# Generating MODFLOW Grids from Boundary Representation Solid Models

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## Abstract

**Complex stratigraphy can be difficult to simulate in MODFLOW models. MODFLOW uses a structured grid that requires that each grid layer be continuous throughout the model domain. This makes it difficult to explicitly represent common features such as pinchouts and embedded seams in a MODFLOW model. In this paper, we describe a method for automatically generating MODFLOW-compatible grids from boundary-representation solid models. Solid models are data structures developed originally for computer-aided design applications that define the geometry of three-dimensional objects. Solid models can be used to represent arbitrarily complex stratigraphy. The elevations defined by the solids are then extracted from the solids in a manner that preserves the continuous-layer requirement imposed by MODFLOW. Two basic approaches are described: The first method adjusts the MODFLOW grid dimensions (layer elevations) to fit the solid model boundaries, and the second method creates a regular MODFLOW grid and adjusts the material properties to match the changes in stratigraphy. One of the main benefits of using solid models to define stratigraphy for MODFLOW models is that it provides a grid-independent definition of the layer elevations that can be used to immediately re-create the MODFLOW grid geometry after any change to the grid resolution.**

## Introduction

When building MODFLOW models (McDonald and Harbaugh 1988), source/sink objects such as rivers, lakes, drains, and recharge zones are represented as scalar parameter values assigned to the cells of a three-dimensional, cell-centered, finite-difference grid. To determine the appropriate parameter values to assign to each cell in the grid, the objects must be discretized. Discretization involves overlaying the objects on the grid cells to determine which cells are associated with each object and computing the proper parameter value (head, conductance, elevation) to assign to the cells.

### The Conceptual Model Approach

This process of discretization has traditionally been performed by manually calculating each parameter value and assigning the values to the appropriate cells. In recent years, this discretization process has frequently been automated through the use of geographic information system (GIS) technology. Model features (including geometry and attributes) are described using points, arcs, and polygons in a GIS database, and the process of discretizing these data to a grid is fully automated. This process of defining model data using GIS objects is often referred to as a "conceptual model" approach (Boisson and Cabal 1998; El-Kadi et al. 1994; Jiansheng et al. 1995; Jiansheng and Smith 1995; Jones and Richards 1996; Jones et al. 2000). The conceptual model approach is a highly efficient modeling technique that allows complex objects to be easily represented, and makes it possible to quickly test multiple-candidate conceptual model scenarious with minimal effort. This increased efficiency ultimately leads to more accurate models.

### Modeling Complex Hydrostratigraphy

To date, most of the developments in the conceptual model approach have focused on the source/sink and boundary condition data; however, a major part of the conceptual model is an idealized representation of the hydrostratigraphy. For a conceptual model to be complete, the three-dimensional stratigraphy must be represented in a grid-independent fashion. Furthermore, this representation must be defined such that the grid layer elevations and material properties (such as Kh, Kv, storage coefficient) can be quickly and automatically discretized to the model grid cells.

For simple one-layer MODFLOW models, the hydrostratigraphy can be easily represented by a pair of surfaces defining the top and bottom elevations of the grid layer and a set of polygons representing the hydraulic conductivity zones. The surfaces can be represented by triangulated irregular networks (TINs), two-dimensional grids, or sets of scattered points defining the elevations and a method for interpolating the elevations to the cell centers.

For more complex, three-dimensional models, representing the hydrostratigraphy in a grid-independent fashion is more challenging. A typical site may include numerous embedded seams, pinchouts, and stratigraphic layers truncated at the surface or bedrock. This type of site is difficult because each of the layers in a MODFLOW grid is continuous throughout the horizontal domain of the model. When representing an object that covers only a portion of the model, the grid layer(s) corresponding to that object must somehow be extended through the rest of the model domain. This typically involves embedding the grid layer within a surrounding unit or connecting the grid layer to another discontinuous object. Thus, representing complex hydrostratigraphy in a grid-independent conceptual model presents several challenges. First, a method must be devised to accurately model the complex geometric relationships inherent in the stratigraphy. Second, a process for mapping the stratigraphic relations to a MODFLOW-compatible grid must be developed. This process should preserve the primary fea-

