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# Documentation for Variable Density Flow Modifications to the USGS Modflow Program

*by*

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AUSTRALIAN
GEOLOGICAL SURVEY
ORGANISATION

# *DOCUMENTATION FOR*

# *VARIABLE DENSITY FLOW*

# *MODIFICATIONS TO THE USGS MODFLOW PROGRAM*

# *(A.G.S.O. RELEASE 1.3)*

*AUSTRALIAN GEOLOGICAL SURVEY ORGANISATION*

*GEOHAZARDS, LAND and WATER RESOURCES DIVISION*

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# DOCUMENTATION FOR VARIABLE DENSITY FLOW MODIFICATIONS TO THE U.S.G.S. MODFLOW PROGRAM

## ABSTRACT

This report presents modifications to a finite difference model and its associated modular computer program (the United States Geological Survey's MODFLOW groundwater flow simulation program). The model simulates variable density groundwater flow in three dimensions. The report includes detailed explanations of the physical and mathematical concepts on which the model is based. The original modular structure of the MODFLOW program has been retained wherever possible.

Variable density groundwater flow within an aquifer is simulated using a block-centered finite-difference approach, with the solution package solving the simulation for freshwater heads. Packages for variable density flow associated with external stresses, such as wells, areal recharge, evapotranspiration, drains, and streams, are also included.

The modifications to the program have been written in FORTRAN 77 and will run without modification on most computers that have a FORTRAN 77 compiler.

The report should be read in conjunction with the original U.S.G.S. MODFLOW documentation.

# CHAPTER 1

# INTRODUCTION

The variable density groundwater flow algorithms implemented in this package are based on those of Kuiper (1983, 1985). MODFLOW was chosen as the base program for the variable density groundwater flow model due to its large number of field applications, its robustness, and its comprehensive software and user documentation.

This document does not replace the documentation supplied with MODFLOW, but should be read in conjunction with it. Where equations from the MODFLOW documentation are referenced, their number is preceded with an "M".

The groundwater flow equation with constant density is used for most groundwater flow studies, as the groundwater density is usually very close to 1 kg/l. In some sedimentary basins with saline aquifers, the groundwater density must be treated as a spatially dependent variable. The density of groundwater is dependent on temperature, pressure and salinity, but is most strongly dependent on salinity. Density changes that occur as a result of thermal and salt transport tend to be much slower than those due to pressure changes. It is therefore reasonable in some situations to regard density as being time independent (Kuiper, 1983). The variable density version of MODFLOW described in this document is best applied in situations where groundwater density varies spatially, but is time invariant over the period of the simulation.

## Equivalent Freshwater Head and Hydraulic Head

In this document, the hydraulic head at a point is defined as the elevation above a datum of the formation water in a well bore penetrating to the measurement point.

Equivalent freshwater heads are used to normalise head measurements in aquifers or other groundwater flow systems that have spatial variations in groundwater density.

The equivalent freshwater head at a given point within an aquifer is defined as "the water level elevation in a well filled with freshwater to a level high enough to balance the existing fluid pressure at that point" (Davies, 1987). The equivalent freshwater head of cell i,j,k, ($h'_{i,j,k}$) can be calculated from the hydraulic head of the cell ($h_{i,j,k}$) using the relationship :-

$$h'_{i,j,k} = ( h_{i,j,k} - CEN_{i,j,k} ) \frac{\rho_{i,j,k}}{\rho_0} + CEN_{i,j,k} \qquad (1)$$

where $CEN_{i,j,k}$ = the elevation of the centre of cell i,j,k.
$\rho_0$ = the density of freshwater

The centre of the model cell is taken to be the average of the top and bottom of the cell if the layer is permanently saturated (layer type 0) or if the hydraulic head is above the top of the cell. Otherwise the centre of the cell is taken to be the midpoint of the hydraulic head in the cell and the bottom of the cell. Note that the equivalent freshwater head varies with elevation within an aquifer (if the relative density is other than unity), necessitating the use of an average freshwater head value (figure 1).

