pulido-Bosch, P. Martínez-Santos, and J. Bellot (2012), Recharge estimation of a small karstic aquifer in a semiarid Mediterranean region (southeastern Spain) using a hydrological model, *Hydrol. Processsses*, *27*(2), 165–174, doi:10.1002/hyp.9200.

van Genuchten, M. Th. (1980), A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sci. Soc. Am. J.*, *44*, 892–898.

Vermeulen, P. T. M., A. W. Heemink, and C. Stroet (2004), Reduced models for linear groundwater flow models using empirical orthogonal functions, *Adv. Water Resour.*, *27*(1), 57–69.

Vermeulen, P. T. M., A. W. Heemink, and J. R. Valstar (2005), Inverse modeling of groundwater flow using model reduction, *Water Resour. Res.*, *41*, W06003, doi:10.1029/2004WR003698.

Vermeulen, P. T. M., C. B. M. te Stroet, and A. W. Heemink (2006), Model inversion of transient nonlinear groundwater flow models using model reduction, *Water Resour. Res.*, *42*, W09417, doi:10.1029/2005WR004536.

Vrugt, J. A., C. G. H. Diks, H. V. Gupta, W. Bouten, and J. M. Verstraten (2005), Improved treatment of uncertainty in hydrologic modeling: Combining the strengths of global optimization and data assimilation, *Water Resour. Res.*, *41*, W01017, doi:10.1029/2004WR003059.

Vrugt, J. A., C. J. F. ter Braak, C. G. H. Diks, B. A. Robinson, J. M. Hyman, and D. Hidgon (2009), Accelerating Markov chain Monte Carlo simulation by differential evolution with self-adaptive randomized subspace sampling, *Int. J. Nonlinear Sci.*, *10*(3), 273–290.

Vrugt, J. A., G. H. Schoups, J. W. Hopmans, C. Young, W. W. Wallender, T. H. Harter and W. Bouten (2004), Inverse modeling of large-scale spatially-distributed vadose zone properties using global optimization, *Water Resour. Res.*, *40*, W06503, doi:10.1029/2003WR002706.

Young, P. C., and M. Ratto (2009), A unified approach to environmental systems modeling, *Stochastic Environ. Res. Risk Assess.*, *23*, 1037–1057.

Young, P. C., and M. Ratto (2011), Statistical emulation of large linear dynamic models, *Technometrics*, *53*, 29–43.

Zhu, J., and D. Sun (2009), Effective soil hydraulic parameters for transient flows in heterogeneous soils, *Vadose Zone J.*, *8*, 301–309, doi:10.2136/vzj2008.0004.