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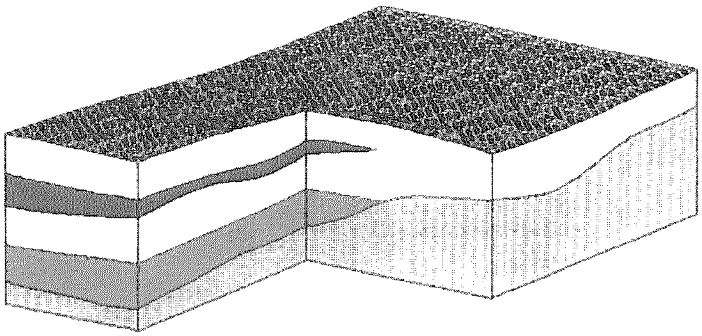


Figure 1. A sample solid model in cutaway view.

tures of the stratigraphy and at the same time generate a grid with continuous layers.

To date, little work has been done in defining a grid-independent representation of hydrostratigraphy specifically for use with MODFLOW models. Waddell and Cave (1998) describe a GIS database for storing grid-independent layer data for use with MODFLOW. The approach they describe is powerful and flexible; however, because the approach was based on layers of two-dimensional grids, the conversion to the MODFLOW arrays was not fully automated. In this paper, we present a new method for defining three-dimensional conceptual models based on boundary representation solid models. This method includes an algorithm for automatically mapping complex stratigraphic relationships to a MODFLOW-compatible grid. The algorithm is ideally suited for generating MODFLOW grids for use with the new Layer Property Flow (Harbaugh et al. 2000) and Hydrogeologic Unit Flow (Anderman and Hill 2000) packages in MODFLOW 2000.

## Solid Models

The most common method for representing three-dimensional objects in the CAD/CAM (computer-aided design/computer-aided manufacturing) industry is called solid modeling. The solid-modeling approach completely and unambiguously defines the volume of a three-dimensional object. Solid models can be manipulated via set operations. For example, a new solid can be created by computing the volumetric union, difference, or intersection of two solids. This feature can be a powerful tool when constructing detailed three-dimensional mechanical parts.

While several methods have been developed for defining solid models, the most common method is called "boundary representation." With the boundary-representation method, a solid model is defined by representing the outer surface of the solid. This surface is a collection of individual faces, typically quadrilaterals or triangles. Each face defines either a linear surface patch or higher order surface, such as Bezier or B-spline surface. Whereas the solid modeling method was originally designed for CAD/CAM applications in mechanical and aerospace engineering, the solid modeling approach has been applied with success to three-dimensional geologic structures (Bak and Mill 1989; Bayer and Dooley 1990; Fisher and Wales 1990; Gjoystdal et al. 1985; Jones and Wright 1993). A sample solid model of a set of geologic units is shown in Figure 1. Each component of the stratigraphy is represented by a separate solid. With a properly constructed set of solids, the boundaries of the solids all match precisely with no voids or overlaps.

The advantage of the solid modeling approach is that it is a fully three-dimensional technique, and it can be used to model stratigraphy at almost any level of complexity. Pinchouts, embedded seams, and faults can all be directly represented in the solid model geometry. This feature makes solid models an ideal geometric structure to use for the stratigraphic component of a three-dimensional conceptual model for MODFLOW simulations. The most significant challenge in such an approach is converting an arbitrarily complex solid-model representation of stratigraphy to a MODFLOW-compliant grid with continuous layers. We have developed two approaches for performing this conversion. The first method, called "boundary matching," adjusts the top and bottom elevations of the interior MODFLOW grid layers to match the original solid model geometry as closely as possible. The second approach, called "grid overlay," is a simpler discretization approach that uses a regular grid and adjust the material properties to match the changes in stratigraphy. Both techniques have unique advantages and disadvantages.