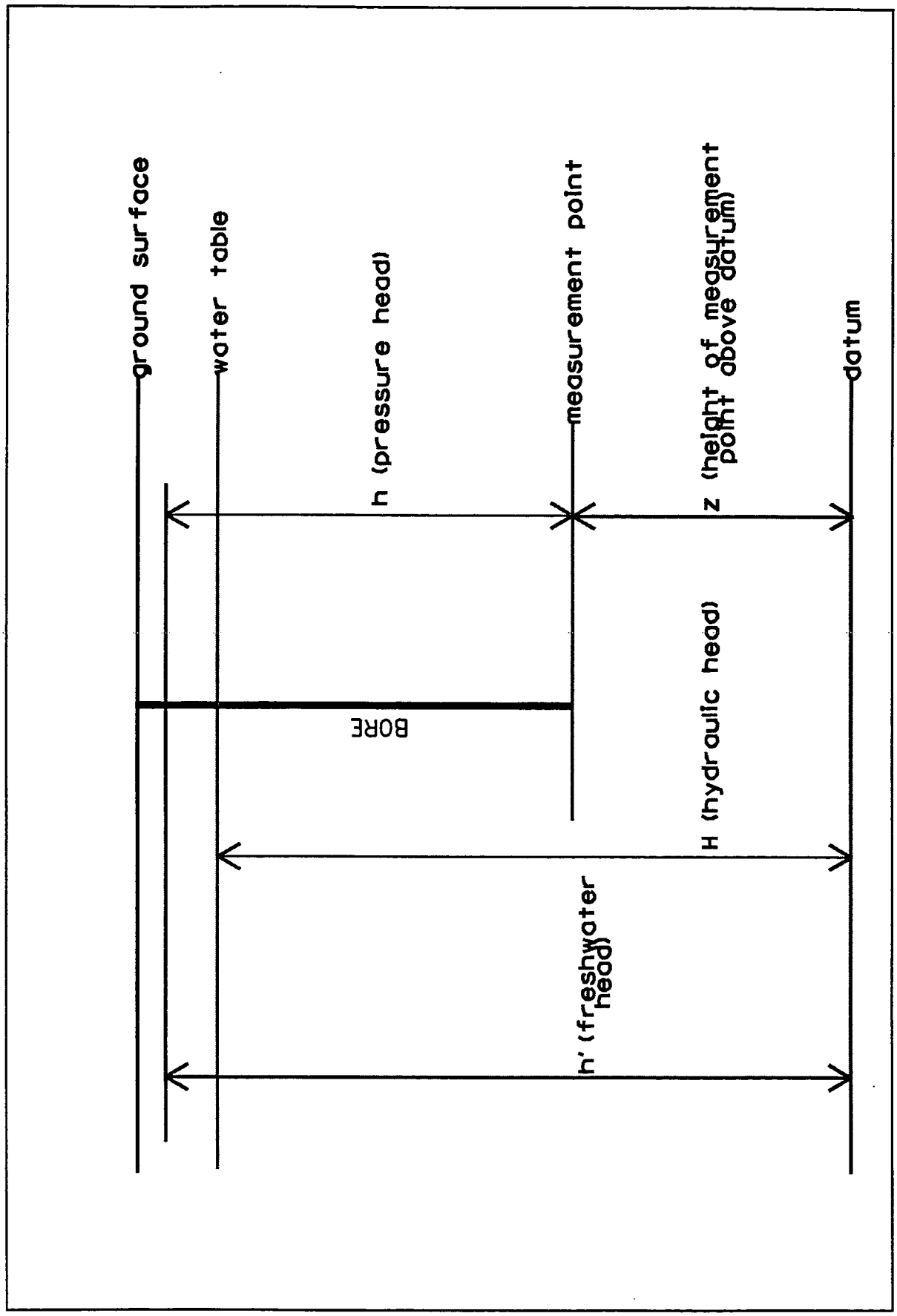


Figure 1: head definitions for variable density.

Therefore, in groundwater flow systems that have variations in groundwater density, it is not reasonable to assume that the water level in an unconfined cell is identical to the freshwater head, nor is it reasonable to assume that the hydraulic head in a confined model cell is identical to the freshwater head.

