CHAPTER 1
Modeling basics

Chapter summary

Regardless of whether the subject to be modeled is a groundwater flow system, the growth of a bacterial colony, the flight of a projectile shot from a cannon, or any other system, the construction of a model is not a simple step-by-step procedure. Because the modeler must make decisions about which processes should be included in the model and which will be neglected, what domain will be used, and so on, the development of a model is as much art as science. Notwithstanding the creative aspects of model development, there are some simple but important rules that should be followed. In this section, we will examine three basic rules for model development, briefly discuss some important aspects of model formulation, and make some suggestions for evaluating a model's performance. These rules and suggestions will form the basis for all of the examples of model development in the following chapters.

1.1 Learning to model

How to develop a model of a physical system, when to believe and when not to believe the model output, and how to determine whether the model predictions have any relevance to real life are common and central questions that must be answered by the would-be modeler every time a new situation is encountered. Most commonly, modelers are shown how to use a software package (or asked to read the documentation for a software package), and then assumed to be sufficiently competent to produce reliable predictions of system behavior. Even a moment's reflection will show that this is a nonsensical way to go about learning the craft of modeling, and this attitude has been largely responsible for the proliferation of bad models and the subsequent lack of confidence in modeling (and modelers).

Ideally, a modeler would gain experience and a deep understanding of the process of model development while working as an "apprentice" under a skilled modeler. This desirable state of affairs is seldom met with in the real world, however. The purpose of this book is to provide some guidance for those aspiring

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modelers who do not have the advantage of serving such an apprenticeship. Although not a substitute for the teaching and advice of an experienced modeler, it is to be hoped that the rules and examples in this and the following sections will at least keep the novice modeler from falling into some of the more obvious pitfalls associated with the mathematical modeling of physical systems.

1.2 Three cardinal rules of modeling

It is probable that, over time, many hundreds of “rules” have been made up regarding the construction, evaluation, and application of mathematical models. Most of these purported rules would be better classified as “suggestions,” “considerations,” or even, in some cases, as “superstitions.” Over many years of making and using models, however, I have become convinced that the following three cardinal rules should be followed at all times in the development of a mathematical model:

1. Always know exactly the objective of model development.
2. The model you develop should be appropriate for the available data.
3. Start with the simplest possible model of the system, even if it is completely unrealistic. Once you thoroughly understand this preliminary model, add complexities to the model *one at a time* until you arrive at a satisfactory representation of the system.

In my experience, all three of these rules are routinely overlooked by modelers, and many poor and inappropriate models have resulted. We will briefly consider each of these rules here, but, more importantly, they are bound into the fiber of every model developed in the following chapters.

1.2.1 Rule 1: Know your model objective

It is common for a modeler to start a modeling investigation with the objective of “making a model of the aquifer” or with a similarly vague idea of what is to be accomplished. I cannot state strongly enough that a modeler must know exactly what s/he is trying to accomplish before ever putting pen to paper (or typing an input parameter). The more precisely the objectives of the model are known, the more likely the investigation will be successful. Make a habit of writing down the objective of your model, and be ready and willing to reduce your objective to a single sentence. The objective “to model the wells in the Grande Ronde Aquifer” is a very poor statement of purpose; a better (although still insufficient) objective is “to determine the influence of pumping well MW-4 on nearby wells.” Better yet (and possibly sufficient to begin an investigation) is “to estimate the change in head in wells MW-1 and MW-3 that results from a 24-hour constant rate pump test in well MW-4.” The examples in the following chapters always include a statement of that which is to be found; hopefully, after working through the examples, the reader will have a clear idea of how to formulate model objectives.

Although the temptation to "just get modeling" and "show some results" may be strong, you will always be better off if you first make certain you understand exactly what it is you want to achieve, and formulate a plan to reach that goal.

1.2.2 Rule 2: Make your model appropriate for your data

Hydrogeologists and environmental scientists are often working in data-poor environments. There is usually little to be gained from building a three-dimensional (3D), coupled saturated–unsaturated zone model with heterogeneous property sets when the only data to constrain the model come from a single aquifer test. Often in these situations a simple analytical model will give results that are as reliable as (or more reliable than) a complex numerical simulation. Furthermore, complex numerical simulations are often misleading, since it is tempting to think that, because they are complicated, they are realistic. What non-modelers (and many modelers) are unaware of is the fact that any computer model is solving the same equations that the modeler can write down with a pencil and paper. If there are few data to support the added complexity in terms of spatially varying properties, time-dependent recharge or boundary conditions, and so on, then the complicated numerical simulation may in fact be a worse representation of the system than a greatly simplified analytical model.