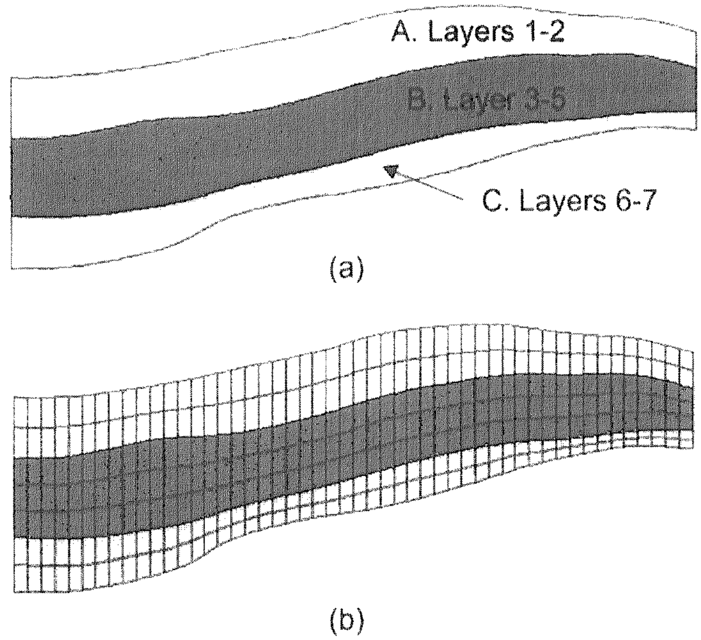



Figure 2. (a) A set of simple solids with grid layer assignments; (b) the MODFLOW grid resulting from the layer assignments.

## Boundary-Matching Approach

The goal of the boundary-matching approach is to ensure that each upper and lower boundary defined by the solid model is precisely matched by a layer boundary in the MODFLOW grid. The six basic steps involved in this are:

1. The modeler creates a set of solid models representing the stratigraphy and assigns a grid layer range to each solid.
2. The modeler creates a MODFLOW grid that surrounds the solids in XY and has the desired number of layers. Cells outside the domain of the solids in XY are made inactive.
3. A vertical ray at the center of each vertical column of cells in the grid is intersected with the solids to create a list of intersection elevations. The solids above and below each intersection are recorded.
4. For each intersection in the list, the index for the grid layer just below the intersection is determined from a set of rules and the layer ranges assigned to the solids adjacent to the intersection.
5. Using the layer indices assigned to the intersections, the top and bottom elevations and the material properties are automatically assigned to the cells in the grid.

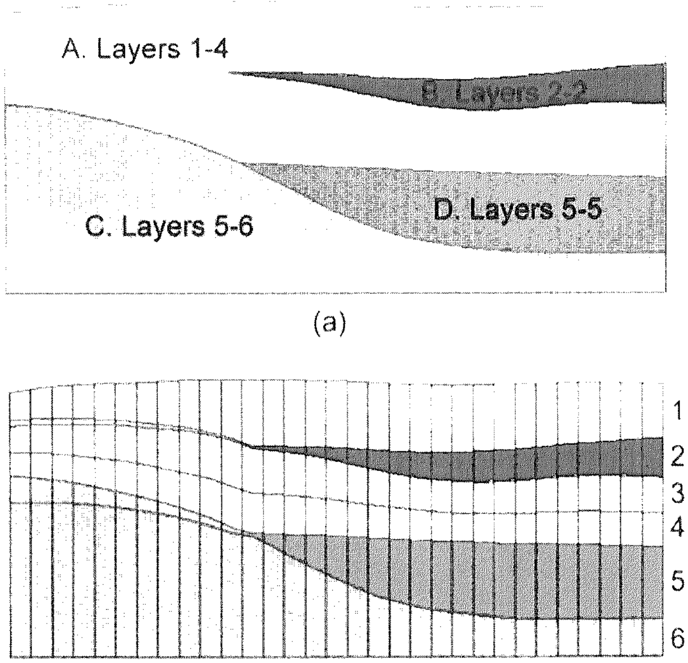



**Figure 3. (a) Grid layer assignments for a set of solids with pinchouts; (b) the MODFLOW grid resulting from the layer assignments.**

6. The elevations are iteratively adjusted to provide a smooth transition of the grid layer geometry.

This approach assumes that the MODFLOW model being used allows for an explicit definition of the top and bottom elevations of each grid layer, as is the case with MODFLOW 2000.

