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MODFLOW: AN INSIGHT INTO THIRTY YEARS DEVELOPMENT OF A STANDARD NUMERICAL CODE FOR GROUNDWATER SIMULATIONS

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Of all the groundwater flow models widely available, the U.S. Geological Survey three-dimensional modular finite-difference, groundwater flow model, MODFLOW, is regarded by many as the most widely used by government agencies and consultancy firms. The model was first developed in 1984 and since then many changes, updates and corrections have been introduced to the program, simultaneously with its growing use. Since its establishment as a world-wide standard for groundwater flow modeling, many programs have been developed to link MODFLOW to other codes that use groundwater flow information in porous saturated media. Processes such as solute transport, variable density flow, multiphase and unsaturated flow, integrated surface water and groundwater flow, parameter estimation, groundwater management and optimization etc., may all be modeled using programs that solve a system combining the process governing equations with the groundwater flow equation, solved by MODFLOW. In this study, a summary of the development of the different versions of MODFLOW, and their specific features and references, is given. The development of the code design, usability regarding data input and output, pre- and post-processing facilities, capabilities, maintenance and a range of applications are presented. The code limitations related to the conceptual model, the mathematical solutions, hardware and software requirements are discussed, along with suggestions for improving the model accuracy and potential future developments of the code.

INTRODUCTION

Of all the groundwater flow models widely available, the U.S. Geological Survey three-dimensional modular finite-difference, groundwater flow model, commonly referred to as MODFLOW, is regarded by many as the most widely used by government agencies and consultant firms. The program was first developed in 1984 by McDonald and Harbaugh from the United States Geological Survey (USGS). So far, MODFLOW is most likely known under four version names: MODFLOW-88 [1], MODFLOW-96 [2], MODFLOW-2000 [3] and finally

MODFLOW-2005[4]. It was originally written using FORTRAN 66 and then modified in 1988 to use FORTRAN 77 for the three first versions and then to use Fortran 90 for MODFLOW-2005.

MATHEMATICAL MODEL AND DEVELOPMENT

MODFLOW solves the partial differential equation that describes three-dimensional groundwater flow in a saturated porous media. The model assumes a flow process involving a single fluid, basically water, with constant parameters (density, viscosity and temperature), in a single phase (liquid). The phase flow is assumed to be laminar and linear, and Darcy's conditions are assumed to be applicable. The principle directions of the hydraulic conductivity are assumed to be parallel to the Cartesian co-ordinate axes and do not vary within the system. Using standard MODFLOW notation, the equation solved is given as [1]:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-W=S_s\frac{\partial h}{\partial t} \qquad (1)$$

where K_{xx}, K_{yy} and K_{zz} are values of the hydraulic conductivity in the x, y and z co-ordinate axes, [LT^{-1}]; h is the potentiometric head [L]; W is a volumetric flux per unit volume and includes sources and/or sinks [T^{-1}]; S_s is the specific storage of the porous material [L^{-1}]; and t is time [T]. MODFLOW allows the three types of boundary conditions to be simulated, namely the Dirichlet, the Neumann and the Cauchy conditions. Eq. (1), together with specification of flow and/or head conditions at the boundaries of an aquifer system and specification of initial-head conditions, forms the mathematical model of a groundwater flow system solved by the program.

MODFLOW uses the finite difference numerical method to solve the groundwater flow mathematical model stated above. The spatial domain of the aquifer system is discretised using a structured block-centred grid. Each cell of the mesh is located by its row, column, and layer. An implicit formulation of the equation time-variables is used. The time derivative of the head is approximated using a backward-difference approach. Following these discretisation conventions, Eq. (1) yields a system of equations which can be written in matrix form. The resulting matrix equation is solved by an iterative method. The MODFLOW-88 version incorporates the strongly implicit procedure (SIP) and the slice-successive over-relaxation (SOR) methods only [1]. In MODFLOW-96, the preconditioned conjugate gradient (PCG) method was added as an alternative solver package [5]. This version accounts also for a new direct solver (D4) based on Gaussian elimination [6]. In MODFLOW-2000, another solver based on an algebraic multigrid iterative method (AMG) is included using a linking package to MODFLOW, called LMG [7]. The latest development in solvers techniques in MODFLOW included the geometric multigrid solver (GMG), based on a conjugate gradient preconditioned by cell-centered multigrid algorithm [8], and the preconditioned conjugate gradient solver with improved nonlinear control (PCGN) [9].

Many changes, updates and corrections were introduced to the program simultaneously with its growing use. In the four main versions of MODFLOW, the code was designed to have a modular structure consisting of the following basic entities: packages, procedures, modules and, in latest MODFLOW-2000 versions and MODFLOW-2005, processes and subroutines.