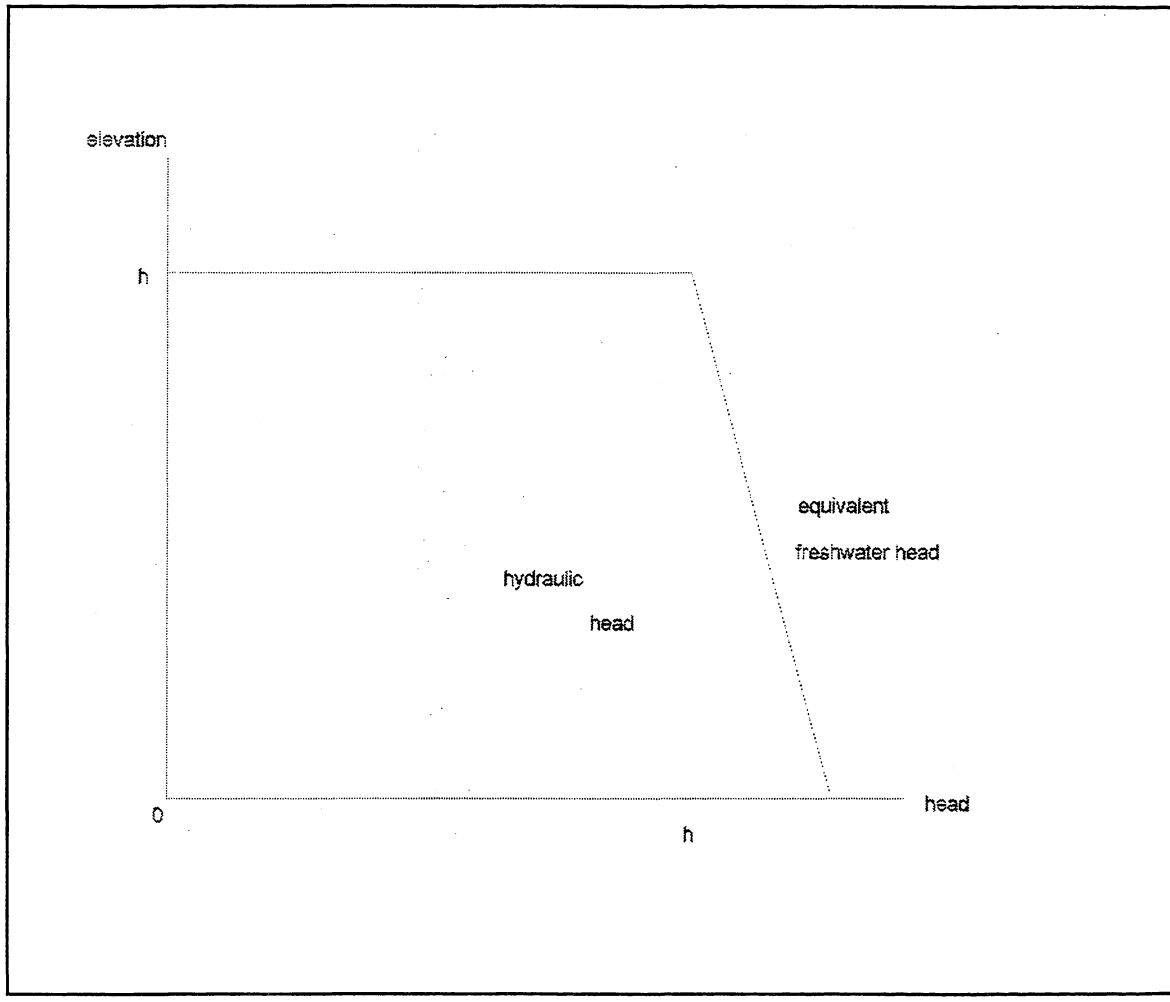


**Figure 2**: Variation of equivalent freshwater head with elevation within a single model cell

Hydraulic heads should be used in all situations where the determination of a model parameter is dependent on the water level of a cell. For example, in transient simulations specific yield or specific storage will be used to determine the flow from storage in a cell. If the cell is confined, the product of confined storage coefficient, fluid density, and the change in equivalent freshwater head between the last

two iterations, divided by the length of the time step (compare with equation M.60) is used to determine the mass flow from storage. If the cell is unconfined, the product of the unconfined storage coefficient, fluid density, and the change in water level (hydraulic head) divided by the time step length (compare with equation M.61) gives the mass flow from storage. Hydraulic conductances in convertible layers must also be calculated from hydraulic heads, in conjunction with hydraulic conductivity values and cell dimensions.

The volumetric budget appropriate to a constant density simulation is no longer sufficient for a variable density simulation, the modified version of MODFLOW now calculates the mass budget of the simulation. The mass budget is based on the conservation of groundwater mass.

