Model Abstraction in Subsurface Flow and Transport Modeling

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Abstract: Model abstraction (MA) is a methodology for reducing the complexity of a simulation model while maintaining the validity of the simulation results with respect to the question that the simulation is being used to address. The MA explicitly deals with uncertainties in model structure and in model parameter sources. It has been researched in various knowledge fields that actively use modeling. We present (a) the taxonomy of MA techniques being applied in subsurface hydrologic modeling, (b) the systematic and comprehensive procedure of the MA implementation including (1) defining the context of the modeling problem, (2) defining the need for the MA, (3) selecting applicable MA techniques, (4) identifying MA directions that may give substantial gain, and (5) simplifying the base model in each direction. The need in MA may stem from (a) difficulties to obtain a reliable calibration of the base model, (b) the error propagation making the key outputs uncertain, (c) inexplicable results from the base model, (d) excessive resource requirements of the base model, (e) the intent to include the base model in a larger multimedia environmental model, (f) the request to make the modeling process more transparent and tractable, and (g) the need to justify the use a simple model when a complex model is available. The MA (a) can result in the improved reliability of modeling results, (c) make the data use more efficient, (c) enable risk assessments to be run and analyzed with much quicker turnaround, with the potential for allowing further analyses of problem sensitivity and uncertainty, and (d) enhance communication as simplifications that result from appropriate MAs may make the description of the problem more easily relayed to and understandable by decision-makers and the public.

Keywords: Groundwater; Vadose zone; Modeling; Flow, Transport.

1. INTRODUCTION

Models of water flow and solute transport in soils, sediments, and porous rocks seek to represent complex and highly transient subsurface systems. Usually, the complexity of flow and transport pathways at the specific site may be easily perceived, but it is often difficult to represent it in mathematical equations of the model without making strong simplifying assumptions (Beven, 2002). This implies that several different structures of the model could be consistent with the available observations.

It has been amply demonstrated in various modelling applications that the increase in complexity of the model does not necessarily mean the increase in its accuracy (Pachepsky et al. 2006). This indicates an opportunity to simplify models. Model abstraction is the methodology for reducing the complexity of a simulation model while maintaining the validity of the simulation results with respect to the question that the simulation is being used to address (Frantz, 1995). The objective of this work has been to identify MA techniques that may be appropriate for characterizing and simulating water flow and contaminant transport in vadose zone.

2. MODEL ABSTRACTION TECHNIQUES

2.1. Background

The first comprehensive discussion of model simplification was presented by Meisel and Collins (1973), and the first summary of techniques to simplify models was compiled by Ziegler (1976). Innis and Rextad (1983) listed 17 categories of simplification techniques in ecological modeling and emphasized conditioning model simplification to the purpose of modeling.

Fishwick (1995) introduced the multiresolution modeling as use of two or more models of different complexity for the same system. Davis and Bigelow (2003) discussed strengths and weaknesses of models of different complexity, and noted that the fundamental knowledge about the system not the only important knowledge (or even the *most* important knowledge) for the decision-making. A significant part of our knowledge of the world is low-resolution. Bigelow and Davis (2003) noted that both the insightful strategy-level analysis and the decision support typically require relatively simple models. Model simplification has also been recently advocated as a tool to improve the usefulness of complex ecological models by joint exploration of the behavior of a complex model and of its simplified counterpart (Van Ness and Scheffer, 2005).

2.2 Taxonomy of MA techniques for subsurface flow and transport models

The categories of MA techniques relevant to flow and transport modeling are presented in Fig. 1. Two large targets of abstraction are (1) the model structure, i.e. the formal description of specific processes and their interactions that affect flow and transport variables, and (2) the parameter determination, i.e. the estimation of constant and functions serving as coefficients in model equations. Although model calibration is considered to be a mandatory procedure in flow and transport modeling applications, a preliminary estimation of model parameters and their variability is useful in both setting initial values of parameters for the model calibration and using non-calibrated model in pilot studies and field campaign designs. Each category of the classification in Fig. 1 represents a variety of specific procedures and techniques. The comprehensive list of those techniques is given in (Pachepsky et al., 2006).

