

A Unified Modeler's Workbench: Workflow-Driven Conceptual and Numerical Modeling

WAYNE HESCH¹ & SERGUEI CHMAKOV²

¹ Schlumberger Water Services, 72 Victoria Street South, Suite 202, Kitchener, Ontario, Canada, N2G 4Y9
whesch@slb.com, ²schmakov@slb.com

Abstract

In order for a groundwater model to be accurate, reliable, and robust, it requires a tremendous amount of information and understanding of the aquifer. The first step in developing a groundwater model, and perhaps the most important, involves the design of a conceptual model. Developing a good conceptual model requires compiling detailed information on the geological formations, groundwater flow directions, recharge, surface water, hydraulic parameters, extraction or injection from wells, and the groundwater quality.

Today's groundwater modeler has at his/her disposal, a variety of tools and data sources for designing a conceptual model. The challenge is bringing together this data into one common application. A revolutionary new tool encourages a conceptual approach to groundwater modeling. The steps for conceptual and numerical modeling are presented in a workflow-driven graphical user interface (GUI), using terminology that is familiar to the modeler. The conceptual model is developed independent of any particular numerical simulator, allowing the freedom to generate or update multiple numerical models of different types (MODFLOW, FEFLOW, and Analytical). Using a conceptual model also allows for generating a variety of numerical discretizations from the same source, such as a variety of finite difference grids (deformed, uniform) or finite element meshes. The results from multiple models can be compared in a 3D environment in order to assess uncertainty and improve model credibility.

Key words groundwater modeling, conceptual modeling, MODFLOW, FEFLOW, groundwater-surface water

INTRODUCTION

The groundwater modeler has to deal with different types of uncertainties, in particular with parameter uncertainties (Hill, 2007, Doherty 2007) and conceptualization uncertainties (Poeter, 2006). In order to handle conceptualization uncertainty, the modeler needs to create a reasonable set of different alternative conceptual models. This in turn, produces a demand for the software giving the modeler a tool for developing such conceptualizations. Currently the cost of developing such alternative models is usually so prohibitive that the majority of the projects can only afford to explore the effects of parameter uncertainties.

The goal of this paper is to present a conceptual approach to groundwater modeling that addresses these issues. This approach allows the modeler to maintain a number of conceptual models within a single project and provides an easy way to generate a number of different numerical models from the same conceptual source.

WORKFLOW OVERVIEW

Groundwater models require a number of steps that must be completed in a specific sequence in order to satisfy a particular goal. Traditional groundwater modeling software fail to provide a logical roadmap for navigating these steps, requiring a steep learning curve, and often lead to user confusion and frustration. Users must resort to step-by-step tutorials, training, or learn by trial-and-error, all of which can be tedious and costly. Another challenge – raw data are usually handled outside of the model building workflow. Workflows for creating groundwater meaningful objects from the raw data are usually left beyond the graphical user interfaces for simulation software, which makes it difficult

to trace the final model to the original data.

A new generation of Visual MODFLOW Flex software (VMOD Flex) presents the groundwater modeling steps in an intuitive, workflow-driven graphical user interface (GUI). During progression through the workflow, visual feedback allows the user to see what states are completed, and where he can go next. This approach prevents the user from getting lost and helps to keep him focused on what is required at a particular state. This is accomplished by adhering to the “minimum distraction” GUI principle, where only the appropriate workflow states are exposed to the user.

The model building process is presented in a natural workflow from: Data Processing => Conceptual Model => Numerical Model => Simulation => Analysis of Results