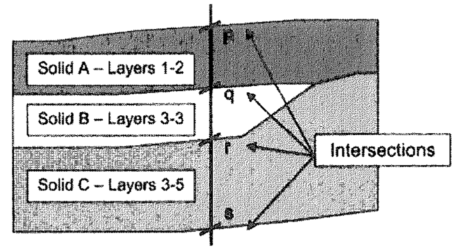
Each of these steps will now be described in more detail.

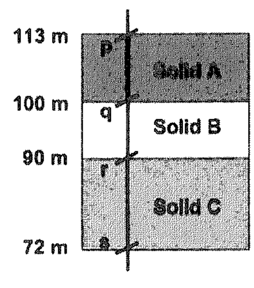
### Step 1: Assigning Layer Ranges to Solids

The first step in the boundary-matching approach is to create the set of solids defining the stratigraphy and assign a "layer range" to each of the solids. The layer range represents the consecutive sequence of layer numbers in the MODFLOW grid that are to coincide with the solid model. A sample set of layer range assignments is shown in Figure 2a. The example in Figure 2 is a case in which each solid is continuous through the model domain and there are no pinchouts. Each of the solids is given a layer range defined by a beginning and ending grid layer identification. The resulting MODFLOW grid is shown in Figure 2b.

A more complex case with pinchouts is illustrated in Figure 3a. Solid A is given the layer range 1-4, and the enclosed pinchout (Solid B) is given the layer range 2-2. The set of grid layers within the defined range that are actually overlapped by the model may change from location to location. The layer range represents the set of grid layers potentially overlapped by the solid anywhere in the model domain. For example, on the left side of the problem shown in Figure 3a, Solid A covers grid layers 1, 2, 3, and 4. On the right side of the model, Solid A is associated with grid layers 1, 3, and 4 because the enclosed solid (Solid B) is associated with Layer 2. Likewise, Solid C is associated with grid layers 5 and 6 on the left side of the model but only with Layer 6 on the right side of the model, where Solid D is associated with Layer 5. The resulting MODFLOW grid is shown in Figure 3b.

When assigning layer ranges to solids, care must be taken to define associations that are topologically sound. For example, because Solid B in Figure 3a is enclosed by Solid A, Solid B could not be assigned a layer range that is outside the layer range of Solid A.




| Intersection List | |
|---|---|
| Intersection p | Solid Above – None<br>Solid Below – Solid A<br>Elevation – 113 m |
| Intersection q | Solid Above – Solid A<br>Solid Below – Solid B<br>Elevation – 100 m |
| Intersection r | Solid Above – Solid B<br>Solid Below – Solid C<br>Elevation – 90 m |
| Intersection s | Solid Above – Solid C<br>Solid Below – None<br>Elevation – 72 m |

(c)

| Intersection List | |
|---|---|
| Intersection p | Layer Index - 1<br>Elevation – 113 m |
| Intersection q | Layer Index - 3<br>Elevation – 100 m |
| Intersection r | Layer Index - 4<br>Elevation – 90 m |
| Intersection s | Layer Index - 6<br>Elevation – 72 m |

(d)

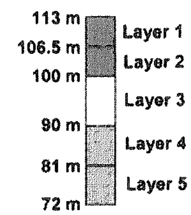



**Figure 4. (a) Sample intersection formed by vertical ray; (b) intersection elevations; (c) intersection records; (d) layer indices assigned to intersections; (e) grid layer elevation assignments.**

### Step 2: Creating the Grid

Once the layer associations are made, the next step is to create the grid. The grid must be created with a number of layers that is consistent with the grid layer assignments made in the previous step. For example, the solids shown in Figure 3 would require a grid with six layers. At this point, an arbitrary set of top and bottom elevations can be assigned to each of the grid layers. The actual elevations will be assigned in subsequent steps.