Packages are entities that describe a hydrologic capability or a solution method. The control of operations with these different packages is also included in a separate one, called Basic Package (BAS). Packages in the final four versions of MODFLOW are given in Table 1. Procedures are pieces of the program that structure its logic in a simple way. Thus, the program flowchart is designed as a sequence of these procedures. Each procedure is defined by the task that is achieved. Modules or subroutines are smaller pieces of the program that are combined within a single procedure for a single package. Calls of different modules, which belong to different packages, in the proper procedural sequence, are operated by the MAIN program.

Table 1. MOFLOW flow packages versus versions.

Packages	MODFLOW-88 Version 2.6	MOFLOW-96 Version 3.3 h	MODFLOW-2000 Version 1.19.01	MODFLOW-2005 Version 1.11.0
Advective-Transport Observation Package (ADV)	–	–	ADV2	ADV2
Basic Package (BAS)	BAS2	BAS5	BAS6	BAS7
Block-Centered Flow Package (BCF)	BCF3	BCF5	BCF6	BCF7
Time-Variant Specified-Head Package (CHD)	CHD1	CHD1	CHD6	CHD7
Coupling DAFLOW Model to MODFLOW (DAF)	–	–	DAF1	–
Direct Solver (DE4)	DE45	DE45	DE45	DE47
Drain Package (DRN)	DRN1	DRN5	DRN6	DRN7
Drains with Return Flow Package (DRT)	–	–	DRT1	DRT7
Evapotranspiration with a Segmented Function Package (ETS)	–	–	ETS1	ETS7
Evapotranspiration Package (EVT)	EVT1	EVT5	EVT6	EVT7
Flow and Head Boundary Package (FHB)	–	FHB1	FHB1	FHB1
Gaging Stations Package (GAGE)	–	–	GAG5	GAG7
General Finite Difference Flow Package (GFD)	GFD1	GFD1	–	–
General Head Boundary Package (GHB)	GHB1	GHB5	GHB6	GHB7
Geometric Multigrid Solver (GMG)	–	–	GMG1	GMG7
Horizontal Flow Barrier Package (HFB)	HFB1	HFB1	HFB6	HFB7
Hydrogeologic-Unit Flow Package (HUF)	–	–	HUF2	HUF7
Hydrograph Package (HYD)	–	HYD1	HYD1	HYD7
Interbed Storage (subsidence) Package (IBS)	IBS1	IBS1	IBS6	IBS7
Lake Package (LAK)	–	–	LAK3	LAK7
Algebraic Multigrid Solver (LMG)	–	–	LMG1	–
Link to MT3DMS Contaminant-Transport Model (LMT)	–	–	LMT6	LMT7
Layer-Property Flow Package (LPF)	–	–	LPF1	LPF7
Drawdown-Limited Multi-Node Well Package (MNW)	–	–	MNW2	MNW2
Preconditioned Conjugate Gradient (PCG)	PCG2	PCG2	PCG2	PCG7
Preconditioned Conjugate Gradient with Improved Nonlinear Control (PCGN)	–	–	–	PCGN2
Recharge Package (RCH)	RCH1	RCH5	RCH6	RCH7
Reservoir Package (RES)	RES1	RES1	RES1	RES7
River Package (RIV)	RIV1	RIV5	RIV6	RIV7
Stream - Flow Routing to include Unsaturated Flow Package (SFR)	–	–	SFR2	SFR7
Strongly Implicit Procedure Package (SIP)	SIP1	SIP5	SIP5	SIP7
Slice Successive Over-Relaxation Package (SOR)	SOR1	SOR5	SOR5	–
Streamflow-Routing Package (STR)	STR1	STR1	STR6	STR7
Subsidence and Aquifer System Compaction Package (SUB)	–	–	SUB1	SUB7
Seawater Intrusion Package (SWI)	–	–	–	SWI2
Subsidence and Aquifer-System Compaction Package (SWT)			SWT1	SWT7
Transient Leakage Package (TLK)	TLK1	TLK1	–	–
Utility Package (UTL)	UTL1	UTL5	UTL6	UTL7
Unsaturated Zone Flow (UZF)	–	–	–	UZF1
Well Package (WEL)	WEL1	WEL5	WEL6	WEL7

The main change in code design was noted in the MODFLOW-2000 version where processes entities have been introduced for the first time in the program flowchart. Processes are more general entities as they define part of the code that solves a fundamental equation by a specified numerical method. This new modularization concept has given a new dimension to the expansion of MODFLOW as it allows additional groundwater mechanisms to be modeled. In MODFLOW-2000, four processes are included, namely: groundwater flow process (GWF), observation process (OBS), sensitivity process (SEN) and parameter-estimation process (PES). The overall program operation and data structure set-up used by these processes are controlled by a separate general process called the Global Process (GLO). Two processes for groundwater transport (GWT) modeling and groundwater management (GWM) have also been added for MODFLOW-2000/2005 as optional packages [3], [4] and [10].

