CHAPTER 1 Introduction

MODFLOW-2005 is a new version of the finite-difference ground-water model commonly called MODFLOW. This report documents the ground-water flow part of MODFLOW-2005. The primary objectives of the new version are the same as for prior versions: the program can be readily understood and modified, is simple to use and maintain, easily executed on a variety of computers with minimal changes, and is efficient with respect to computer memory and execution time.

History

Prior to the development of MODFLOW, the two- and three-dimensional finite-difference models described by Trescott (1975), Trescott and Larson (1976), and Trescott, Pinder, and Larson (1976) were used extensively by the U.S. Geological Survey (USGS) and others for the computer simulation of ground-water flow. The first version of MODFLOW (McDonald and Harbaugh, 1984) was the result of the need to consolidate all the commonly used simulation capabilities into a single code that was easy to understand, use, and modify. This first version was developed between the spring of 1981 and the winter of 1983. That model code was originally called the USGS Modular Three-Dimensional Finite-Difference Ground-Water Flow Model, but the model became known as MODFLOW several years later. This was developed using the Fortran 66 computer language.

Revised documentation was released in the report series Techniques of Water Resources Investigations (TWRI) (McDonald and Harbaugh, 1988). The program was largely the same as the 1984 version, but small changes were made to make the code conform to Fortran 77 rather than Fortran 66. This first version of MODFLOW is called MODFLOW-88.

By the early 1990s, MODFLOW had become the most widely used ground-water flow model both within and outside the USGS. Many additions had been made to expand MODFLOW's capabilities. For example, more elaborate representation of the relation between streams and an aquifer was developed (Prudic, 1989). Leake and Prudic (1991) developed a package to represent subsidence. Two preconditioned conjugate-gradient packages were developed (Kuiper, 1987; Hill, 1990). An overall update to MODFLOW, called MODFLOW-96, was published (Harbaugh and McDonald, 1996a and 1996b). MODFLOW-96 was a relatively minor update primarily to improve ease of use.

MODFLOW was originally conceived solely as a ground-water flow model. The authors viewed the solution of additional related equations as something to be done in separate programs. An example of a related equation is a transport equation that uses flows computed by the ground-water flow equation. Another example is parameter estimation, which solves an additional equation to compute optimal hydraulic parameters that result in the best match to real-world observations. By the late 1990s, there was a growing belief by many developers of modeling programs that combining such related capabilities into a single program promised to make development and use easier; therefore, the decision was made to broaden the scope of MODFLOW to allow capabilities such as transport and parameter estimation to be directly incorporated.

To facilitate the incorporation of related equations into MODFLOW, an expansion of the modular design was required. The result, which became MODFLOW-2000 (Harbaugh and others, 2000), was the addition of "Process," which is defined as parts of the code that solve a major equation or set of related equations. The part of the code that solves the ground-water flow equation became the Ground-Water Flow (GWF) Process. Three processes, Observation, Sensitivity and Parameter Estimation, aid calibration and model evaluation (Hill and others, 2000). Solution of the transport equation is the Ground-Water Transport Process (Konikow, Goode, and Hornberger, 1996) and the management of ground-water is the Ground-Water Management Process (Ahlfeld, Barlow, and Mulligan, 2005).

MODFLOW-2005 is similar in design to MODFLOW-2000. The expanded concept of processes continues as in MODFLOW-2000. The primary change in MODFLOW-2005 is the incorporation of a different approach for

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managing internal data. Fortran modules are used to declare data that can be shared among subroutines. This allows data to be shared without using subroutine arguments. As a result of using Fortran modules, a change in terminology for MODFLOW has been made. MODFLOW subroutines were originally called modules in a generic sense. The generic term module has been eliminated and replaced by the term subroutine.

Overview of Design

The goals for MODFLOW-2005, as for all prior versions of MODFLOW, can be easily stated: the program is easy to understand, use, enhance, and modify. These goals interrelate to some degree; for example, it would be difficult to use the code if it could not be understood. MODFLOW uses a modular structure wherein similar program functions are grouped together, and specific computational and hydrologic options are constructed in such a manner that each option is independent of other options. Because of this structure, new options can be added without the necessity of changing existing options. The model may be used for either two- or three-dimensional applications. Input procedures have been designed so that each type of model input data may be stored and read from separate external files. User-specified formatting allows input data for the grid to be read in almost any format without modification to the program. The output of model results is also flexible; the user may select which data to output, the frequency of output, and for some data, the format of the output.