After creating the grid and before proceeding to the next step, the active/inactive zones of the grid must be defined. This can be accomplished by projecting the outline of the solids in plan view to the XY plane to create a polygon defining the model domain. The midpoint of each of the cells in the grid is then compared with this polygon, and the cells that are outside the polygon are marked as inactive (the corresponding value in the IBOUND arrays is set to zero).

### Step 3: Ray/Solid Intersection List

Once the grid is created, the next step in the boundary-matching algorithm is to create the ray/solid intersection list. One list is created for each vertical column of cells. A ray is an imaginary vertical line that passes through the centroid of each grid cell in the column. A sample ray is shown in Figure 4a. An intersection record is created for each instance the ray intersects a solid. The ray/solid intersections are sorted into a list as shown in Figures 4b and 4c. For each intersection, the solid above the intersection, the solid below the intersection, and the elevation of the intersection are stored.

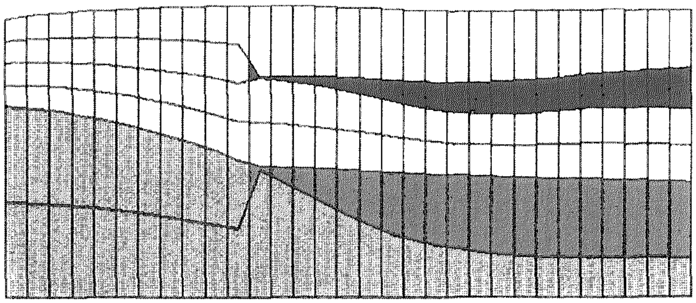


**Figure 5. MODFLOW grid for sample problem after assigning elevations and material properties. Smoothed version is shown in Figure 3b.**

## Step 4: Assigning Layer Indices to Intersections

The ray/solid intersection list identifies the sequence of solids at the center of each vertical column of cells. Each solid intersected by the ray appears in the list either twice or a multiple of two times. If the solid is a normal stratified layer or an embedded seam, it appears in the list twice. If the solid contains embedded seams, it appears multiple times in the list.

After creating the ray/solid intersection list, the next step is to parse through the solids in the list and determine which set of grid layers are associated with each section in the ray/solid intersection list. This determination is made using the layer range assignments made in Step 1.

When resolving the solid/grid layer associations, a layer index is assigned to each intersection in the list. The index represents the number of the grid layer just below the intersection. Once a layer index has been assigned to reach intersection, assigning the grid layer elevations is easily accomplished. When assigning the layer index to the intersections, one of four cases can occur: the first intersection, normal stratified layer, overlapping layers, or the last intersection. In each case, the layer index is assigned differently.

### *The First Intersection*

If the intersection corresponds to the first intersection in the list, assigning the layer index is trivial. The layer index is simply the top layer in the layer range assigned to the solid just below the intersection. For our sample problem (Figure 4), this index is one.

### *Normal Stratified Layers*

In the case of normal stratified layers, the layer ranges assigned to the solids above and below the intersection do not overlap. The top index of the layer range of the solid just below the intersection is equal to the bottom index of the layer range of the solid above the intersection plus one. For the sample problem in Figure 4, Intersection q corresponds to the normal stratified layers condition. For this case, the layer index assigned to the intersection is the top layer of the layer range of the solid just below the intersection. For Intersection q, the layer index would be three.

### *Overlapping Layers*

The most complicated case is that of overlapping layers. In this case, the bottom index of the layer range of the solid above the intersection is greater than or equal to the top index of the layer range of the solid below the intersection. For the sample problem in Figure 4, Intersection r corresponds to this condition because the layer range for Solid A is 3-3 and the layer range for Solid B is 3-5. In general, there are two scenarious possible: Either the top solid engulfs the bottom solid or the bottom solid engulfs the top solid.

*Top Solid Engulfs Bottom*

For the case where the top solid engulfs the bottom, the layer range for the bottom solid is a subset of the layer range for the top solid. When this occurs, the bottom grid layer of the solid above the intersection is greater than or equal to the bottom grid layer of the solid below the intersection. In this case, the index for the intersection is set to the top grid layer of the bottom solid. An example of this type of scenario would be an intersection at the bottom of the upper embedded seam in Figure 3a.