LIMITATIONS AND IMPROVEMENTS

(i) Conceptual model-related limitations and improvements:

As stated before, MODFLOW is formulated to simulate saturated groundwater flow in porous media. Accordingly its applicability is restricted to the simulation of this hydrogeological process. Thus, MODFLOW cannot be applied alone in several commonly occurring situations that involve other physical processes such as flow in vadose zones, density dependent flow, multiphase flow or surface processes. Many works have been conducted to overcome these limitations. Indeed, in 2002, a program that simulates variable-density, transient, ground-water flow in three dimensions was developed by USGS combining MODFLOW and MT3DMS into a single program called SEAWAT. Later version accounts for multi-species solute and heat transport [11]. Moreover, in MODFLOW-2005, a new package for simulating regional seawater intrusion in coastal aquifer systems (SWI) was introduced, representing variable-density flow with discrete zones of uniform or linearly varying density [12]. No vertical discretization of the aquifer is needed. However, no package for heat transport has been developed for MODFLOW-2005 so far, as it was for variable density flow (SWI).

Downward seepage from lakes (LAK), rivers (RIV), reservoirs (RES) and streams (STR) is limited to situations where the head is the underlying aquifer and is always above the bottom elevation of the surface water feature and the bottom elevation of the layer containing the feature. To overcome this limitation, in later versions of MODFLOW-2000, a Streamflow-Routing package (SFR) was embedded to allow for the addition and subtraction of water from runoff, precipitation, and evapotranspiration within each stream reach considering unsaturated flow between streams and aquifers. The (SFR) package is linked to the Lake (LAK) package and integrated with the Ground-Water Transport (GWT) process of MODFLOW. Unsaturated flow is simulated independently of saturated flow within each model cell corresponding to a stream reach whenever the water table falls below the streambed elevation [13]. Limitations related to stream cell large width were discussed in Ou *et al.* [14], where a new Cross-section Streamflow Routing (CSR) package compatible with MODFLOW 2005, capable of simulating accurately variation of stream-aquifer interactions and streambed heterogeneity in longitudinal and transverse directions, was presented. Recently, a Surface-Water Routing Process (SWR1) package was developed in to simulate one-dimensional and two-dimensional surface-water flow for MODFLOW-2005 [15].

MODFLOW contains also several limitations to reproduce elevation profiles of the free surface along open drain channels. The Drain Module available within MODFLOW simulates groundwater flow to open drain channels as a linear function of the difference between the hydraulic head in the aquifer and the hydraulic head in the drain, where it considers a static representation of water surface profiles along drains. Rodriguez *et al.* [16] use the one-dimensional computer code for open surface water calculations HEC-RAS, to iteratively estimate hydraulic profiles along drain channels in order to improve the aquifer/drain interaction process.

MODFLOW also includes other limitations related to the representation of certain mechanisms within packages. Thus, the recharge package (RCH) provides unphysical predictions for unconfined systems, if the water table reaches, or is above land surface. In addition, the (RCH) package does not process a distributed recharge and discharge to groundwater. Dong *et al.* [17] developed an effective method based on the recharge (RCH) package to simulate areal recharge and discharge for MODFLOW2000/2005.

The simulation of wells with the well package (WEL) is limited to withdrawal at a specified rate from individual cells, and short term transient effects between cells and wells, important in aquifer test analysis, are not simulated. Some of these limitations have been overcome by the development of new package, namely the drawdown-limited multi-node well (MNW) package that has been included in MODFLOW-2000/2005 and GWT versions to allow the simulation of multi-node wells that are completed in multiple aquifers or in a single heterogeneous aquifer, partially penetrating wells, horizontal wells and non-vertical wells [18]. Hydraulic characteristics can be defined for each multi-node well. However, input and output files are complex to build and not easy to read. Use of pre- and post processors is highly needed.

Performance and errors that can be generated by the different interpolation techniques used to approximate hydraulic parameters on cell surfaces in MODFLOW have not been investigated so far.

(ii) Mathematical solution-related limitations and improvements:

Some of the limitations related to finite difference formulations in MODFLOW include the inability of rectilinear grids to conform the model to geometric, topographic or lithologic features. Moreover, steep and rapid changes in the vicinity of hydraulic features, such as pumping/injection wells, lakes, rivers, drains, etc., cannot be captured accurately due to the relatively large distances between adjacent nodes. Mehl and Hill [19] presented a local grid refinement method for three-dimensional block-centred finite difference meshes using shard nodes, as incorporated in MODFLOW-2005 using package (LGR). For realistic problems, this new feature improves model accuracy which is controlled by convergence criteria, as defined by the user. However, fine grids can result in long computer processing times that prohibit the many model runs often needed to understand the system dynamics and calibrate the model. In 2013 the USGS released a new version, called MODFLOW-USG [20], based on a control volume finite difference (CVFD) formulation to allow structured and unstructured grid types, including nested grids and grids based on a variety of cell shapes. Flexibility in grid design can be used to focus resolution along rivers and around wells, for example, or to subdiscretise individual layers to better represent hydrostratigraphic units.