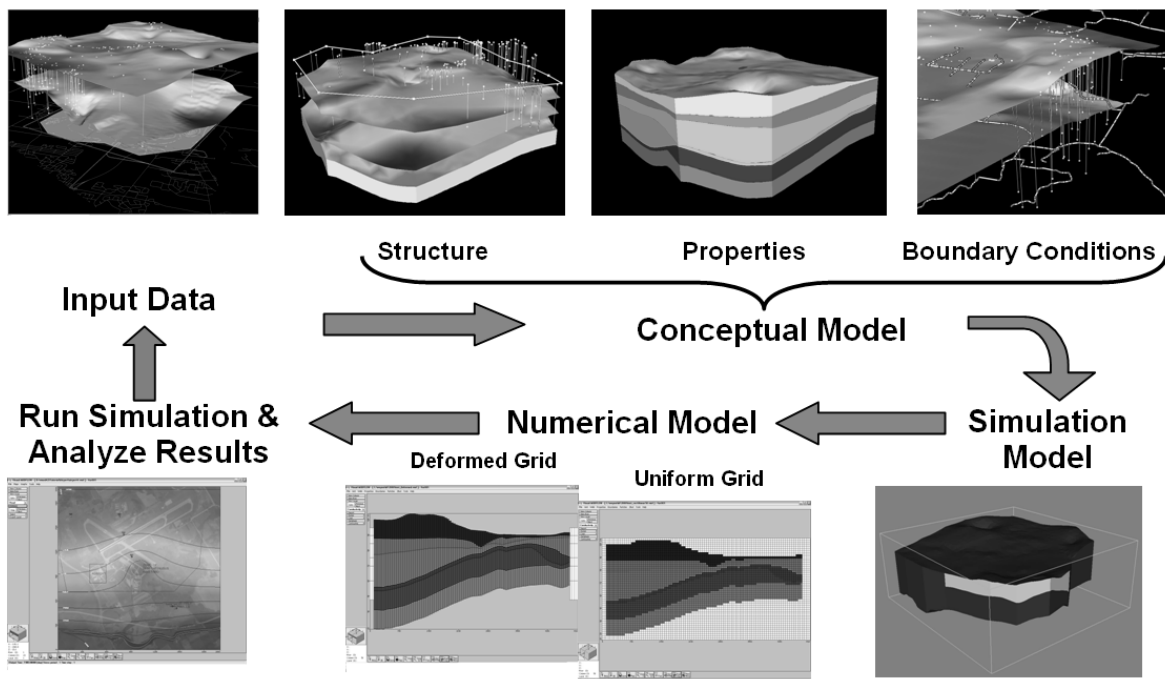


Fig. 1 General workflow overview

Data processing

VMOD Flex provides a workspace for organizing and management of the raw data. The object complexity ranges from rather simple ones such as points, polylines, polygons and surfaces to as complex as wells (vertical, deviated, or horizontal), or vertical cross-sections.

These objects all share a common characteristic: they are not required to carry any hydrogeological semantics. The objects at this level are considered to be just pure geometry with attached attributes having little or no semantics with respect the modeling goal. This is the way how VMOD Flex allows the modeler to load the raw data in the context of the modeling project and organize them for future use depending on the modeling objectives. At all times the raw data stored in the objects are left intact and kept grid and mesh-independent.

All objects can be imported from a variety of data sources such as Digital Elevation Models (DEM),

shapefiles, spreadsheets, databases, or created manually. The list of supported formats is open and can be extended as necessary. To facilitate import of geographical information, VMOD Flex supports a number of geographic and projected (UTM, State Plane, ETRS89) coordinate systems and transformations between them. Local Cartesian (non-earth) coordinate systems are also supported.

Although these objects may not be used directly in the numerical model, they serve as its building blocks. To facilitate this, each object exposes a set of operations to change its own state or generate other objects. Possible examples of operations includes creating surfaces from points using various interpolation methods, spatial transformation like shifting and rotating, converting points to polylines, etc. Operations may include another object's as operands, for instance it is possible to drape a polygon on a surface. To facilitate traceability of the model, each object carries with it a revision history: the creation date and the author of the object, what other data were used, and what operations were applied to it.

Viewing and Editing

Another feature of VMOD Flex is a set of 2D and 3D viewers and editors. Rather than limit the user to a set of fixed views of the model being developed, VMOD Flex introduces a concept of universal viewers and editors. Any object created in the project workspace can be visualized provided it exposes a set of pre-defined programmatic interfaces. The modeler can display a number of 2D and 3D views and have different objects simultaneously visualized in those views.

The editing process includes geometry editing and attributes editing. Geometry editing can be performed concurrently in a graphical or tabular view thus allowing for increased level of control on the object geometry changes. If the object being edited is simultaneously visualized in other graphical views, all the changes are reflected live in those views during the editing session. To increase usability all editing includes multi-level undo capabilities.

Attribute editing is based on a selector mechanism that allows the modeler to delineate zones in data objects where attributes of the object's geometrical elements can be specified in a uniform way. Each zone is assigned a particular method for defining attributes. There are a number of methods that can be used to define the attributes: constant value, linear interpolation between nodes, values from a surface data object (imported from DEM), values from a set of river gauge stations, etc. Once again, the modeler can make use of data objects loaded into the data workspace – for instance assign river stage from a DEM imported during the course of data management activity. This mechanism is similar to the one used in Visual MODFLOW (Chmakov, 2003) to handle the MODFLOW Stream Routing Package (STR) (Prudic, 1989).