*Bottom Solid Engulfs Bottom*

For the case where the bottom solid engulfs the top, the layer range for the top solid is a subset of the layer range for the bottom solid. This can be detected by checking to see if the bottom grid layer of the solid above the intersection is less than the bottom grid layer of the solid below the intersection. In this case, the layer index for the intersection is set to the bottom grid layer of the top solid plus one. For the example problem in Figure 4, Intersection r corresponds to this condition. The layer index for Intersection r would be set to four.

### *The Last Intersection*

The final category that is handled by the algorithm occurs when the last intersection in the list is encountered. In this trivial case, the index is set to the one greater than the bottom index of the layer range of the solid below the intersection. For the sample problem in Figure 4, Intersection s corresponds to this condition. The layer index for Intersection s would be set to six.

At this point, all of the layer indices for the intersections have been assigned and elevations and material properties are ready to be assigned to the MODFLOW layers. The complete list of layer indices for the sample problem in Figure 4a is shown in Figure 4d.

## Step 5: Assigning Elevations and Material Properties

The next step is to use the layer indices assigned to the intersections in Step 4 to assign the grid layer elevations and material properties to each of the cells. Each ray/solid intersection list is traversed and the pairs of intersections are used to make the elevation and material assignments. The grid cell elevations assigned at this step for the sample problem are shown in Figure 4e. Note that each pair of intersections corresponds to one or more layers of cells. For example, Intersection q and r correspond to a single grid layer because the difference in the layer index assigned to the indices is one. However, Intersections r and s correspond to two grid layers and an elevation for the boundary between the two intersections is linearly interpolated.

## Step 6: Smoothing the Elevations

The MODFLOW grid corresponding to the solid shown in Figure 3a is illustrated in Figure 5. At this point, the elevations and the material properties have been assigned to the grid as described in the previous section. When assigning the elevations, each vertical column of cells is treated independently of the adjacent vertical cells. As a result, there are extreme elevation changes from one column to the next at locations where the solids pinch out. The final step in the solid-to-grid conversion process is to adjust the elevations to smooth out these transition points.

The cell elevations are smoothed using an iterative process similar to the Laplacian smoothing process used to smooth finite-element meshes (Canann et al. 1998). The typical approach used in a

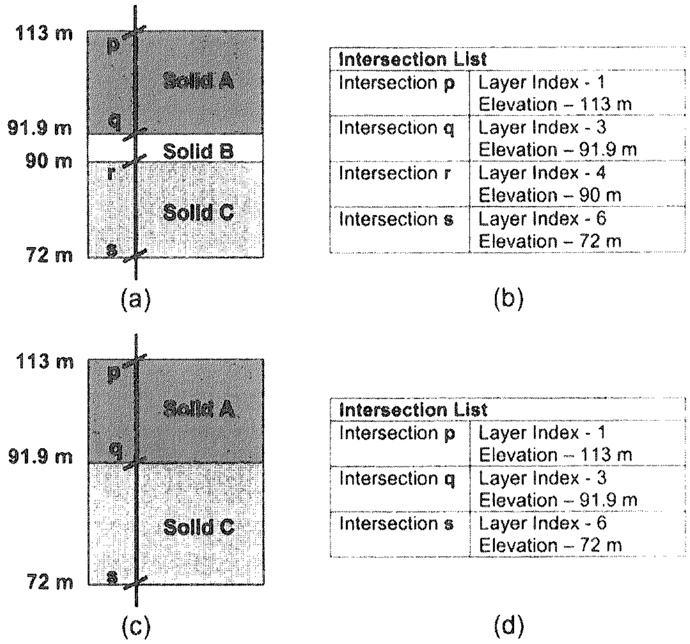



**Figure 6. Removing thin solids from intersection list: (a) solids intersected by vertical ray, (b) original intersection list, (c) solids after removal of Solid B, (d) modified intersection list.**

smoothing process is to set the cell top/bottom elevation equal to the average of the four adjacent cell elevations at each iteration. This process is repeated for a given number of iterations or until the change in elevation is less than a specified limiting value. Figure 3b shows the grid in Figure 5 after smoothing is completed. At this point, the solid-to-MODFLOW-grid conversion process is complete.