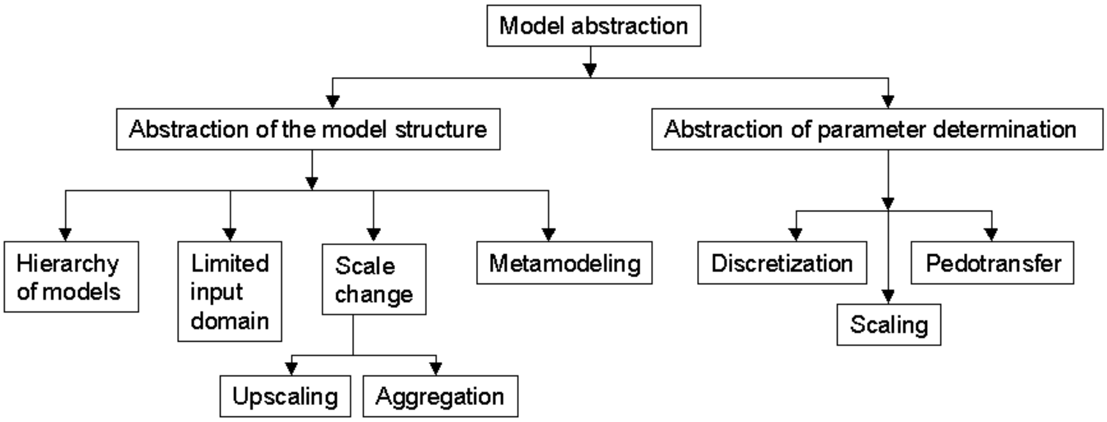

Figure 1. Categories of model abstraction techniques relevant to flow and transport modeling in subsurface hydrology

2.3 Hierarchies of models.

A pre-defined hierarchy of models has been suggested for flow and transport in structured media (Altman et al., 1996). Figure 2 shows a schematic representation of increasingly complex models that may be used to simulate preferential flow and transport in macroporous soils or unsaturated fractured rock. Similar hierarchies have been suggested for solute and colloid transport modeling.

2.4 Delimited input domain

Some features or processes may be not relevant for a given class of scenarios or for a given set of model outputs. A reduction of the spatial dimensionality is one application of these techniques. Delimiting input domain may allow rejection of the models in the hierarchy of Figure 2 based upon the type of flow being encountered. For example, the absence of saturated or near-saturated flow may make it possible to use the equivalent continuum models, whereas the presence of saturated flow may warrant the use of the dual-porosity or dual-permeability flow models.

2.5 Scale change – upscaling

This category of MA recognizes the need in altering model structure when the spatial scale changes. Model equations, variables and parameters change. The differences among the upscaling techniques are related to introducing additional relationships to compensate for the loss of information that occurs after upscaling Upscaling may involve also the reduction of dimensionality. To be efficient, upscaling techniques have to use the correct statistical representation of rare features at the fine scale, because these features often govern the media behavior at the coarse scale. For example, macropores are rare in soils and are easy to miss during the core-scale sampling, but they control water flow and solute transport at field scales.

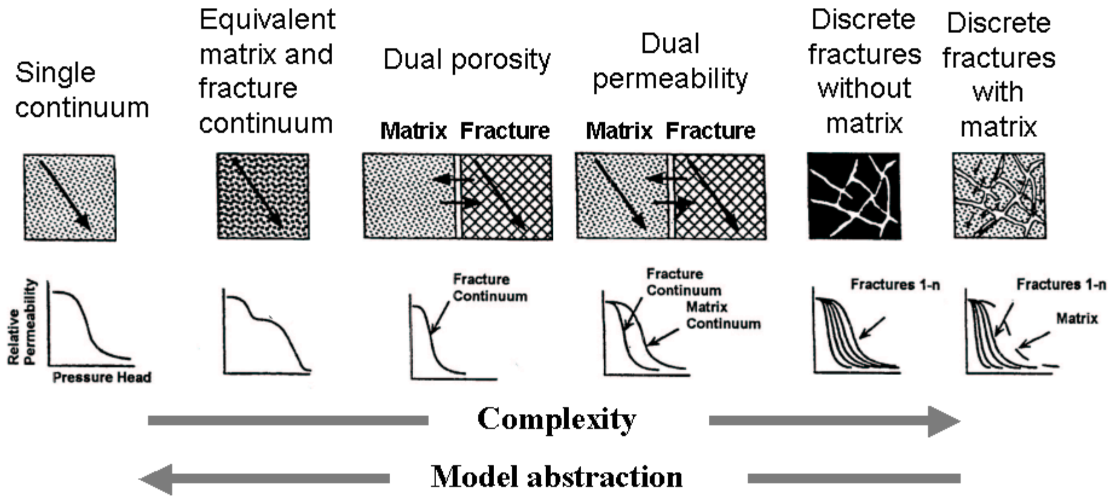

Figure 2. Hierarchy of models to simulate water flow and solute transport in structured soils or in unsaturated fractured rock (after Altman et al., 1996)