The zone based approach for assigning and editing the attributes does not depend on the object dimension, and is similarly used for attributes of 2D and 3D objects. This mechanism is used for defining both property and boundary condition attributes.

Conceptual Model

The Conceptual Model in VMOD Flex is represented by a workspace that is separate from that of the raw data. Similar to the data workspace, the content of the conceptual workspace is comprised of objects. The difference between the objects in the conceptual model and the data workspace is that conceptual model workspace objects must have particular semantics and adhere to business rules specific to the conceptual model objects.

The Conceptual Model (CM) workspace contains a fixed structure of folders for organizing the CM objects. In contrast to the data workspace, there is no option to have arbitrary objects in the conceptual model – the CM structure is fixed and the modeler typically builds CM objects using data objects as building blocks. The modeler can create as many conceptual models as (s)he wants, using objects from data workspace.

Every conceptual model is comprised of three sub-models: Structural Model, Property Model and Boundary Condition Model, each one with its own (fixed) structure. Accordingly, the CM creation workflow includes creating these models in succession.

The Structural Model (SM) consists of a bounding polygon and a set of horizons; the horizons represent the geological structure of the site. Typical SM creation workflow assumes creating horizons from surfaces existing in the data workspace (surfaces can be imported or created from 2D-XY scatter points, cross-section interpretations, or borehole log contact points). At this step, VMOD Flex enforces business rules for different types of horizons (base, erosional, conformable, and discontinuous (**Figure 2**)) by properly modifying the original surfaces used for horizon creation. This simplifies the process of designing pinchout and discontinuous layers. The volumes in between the horizons constitute the structural zones used later on for property modeling.

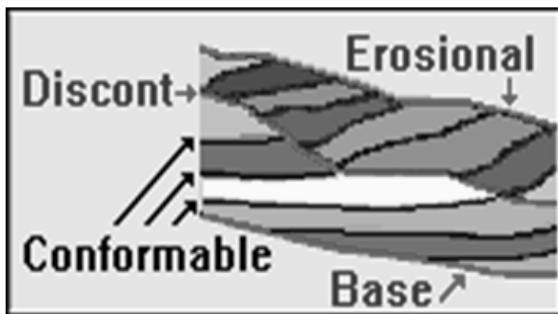


Fig. 2 Horizon Types

At the next step the property zones are created using structural zones as the compartmental basis; the modeler has an option to further subdivide the compartment structure provided by the structural model using data objects such as polygons and surfaces in order to create more property zones. Based on these property zones the modeler assigns property attributes required by the modeling objectives.

The most complex part of conceptual modeling is defining the Boundary Conditions (BC). In essence, these are independent models ranging from relatively simple ones that are incorporated in the main simulator (like River BC in MODFLOW) to rather complex models like MIKE 11 (Havnø et al, 1995) providing very detailed model for channel flow. In both cases, however, the external models share the same geometry (river network) but require a different set of model attributes. In the first case (MODFLOW River BC), it is sufficient to specify just a few attributes; in the second case (MIKE 11) there is a complex workflow defining the model which is linked together through OpenMI interface. On the VMOD Flex side, however, specifying MIKE 11 as the BC model of choice is rather simple – the modeler should just specify a path to the .omi manifest of the respective MIKE 11 project (Graham, Chmakov et al., 2006). A simplified linking, where boundary conditions for the numeric model are taken from another model – numerical or analytical – can also be handled this way.

Numerical Model

On the conceptual level a numerical model is represented by its simulation domain. Each simulation domain can have one or more numerical grid or meshes attached to it, which defines the horizontal discretization. The grid (mesh), though not linked to the conceptual model, is defined in this workspace only at the time of translating the conceptual model to the numerical model. It is important to emphasize, that in the contrast to the conventional approach, the numerical grid/mesh is not used as the definition domain for the model properties – it only serves as one of the inputs to the process of translating a conceptual model to the numerical one.

If the project objectives change, a new grid or mesh type and corresponding numerical model can be easily generated (**Figure 3**), or existing ones updated, from the conceptual objects. This way the modeler can explore different modeling scenarios by changing discretizations, boundary conditions or, ultimately, even switch to another main simulator (MODFLOW, FEFLOW, etc.)