MODFLOW-2005 is written in the Fortran 90 (American National Standards Institute, 1992) programming language. Programs written in standard Fortran are highly portable. Use of non-standard features has been carefully avoided so that MODFLOW-2005 will run, without modification, on most computers. Minor modification, however, may be necessary or desirable on some computers.

The GWF Process of MODFLOW has been divided into "packages." A package is the part of the program that deals with a single aspect of simulation. For example, the Well Package simulates the effect of wells, the River Package simulates the effect of rivers, and the Strongly Implicit Procedure Package solves the system of simultaneous finite-difference equations. Many of the packages represent options that the user may or may not have occasion to use. The fundamental method in Fortran for dividing a program into pieces is subroutines, so each package consists of multiple subroutines. The MAIN Program calls the various subroutines of the packages in the proper sequence to simulate ground-water flow.

When additional processes are included, each process is similarly divided into packages. A single code for all processes combined could become quite large. Accordingly, the authors consider it acceptable to have multiple versions of MODFLOW that consist of various combinations of processes rather than one giant version containing all processes. Thus, MODFLOW is not necessarily a single program, but all MODFLOW programs include the GWF Process.

MODFLOW-2005 makes use of Fortran modules for storing and sharing data. Each package includes one or more Fortran modules that declare the shared data for that package. The modules are designed so that data for multiple model grids can be simultaneously defined. Support for multiple grids makes it possible to incorporate local grid refinement (Mehl and Hill, 2004) into MODFLOW. The details of writing code that supports multiple grids are included in Chapter 9; however, new packages added to MODFLOW are not required to support multiple grids.

Organization and Scope of This Report

MODFLOW-2005 is being released initially with only the Ground-Water Flow (GWF) Process. This report consolidates the documentation of the GWF Process. The documentation since MODFLOW-88 has been increasingly dispersed. Documentation for MODFLOW-96 and MODFLOW-2000 was not complete by itself and referred extensively to the MODFLOW-88 documentation. This report documenting MODFLOW-2005 is similar to McDonald and Harbaugh (1988); the fundamental concepts, programmer information, and user input instructions for ground-water flow are entirely contained in this one report. There will still be a need to refer to additional reports for capabilities added to MODFLOW, including additions of processes and capabilities to simulate additional hydrologic features.

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The purpose of this report is to describe the mathematical concepts used in the GWF Process of MODFLOW-2005, the program design, the input needed to use it, and programming details. Two preliminary chapters describe topics relating to the overall program; Chapter 2 derives the finite-difference equation that is used in the model, and Chapter 3 describes the overall design of the program. The core packages are described in Chapters 4-7. Chapter 4 describes the Basic Package, which handles a number of administrative tasks for the program as a whole. Because the Basic Package deals with administrative tasks for the entire program, part of Chapter 4 also deals with overall program design. Chapter 5 describes details of how flow through a porous medium is simulated. Chapter 6 describes the simulation of hydrologic stresses, or external sources and sinks. The description of each stress consists of the physical and mathematical concepts and the derivation of the terms that incorporate the stress into the flow equation. For example, in the section on the River Package, an equation is derived that approximates flow through a riverbed, and a discussion is provided to show how that equation can be incorporated into the finite-difference equation. Chapter 7 describes numerical solvers. Chapter 8 describes input instructions for all of the packages, including instructions for the utility subroutines that are used by various packages to perform common tasks. Chapter 9 provides programmer documentation. A sample problem is included in an appendix.

The programmer documentation in Chapter 9 defines the shared data for the GWF Process as a whole and for each package within the GWF Process. The programmer documentation also includes a list of the subroutines in each package, followed by descriptions of the subroutines. The subroutines are not fully documented for all packages because many packages are similar. Only one package of each type is fully documented. The solvers are rarely modified by users, so these are not fully documented here. In situations where this information is needed, prior references can be used.

The packages documented in this report are:

Basic Block-Centered Flow Layer-Property Flow Horizontal Flow Barrier Well Recharge General-Head Boundary River Drain Evapotranspiration Strongly Implicit Procedure Preconditioned Conjugate Gradient Direct Solver