2.6 Scale change – aggregation

Change of scale also leads to a change of the model governing equations and parameters with these techniques. However, unlike in upscaling, no relationship is assumed between model parameters at fine and coarse scales. Parameters of the coarse-scale model are deemed to be lumped. An example is using a bucket-type soil water flow model at the field scale whereas Richards equation is used at the soil profile scale (Fig. 2). Soil water retention is parameterized with the field capacity at coarse scale and with soil water retention curves at the fine scale. No relationship between the coarse scale and fine scale parameters exists, because there is no reliable relationship between the water content at field capacity and soil water content at any specific values of soil water tension. Aggregation can be also done without the change in the model equations by combining several soil horizons or geologic strata. Attempts to determine the effective hydraulic properties of the equivalent soil profile from the layer properties have shown that the effective properties depend not only on layer properties but also on the type of the predominant water regime (infiltration or evaporation).

Aggregation should be distinguished from the model coarsening, when the support is increased without explicit recognition of the increasing non-homogeneity within it. In the latter case, no MA is actually performed.

2.7 Metamodeling

Metamodeling, also known as the repromodeling (Meisel and Collins, 1973) creates a relatively small and simple empirical model intended to mimic the behavior of a large complex model, that is, to reproduce the object model's input-output relationships. (Davis and Bigelow, 2003). A common way to develop a metamodel is to generate "data" from a number of large-model runs and then to use the statistical methods to relate the model input to the model output without attempting to understand the model's internal working. Artificial neural networks and classification and regression trees, along with statistical regressions, became a popular means to build metamodels.

Based on pure statistics, metamodels undoubtedly have problems, e.g. (a) the inability to provide a sensible explanation of results to a decision-maker, (b) the failure to represent multiple critical components; if a system failure is modeled and the system fails if any of several components fail, then metamodels may not simulate that, instead predicting that a weakness in one component can be compensated by greater strength of another, (c) non-reliable sensitivity of metamodels, and (d) shortcomings in representing the whole input space. (Davis and Bigelow, 2003).

2.8 Discretization

In some cases, using a set of discrete values of parameters instead of their continuous values leads to substantial simplifications. This simple but very important abstraction is commonly used in flow and transport modeling by employing soil and geological textural maps to define soil or sediment "units" that have the same hydraulic properties

2.9 Scaling

When the model coarsening is performed, i.e. the support is increased but no changes in the model structure is made, the scale-dependence in model parameters will be most probably encountered, because the larger units of the hierarchical structures in soils or sediments are enclosed in the extended support volumes. Scaling relationships are usually applicable within one to two orders of magnitude scale change.

2.10 Parameter estimation with pedotransfer functions

Parameters of the water flow models in variably saturated porous media are nonlinear functions of matric potential or water content. These parameters are notoriously difficult to measure. A substantial effort has been made to estimate these parameters from the data available from soil survey or borehole logs. The empirical functions used for such estimating are often called pedotransfer functions (PTF). An extensive work has been done to develop them. The first book on this topic (Pachepsky and Rawls, 2004) provides an overview of these fast-developing studies.

The reliability of PTFs can be estimated by re-sampling with the data set used in the PTF development, or by using an independent data set. The re-sampling methods, however, do not render any information about the reliability of PTF if it is applied in the region other than that the development data set has been collected at. the accuracy of any PTF outside of its development dataset is essentially unknown, and the use of ensemble predictions from multiple PTFs appears to be beneficial (Pachepsky et al, 2006).

3. IMPLEMENTATION

3.1 Model absraction process

MA is not about developing models, but rather about modifying or replacing them. The MA process starts with an existing *base* model that can be calibrated and used in simulations. The *key output* of the model id defined that provides the necessary and sufficient information to decide on issues of interest.

The MA process includes the following steps.
1. Justify the need for the MA
2. Review the context of the modeling problem
3. Select applicable MA techniques.
4. Determine MA directions and simplify model in each direction.

3.2 Justify the need for MA

The base model may need abstraction for one or more of the following reasons:

- The base model includes a complex description of processes that cannot be observed well and yet need to be calibrated; the calibrated values of parameters of those processes are very uncertain (see, e.g., the excellent example in (Kokkonen and Jakeman, 2001)).
- The base model propagates uncertainty in the initial distributions, parameters, and forcing in a manner that creates an unacceptable uncertainty of the key output.
- The base model produces inexplicable results in terms of the key output.
- The base model requires an unacceptable amount of resources for computations, data pre-processing, or data post-processing, e.g. the base model is not suitable as a part of an operational modeling system that requires real-time data processing.
- The base model lacks transparency to be explicable and believable to the users of the key output. The lack of transparency of the base model is the reason for abstraction that arises from the perception of potential users or critics of simulation results. The MA justification in such case is outside of the modeling project per se.