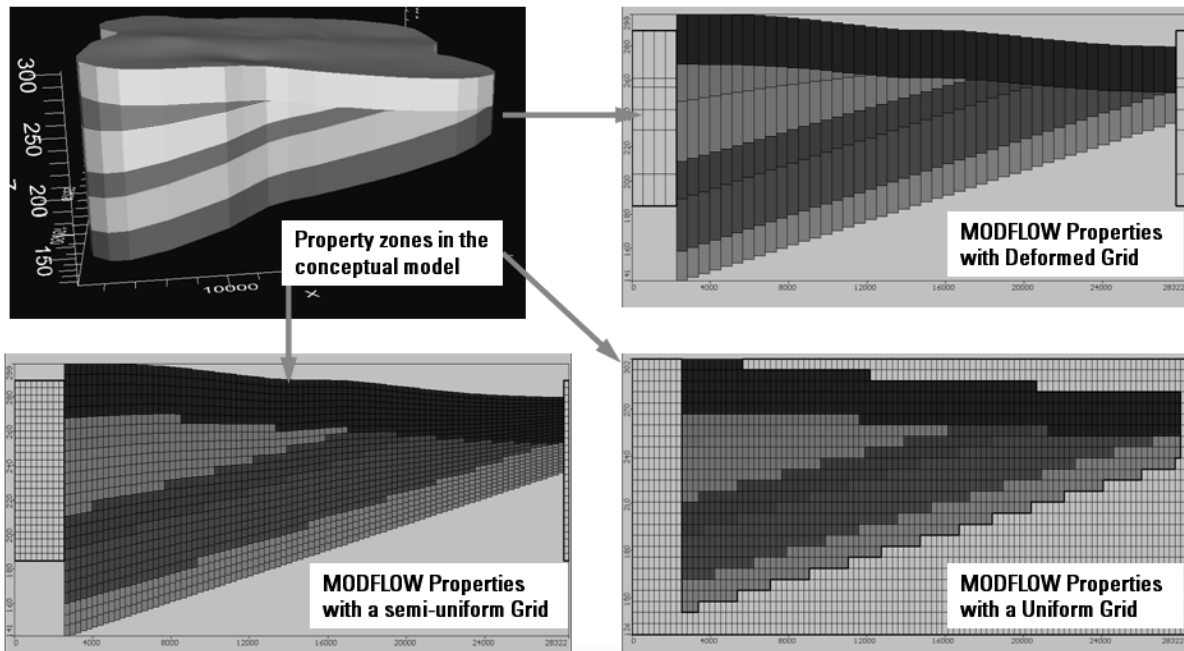


Fig. 3 Different vertical grid types generated from the same conceptual model

Most three-dimensional numerical models use vertical discretization that primarily accounts for geological layers. In some cases, this is not sufficient as it can create small pinchout layers with instabilities. Using VMOD Flex it is possible to generate model layers that are independent of the geologic structure. During conversion to the numerical model, properties are upscaled based on geometry, using a weighted average method to provide appropriate representation of the conceptual model properties. Examples of different vertical finite difference grids, with properties, are shown in **Figure 3**, while examples of two different vertical finite element meshes are shown in **Figure 4**.