It should be said that many clients, regulatory agencies, and other downstream users of model output will push for complex numerical simulations in spite of the paucity of data to support such simulations. Although economic, political, or regulatory pressures may force a modeler to undertake the development of 3D simulations when only 1D simulations are justified, or a transient model when a steady-state model would do, the modeler should at all times be aware of the limitations of the models s/he is working with. By following Rule 3 (Section 1.2.3), the savvy modeler will be able to develop the more complex model demanded by the client while still maintaining her or his integrity and a high standard of modeling ethics.

1.2.3 Rule 3: Start simple and build complexity

When faced with a complex and difficult real-life situation, it is tempting to start out by developing a model that includes the most important processes. For example, if the goal is to understand the impact of a pumping well on other nearby wells, a novice modeler might want to build a model that includes variations in the rate of pumping, recharge from rainfall or snowmelt, the influence of changing water levels in a nearby lake, and other similar items that are clearly needed for a realistic representation of the system. The problem is that there is no way, in such a complex conceptualization, for the modeler to determine if the model output makes sense or not. Your first attempt at modeling a system should always be the simplest possible representation. Rather than modeling a 3D transient system, begin by modeling a 1D or 2D steady-state system with no source terms or other complexities. Although this may not be a realistic representation of the system, at least the modeler will know if the results are reasonable. Next, the modeler may add a spatially and temporally constant source term; again, evaluate the results. Do they make sense? Can you convince yourself the output is reasonable? If so, add another complexity, reevaluate, and so on, until the final product is one that you both understand and believe in. Never go on to the next step until you have complete confidence in, and an intimate understanding of, the current step—as well as all the steps that lead to the current step.

1.3 How can I evaluate my model?

Particularly with regard to Rule 3 (Section 1.2.3), one may rightly ask the question: "how do I know my model is giving reasonable results?" There is no easy answer to this question; in part, knowing a model is giving reasonable results is the product of experience with models. There are, however, some simple suggestions that can help to uncover problems with a model; these are described in the following text.

1.3.1 Test model behavior in the limits

The quickest way to begin an examination of model behavior is to check the behavior of a model in the limits. What is the model behavior at time $t = 0$? What about as $t \to \infty$? If you set a parameter to 0 or check the limit as it goes to ∞, is the result what you would expect? These kinds of tests are most readily carried out with analytical models, but, with some ingenuity, they can usually be applied even to complex numerical simulations.

1.3.2 Look for behavior congruent with the governing equations

Even very complex numerical simulations are based on a few well-known equations such as the Laplace equation, Poisson's equation, and the transient diffusion equation. Each of these equations implies particular behaviors, and you should check to make certain your model is behaving in a fashion that accords with your understanding of the underlying governing equations. (We will examine the characteristic behaviors of the most common equations in the following chapters.) Check for maxima and minima, look at the curvature of the predicted model surface, and examine any discontinuities in the output. Are these features present (if you expect them) or not (if you don't expect them), and are they in the appropriate places? It is a good sign if your expectations, based on your understanding of the characteristics of the governing equations, are realized. If the behavior you observe in your model output is different than your expectations, you need to understand why these differences arise before moving forward.

1.3.3 Nondimensionalization

Whenever possible, you should nondimensionalize your model (nondimensionalization is described in Appendix A, and illustrated throughout this text). Note that, although you will rarely be able to nondimensionalize a commercial simulation package, the model is based on mathematical equations that can always be nondimensionalized. Nondimensionalization carries with it a number of benefits; in particular the following:

- Nondimensionalization reduces the governing equations to their most basic functional form, which helps to clarify the expected behavior.
- Examination of the nondimensional form of the governing equation is the easiest and most certain way to identify which parts of an equation are relevant and which parts may be neglected. In this way, simplifications of the original equations may often be made (and, equally important, justified).
- Nondimensional plots of model output are the most compact way of presenting the model results. Admittedly, your target audience may not be equipped to understand dimensionless results; in this case, it is up to the modeler to either present dimensional results or educate their audience regarding the nondimensional ones.
- The nondimensionalization process results in the identification of the controlling dimensionless parameters. These parameters control the behavior of the equation, allowing the modeler to readily identify parameter ranges over which behavioral changes will take place. Furthermore, the dimensionless parameters show the modeler which dimensional parameters can be uniquely identified and which cannot.

1.4 Conclusions

As was stated in Section 1.1, following the rules and suggestions laid out in this chapter won't guarantee success, nor will it make you a modeler (only time and experience will do that). Hopefully, however, the ideas presented here will help you avoid some of the most common traps that inexperienced modelers tend to fall into. In the following chapters, I will develop a number of models; as you follow these developments, watch for the application of these basic principles. Ask yourself how you could apply these principles to your own problems. As with any creative endeavor, there are rules and guidelines that can be applied, but the ultimate responsibility for the final product belongs with the artist.