Other limitations related to the solution methods include the following: 1) MODFLOW sometimes encounters difficulties, or fails to converge, in drying/re-wetting situations, 2) solvers available in MODFLOW are efficient for small or straightforward problems, but become inefficient, or fail altogether, for large and complex problems, 3) MODFLOW's time stepping increases the step size in geometric progression indefinitely, thereby sacrificing robustness, efficiency, and efficient control of simulation output.

Doherty [21] suggested a number of adjustments to the BCF package to improve MODFLOW convergence when dewatered cells were included in the calculations. Potential inaccuracies involving the matrix solvers SIP, SSOR and PCG2 were fully addressed by Osiensky and Wiliams [22]. A comparative discussion about the performance of MODFLOW iterative solvers SOR, SIP, PCG, and AMG, is provided by Mehl and Hill [7] and Detwiler *et al.* [23]. The AMG and GMG solvers were compared in Wilson and Naff [8]. An unstructured preconditioned conjugate gradient (UPCG) solver, using general-purpose graphics processing units (GPGPUs) to improve the performance of MODFLOW has been developed recently in Hughes and White [24] and compared with the PCG solver. However, no detailed comparisons between all the MODFLOW solvers, namely SIP, SSOR, PCG, DE4, AMG and, more recently, PCGN have been undertaken to-date.

(iii) Hardware and software-related limitations and improvements:

The main hardware and software related limitations can be summarised as follows: 1) pre and post-processing facilities are unavailable within MODFLOW-2000 and 2005. In fact, data input/output, grid considerations, and simulation control have complex data structures, particularly when several simulations are involved for calibration, and sensitivity analysis, 2) for large, complex problems, simulation problem dimensions are limited by available computer memory or prohibitively long simulation times,

The USGS has separately developed two basic pre-processors to the MODFLOW program, namely MFI2K, which assist in preparing input data for MODFLOW-2000 [25], and ModelMuse, a graphical user interface (GUI) for creating the flow input files for MODFLOW–2005 [26]. The two programs can be downloaded for free from the USGS software home page. Other programs, which perform post-processing tasks were also developed by the USGS separately (e.g. GW_Chart, MODPATH, Model Viewer, ZONE CONC, ModelMuse). However, due to its growing use and development since its release, more sophisticated pre- and post-processing capabilities have been developed by other organisations and private companies. These facilities include mesh generator, CAD/GIS style tools and functionality, a graphical user interface for 3D views, animation, contour plots, colour postscript output, vector plots, and importing and exporting data facilities. Commercial versions of the MODFLOW software allow most of these options (e.g. GMS, MODELGIS, Visual Modflow, Groundwater Vistas). Most of these commercial software tools have their own in-built pre-and post-processors, as they bring other process simulation codes together (e.g. contaminant transport codes, surface water codes, particle tracking codes). Such functions are increasingly being improved as they represent a highly attractive criterion in software selection by modelers.

To enhance the code accuracy and efficiency related to both memory requirements and computing efforts, parallelization methods have been increasingly used. In 2013, Ji *at al.* [27] developed a graphics processing unit (GPU) based method to parallelize MODFLOW by reorganizing the equations and solving them with the GPU library. Experimental tests show that a 1.6- to 10.6-fold speedup can be achieved for models with more than 105 cells. The efficiency can be further improved by using up-to-date GPU devices. Cheng *et al.* [28] rebuilt MODFLOW on J Adaptive Structured Meshes applications Infrastructure (JASMIN). Test indicated a net improvement in accuracy, processing time and scalability of the code results.

CONCLUSION

MODFLOW has evolved enormously throughout the 30 years of its existence. Many limitations related to its conceptual model, mathematical solution or hardware and software performances have been constantly challenged through the development of new package versions, based on users and developers reporting. MODFLOW-2005 is now a ‘mature’ program for groundwater simulations. Although the model can not simulate all groundwater processes, it can be coupled, through specific packages, to other groundwater simulators, such us MT3DMS, SURFACT, SWAT, TOUGH2 etc., with minor modifications in the input and/or output files or using appropriate pre and post-processors and GIS tools. The model also presents a user defined balance between accuracy and complexity, through choice of grid size, refinement and shapes, matrix solvers, and conceptual approaches.

It can be concluded that the true success of the model and development efforts is largely influenced by the USGS maintenance policy, users and developers reporting problems and the free access to the program and its source code. The hybrid forms of development that borrow the most effective techniques from both research and applications have led to a high performance, open-source program and world-wide standard numerical code used as a reference for groundwater simulations.

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