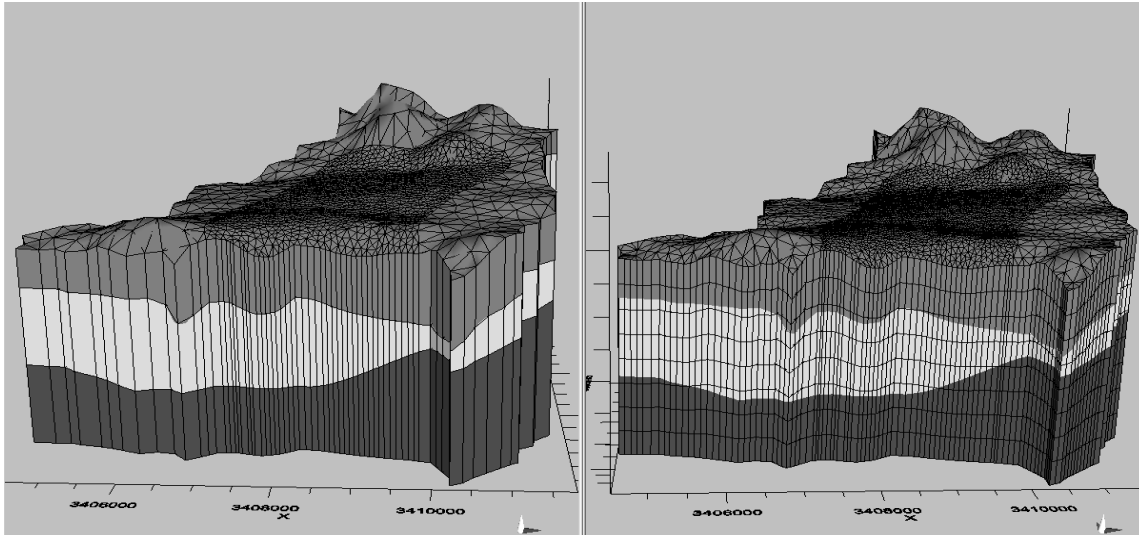


Fig. 4 Different vertical mesh types generated for the same conceptual model; (Deformed (left) and Semi-Uniform (right))

Multi-Model Analysis

A typical groundwater modeling project will go through several iterations: comparing pre-pumping to post-pumping heads, experimenting with various grid types or property distributions, or evaluating several remediation scenarios. Often it is necessary for the modeler to keep a catalog of these models as a form of version control. Within a single project, VMOD Flex allows the modeler to store multiple model runs from one or more numerical grids. The results of the models can be compared in 2D or 3D viewers, or multiple side-by-side views. It is also possible to calculate head differences between different model runs, from the same or different grid types (for example, calculate the drawdown difference at a specific pumping well when using a uniform grid or variably-spaced grid). The best model can be selected, thus improving model credibility.

Data Analysis

Including the numerical grid/mesh into conceptual model allows one to establish a link between the conceptual model and the resulting numerical model(s). The simulation results (heads, concentrations, fluxes, pathlines, charts) can be validated against the original raw field data (borehole logs, cross-sections, GIS and related data), thus improving confidence in the model and simplifying presentation to stakeholders.

SUMMARY AND FUTURE DEVELOPMENT

A fully conceptual, simulator-independent approach to groundwater model building is presented. VMOD Flex software provides integrated conceptual and numerical modeling in an intuitive workflow-driven GUI, and allows for generation of multiple numerical models with minimal effort. Raw data are stored alongside numerical models and simulated results, thus simplifying the process of validating simulated data with observed raw data. This allows the modeler to reduce the uncertainty and improve the model credibility. The current implementation provides support for the MODFLOW and FEFLOW engines. Future plans include extending it to other flow and transport engines and surface water-groundwater simulators.

REFERENCES

- Hill, M., C., Tiedeman, C., R., 2007. *Effective Groundwater Model Calibration: With Analysis of Data, Sensitivities, Predictions and Uncertainties*, John Wiley and Sons.
- Doherty, J., 2007. Model predictive error: how it arises and how it can be accommodated, *Model Care*, 493-498
- Poeter, E., 2006. All Models Are Wrong: How Do We Know Which Are Useful?, *MODFLOW and More 2006, Proceedings v.1*, 11.
- Chmakov, S., Delaney, P., 2003. Grid-Independent, Graph-Based Approach for Supporting the Streamflow-Routing Package in Visual MODFLOW, *MODFLOW and More 2003, Proceedings*, 144-148.
- Prudic, D.E., 1989. Documentation of a computer program to simulate stream-aquifer relations using a modular, finite-difference, ground-water flow model, U.S. Geological Survey Open-File Report 88-729, 113 p.
- Havnø, K., Madsen, M.N. and Dørge, J., 1995. MIKE 11 – A generalized river modeling package, *Computer Models of Watershed Hydrology*, Singh, V.P., Ed., Water Resources Publications, Colorado, USA, (1995), p809-846.
- Graham, D.N., Gijssbers, P.J.A., Gregersen, J.B., 2003. OpenMI: Harmonizing Water Management Through an Open Modelling Interface, *MODFLOW and More 2003, Proceedings*, 121-125.
- Graham, D. N., Chmakov S., Sapozhnikov, A., Gregersen, J. B., 2006. Coupling the MIKE 11 Channel Flow Model to MODFLOW, *MODFLOW and More 2006, Proceedings v.2*, 727-731.