To address the need in abstraction stemming from the uncertainty in calibrated parameter values or in simulation results, set of decision rules has been developed (Pachepsky et al., 2006) based upon the classification proposed by Hill (1998). The decisions are based on (1) statistical characteristics of the parameter, and (2) the model prediction uncertainty. In this analysis, the basic diagnostic measures are: (1) the composite scaled sensitivity of the parameter; (2) coefficient of variation of the parameter; (3) the scale sensitivity of prediction; (4) correlation coefficients between estimated parameters, and (5) the updated correlations coefficients of the parameter. These statistics are directly available or can be computed according to Hill (1998) from the output of calculations with the available from the most widely used universal parameter estimation codes, e.g. UCODE or PEST.

The uncertainty of the key output has to be quantified using probability distribution function to see the expected range of predictions given the uncertainty of inputs. If the range of predictions is unacceptable for the purposes of performance assessment, i.e. the median predicted value cannot be statistically significantly discerned from the critical value of the key output, then the MA can be considered. If the correlations between inputs are known, the uncertainty can be substantially reduced (Reckhow, 1994).

3.3 Review the context of the modeling problem

The context of the modeling problem has to be reviewed to assure the objectiveness and the comprehensiveness of the MA. It needs to be realized what details and features of the problem are omitted or de-emphasized when the abstraction is performed. Neuman and Wierenga (2003) listed the following issues that constitute the context:
1. What is (are) the question(s) that the base and abstracted models are to address? The answer should consider (a) the potential or existing problem in which modeling is one of the solution instruments, (b) the potential or existing causes of the problem, (c) the issues needing resolution, and (d) the criteria to decide on efficiency of the resolution. The key output has to be provided with the spatial and temporal scale at which it is evaluated. Acceptable accuracy and uncertainty of the model output have to be established with the end user input.
2. What kind of data is available to calibrate the base and the abstracted models and to test them with respect to the key output? The essential condition is to have the database as broad as possible. It has to include the data from public and private sources, cover both quantitative and qualitative (expert) information, and encompass both site-specific and generic information.
3. To make sure that the abstracted models are sound, the additional information has to be collected, insuring that the abstracted models include descriptions of all essential processes of flow and transport for given site. This information may be of lower quality compared with the necessary part of the database. However, one has to be sure that some small-scale internal heterogeneities will not have a dominant effect on flow and/or transport at the scale of interest.

3.4 Define applicable MA techniques

MA can lead to simplifications via
- the number of processes considered explicitly,
- process descriptions,
- coarsening spatial and temporal support
- the number of measurements for the reliable parameter estimation,
- reduced computational burden,
- data pre-processing and post-processing.

Each of categories of MA techniques in Fig. 1 includes several techniques to be used at this MA stage. The number of processes can be decreased using abstractions with hierarchies of models, and delimiting input space. Process descriptions can be simplified using abstractions with a hierarchy of models, limiting input domain, and scale change..
It has been often assumed that spatially and temporally averaged values are less prone to the predictive uncertainty. This is generally true for statistically homogeneous and stationary systems. Spatial-temporal fields of water contents, concentrations, and soil water potentials usually do not conform these statistical requirements. Nevertheless, the change of scale may reduce the variability of the data because of the temporal persistence in differences soil water contents in different locations (Grayson and Western, 1998).
If the scale is coarsened but the process description is not changed, one should expect the scale-dependence of parameters. There typically exists a mismatch between the observation scale and computational grid scale. In unsaturated zone modeling, the reliance on laboratory measured hydraulic properties is much higher than in saturated zone projects. Coarsening of the scale typically creates computational grid units that are larger than the laboratory samples. In such case, scaling abstraction techniques have to be applied.

MA does not decrease the number of measurements needed to calibrate the base model. Ultimately, the key output can be obtained from a highly simplified, abstracted model, and yet the base model has to be calibrated and tested to assure that it is able to represent the natural complexity of the hydrological content, and that it can work as a starting point for abstraction.