### *Preventing Thin Cells*

One of the problems with the boundary-matching algorithm is that it can result in thin cells at transition points adjacent to pinchouts (Figure 3b). These thin cells may lead to numerical instabilities in certain situations, such as cell wetting/drying or transport simulations with companion models such as MT3DMS (Zheng and Wang 1999).

Fortunately, the boundary-matching algorithm can be easily modified to avoid thin cells. First, the user must specify a minimum cell thickness. After the layer indices have been assigned to the intersection list in Step 4 for each vertical column of cells, each length of solid (defined by a pair of adjacent intersections) in the intersection list is divided by the number of MODFLOW layers associated with the solid, resulting in a cell thickness. If this cell thickness is less than the minimum thickness, the intersection records and layer indices in the intersection list are modified such that the solid is removed from the intersection list. The space occupied by the thin solid is taken by the solid either just above or just below the solid. For example, a set of sample solids intersected by a vertical ray is shown in Figure 6a, and the corresponding intersection list is shown in Figure 6b. If the minimum thickness for the cells in Solid B is equal to 2.0, then because the thickness of Solid B is 1.9, the solid is removed from the intersection list by removing the record for Intersection r, as shown in Figures 6c and 6d. The space taken by Solid B is then occupied by Solid C.

The grid shown in Figure 7 was generated by applying the boundary-matching algorithm with a minimum thickness criterion to the solids shown in Figure 3a. This grid is superior to the grid shown in Figure 3b in terms of minimizing extremely thin cells.

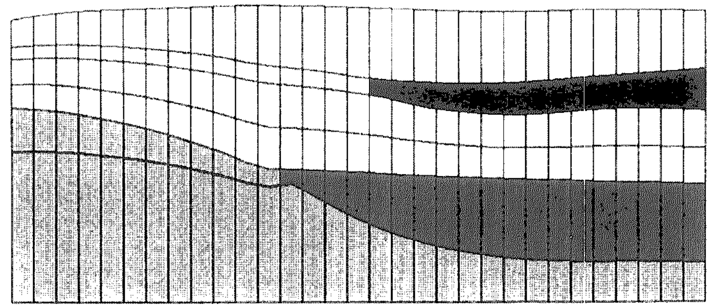


**Figure 7. Results of boundary-matching algorithm after using the minimum cell thickness technique. Compare to Figure 3b.**

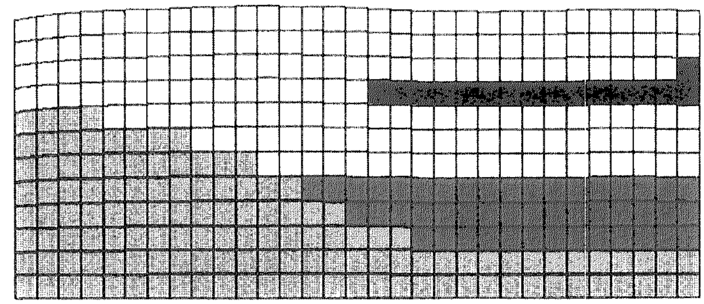


**Figure 8. MODFLOW grid after applying the grid overlay method using the simple discretization approach. Compare to Figure 7.**

## Grid Overlay Method

In cases where the minimum thickness criterion used with the boundary-matching algorithm still does not result in a satisfactory grid, the "grid overlay" conversion method can be used. This method does not accurately preserve interior boundaries, but it is simple and results in more uniform cell size transitioning. With the grid overlay method, a MODFLOW grid of fine resolution and regular vertical spacing is compared with the solid model. Unlike the boundary-matching algorithm, no layer assignments are made to the solids. For each vertical column of cells in the grid, a vertical ray is intersected with the solids and the maximum and minimum elevations of the solids are found. The cell elevations are then linearly interpolated between the top and bottom of the solids. The resulting uniformly spaced cell thicknesses may result in improved model stability, particularly for transport simulations.

Once the elevations are assigned via the grid-overlay method, a simple discretization or an equivalent properties technique can be used to assign the material properties.

### Simple Discretization

The simplest approach is to compare the centroid of each cell with the solids to determine which solid contains the cell centroid. The material properties associated with the solid are then inherited by the cell. The grid resulting from the sample problem of Figure 3a is shown in Figure 8.

### Equivalent Properties

The second approach for assigning properties is a weighted mean procedure, where the property is weighted by the thickness of the units within the MODFLOW layer. In this process, the first step is to compute a ray/solid intersection list for each vertical column of cells. Each cell in the column is then compared with the ray/solid intersection list, and the sequence of solids inside the cell is determined (Figures 9a and 9b). The stratigraphy defined by the solids in the cells is then assumed to follow the simple idealized pattern

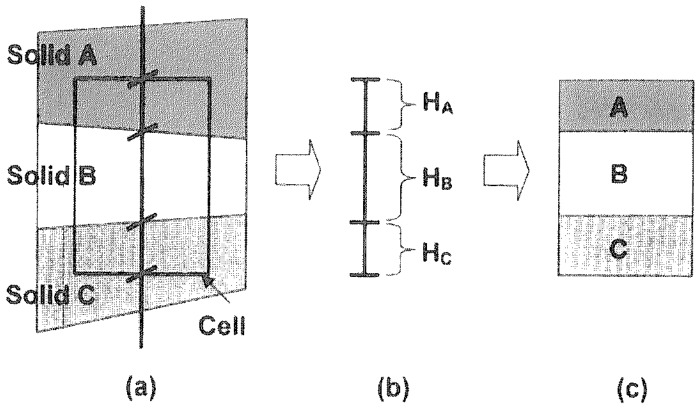



**Figure 9. Determining overlap lengths to use in weighted average formula: (a) side view of cell overlapping solids, (b) ray/solid intersection list, (c) idealized representation of solids inside cell.**

shown in Figure 9c. Using this idealized representation, a set of equivalent material properties can be computed for the cell. For example, the horizontal hydraulic conductivity can be computed using the traditional "flow parallel to strata" equation:

$$k_{heq} = \frac{\sum_{i=1}^{n} k_{hi} H_i}{\sum_{i=1}^{n} H_i} \qquad (1)$$

where $k_{heq}$ is the equivalent horizontal hydraulic conductivity for the cell; $k_{hi}$ is the horizontal hydraulic conductivity for each solid; and $H_i$ is the thickness of each solid in the cell.

A similar equation can be used to compute an equivalent vertical hydraulic conductivity and equivalent storage coefficients.

## HUF Package

A new flow package was recently introduced with MODFLOW 2000, called the Hydrogeologic-Unit Flow (HUF) package. This package is designed to represent complex stratigraphic relationships in a grid-independent fashion. The hydrostratigraphy is represented using a set of hydrogeologic units. Each unit is defined by two arrays, one for the top elevation and one for the thickness. The thickness values can be set to zero in regions of the model where the unit is not present. When MODFLOW is executed, each cell is compared with the corresponding unit elevation arrays, and equivalent hydraulic properties are assigned using the approach described in the previous section.

Solid models are an ideal tool for generating input for the HUF package. Once the ray/solid intersection lists have been generated for each vertical column of cells, the elevations defined by the intersections can be used to directly create the top elevation and thickness arrays used by the HUF package.

## Conclusions

Solid models of hydrogeologic units are a powerful and flexible tool for generating layer elevation data for MODFLOW models. We have presented several algorithms for generating MODFLOW-compliant computational grids from arbitrarily complex stratigraphy data. These techniques make it possible to include embedded seams, truncated layers, and discontinuous alluvial deposits in a MODFLOW model quickly and easily. Including such features can lead to more accurate ground water models. Solid models also provide the layer geometry component of a completely grid-independent conceptual model approach to defining and managing ground water model data.

The algorithms presented in this paper have been implemented in the Groundwater Modeling System (GMS) developed at the Environmental Modeling Research Laboratory at Brigham Young University.

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