3.5 Define and execute model abstractions

MA, in general, results in smaller number of independent parameters to measure/estimate and/or the lesser amount of computations. The particular MA procedure depends on the purpose of abstraction and on the available resources. Each abstraction is a separate sub-project that requires justification, planning, and milestone-metered execution. The feasibility of a particular MA can be judged on the basis of resources spent cumulatively on five stages of the abstracted model application, namely (1) pre-processing, (2) calibration, (3) simulation, (4) post-processing, and (5) reporting. For the specific MA procedure, it is necessary to make sure that the software for using the abstracted model is available, that the output of the abstracted model will be compatible with the available data for calibration and testing purposes, and that the pre- and post processing tools are in place.

4 CONCLUDING REMARKS

An important feature of models abstraction is the explicit treatment of the model structure uncertainty. Unlike the uncertainty in input data, in model parameters, and in scenarios, the effect of

the model structure uncertainty on the uncertainty in simulation results is usually impossible to quantify in statistical terms without making very strong assumptions. .MA is always performed in the uncertainty context.
As it is often not possible to decide which model is "better" or "more correct, " the idea of using an ensemble of models becomes more and more accepted. MA can generate models of different structures in a systematic way, thus creating a model ensemble.

Model abstraction in contaminant hydrology has been used mostly in research. Potential benefits of MA include improvement of understanding and communication of modeling results, more robust predictions, and better understanding of essential factors and their representation in models. This makes MA an attractive methodology for engineering modeling applications.

5. REFERENCES

Altman, S. J., Arnold, B. W., Barnard, R. W., Barr, G. E., Ho, C. K., McKenna, S. A., and R. R. Eaton, *Flow Calculation for Yucca Mountain Groundwater Travel Time,* (*GWTT-95*). SAND96-0819, Sandia National Laboratories, 212 pp., Albuquerque, NM, 1996.

Beven, K., Towards a Coherent Philosophy for Modeling the Environment, *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, 458(2026): 2465-2484, 2002

Bigelow, J. H,. and Davis, P. K., *Implications for model validation of multiresolution, multiperspective modeling (MRMPM) and exploratory analysis*. MR-1750, RAND, 2138, Santa Monica, CA, 2003

Davis, P. K., and Bigelow, J. H,. *Motivated metamodels: synthesis of cause-effect reasoning and statistical metamodeling*, MR-1570, RAND, 2138, Santa Monica, CA, 2003.

Fishwick, P. A., *Simulation Model Design and Execution*, Englewood Cliffs, Prentice-Hall, 1995

Frantz, K. F., A taxonomy of model abstraction techniques, In: Alexopoulos, C., Kang, K., Lilegdon, W. R., and Goldsman, D. (Eds.) *Proceedings of the 1995 Winter Simulation Conference*, pp.1413-1420, 1995.

Hill, C. M., *Methods and Guidelines for Effective Model Calibration,* U. S. Geological Survey Water Resources Investigations Report 98-4005, 90 pp., Denver, CO, 1998.

Innis, G., and E. Rextad, Simulation model simplification techniques, *Simulation*, 41: 7-15, 1983.

Kokkonen, T. S., and A. J. Jakeman, A Comparison of Metric and Conceptual Approaches in Rainfall Runoff Modeling and Its Implications, *Water Resources Research*, 34: 2345-2352, 2001.

Meisel, W. S. and D. C. Collins, Repromodeling: An approach to efficient model utilization and interpretation, *IEEE Transactions on Systems, Man, and Cybernetics*, SMC-3: 349-358, 1973.

Neuman, S. P., Wierenga, P. J., and T. J. Nicholson, *A Comprehensive Strategy of Hydrogeologic Modeling and Uncertainty Analysis for Nuclear Facilities and Sites*, *NUREG/CR 6805*. U. S. Nuclear Regulatory Commission. Washington, D.C. 20555-0001, 2003.

Pachepsky, Y. A., Guber, A. K., Van Genuchten, M. T., Nicholson, T. J., Cady, R. E., Simunek, J., Schaap, M. C. 2005. *Model Abstraction Techniques for Soil Water Flow and Transport. NUREG/CR* U. S. Nuclear Regulatory Commission. Washington, D.C. 20555-0001, 2006 (in press).

Pachepsky, Y.A., and Rawls, W. J. (eds.), *Development of Pedotransfer Functions in Soil Hydrology,* Amsterdam, Elsevier, 2004.

Reckhow, K. H. Water quality simulation modeling and uncertainty analysis for risk assessment and decision making. *Ecological Modelling,* 72:1-20, 1994

Van Ness, E. H., Scheffer, M, A strategy to improve the contribution of complex simulation models to ecological theory, *Ecological Modelling*, 185: 153-164, 2005.

Zeigler, B., *Theory of modeling and simulation,* Wiley and Sons, New York, 1976.