When specifying parameters sets for this program, units of length should be metres, giving mass flow rates in metric tonnes - the program assumes the density of freshwater to be 1 tonne/$m^3$.

## Groundwater Flow Equations

The steady state constant density groundwater flow equation can be modified to allow for variations in fluid density. Following Kuiper's (1983) derivation, the general vector form of Darcy's equation for an isotropic medium is :

$$\bar{q} = \frac{-k}{\mu} \cdot \left[ \nabla p + \rho g \nabla z \right] \qquad (2)$$

where $q$ = specific discharge of the fluid
$k$ = intrinsic permeability tensor of the porous medium
$\mu$ = dynamic viscosity of the fluid
$p$ = pressure of the fluid
$\rho$ = density of the fluid
$g$ = acceleration due to gravity
$z$ = vertical distance measured upwards

With the equivalent freshwater head defined by:

$$h' = \frac{p}{\rho_0 g} + z \qquad (3)$$

where $\rho_0$ =1 tonne/m$^3$

and the hydraulic conductivity tensor K defined by:

$$K = \frac{k\rho g}{\mu} \qquad (4)$$

then Darcy's equation (2) becomes:

$$q = - \frac{K \rho_0}{\rho} \left( \nabla h' + \frac{\rho - \rho_0}{\rho_0} \cdot \nabla z \right) \qquad (5)$$

If the tensor K' is defined as:

$$K' = K \rho_0 = \frac{k \rho_0 \rho g}{\mu} \tag{6}$$

then it follows that:

$$\rho \bar{q} = -K' \left[ \nabla h' + \frac{\rho - \rho_0}{\rho_0} \nabla z \right] \tag{7}$$

The first term within the brackets of the equation (7) is the gradient of equivalent freshwater head. The second term within the brackets is Davies' "density related gravity dependent flow" term, and will only be non-zero where flow includes a vertical component.

The mass flow rate in the vertical direction ($F_z$)can be calculated from:

$$F_z = \int_{Sz} \rho q_z \, ds \tag{8}$$

where $S_z$ is the cross-sectional area of the vertical flow path.

If the z-axis of the model grid is parallel to the z-axis of the conductivity tensor, then the mass flow rate between two vertically adjacent model cells is given by:

$$F_z = \Delta x_i \, \Delta y_i \, K_{zz} \, \rho_0 \left[ \frac{\partial h'}{\partial z} + \frac{\rho - \rho_0}{\rho} \right] \tag{9}$$

where $\Delta x_i$ and $\Delta y_i$ are the horizontal diomensions of the model cell.

In finite difference form, the above equation may be expressed as:

$$F_z = \frac{\Delta x_i \, \Delta y_i}{\Delta z} K_{zz} \, \rho_0 \left[ \Delta h' + \frac{(\rho_1 - \rho_0) \, b_1 + (\rho_2 - \rho_0) \, b_2}{2 \, \rho_0} \right] \tag{10}$$

where $b_1$ and $b_2$ are the vertical thicknesses of each model cell, and $\rho_1$ and $\rho_2$ are the densities of the groundwater in cells 1 and 2 respectively. Note that the bracketed parameters in equation (10) above are equivalent to the difference between the environmental heads at the centers of the two cells (Lusczynski, 1961). The second term inside the brackets is the harmonic mean of the difference between the density of the fluid in the cell and the reference freshwater density.

Mass flow in the horizontal direction parallel to the x axis is given by:

$$F_x = \int_{Sx} \rho \, q_x \, ds \tag{11}$$

The mass flow rate between two horizontally adjacent model cells, whose centers differ in elevation by $\Delta z$, can be expressed as:

$$F_x = A_x \, K_{xx} \, \rho_0 \left[ \frac{\Delta h'}{l} + \frac{\rho - \rho_0}{\rho_0} \, \frac{\Delta z}{l} \right] \tag{12}$$

The cross-sectional area of the flow path ($A_x$ in equation (12), can be approximated from the product of the widths of the two cells parallel to the y-axis and the harmonic mean of the thicknesses of the two cells:

$$A_x = \Delta y \left( \frac{b_1 \, \Delta x_1 + b_2 \, \Delta x_2}{\Delta x_1 + \Delta x_2} \right) \tag{13}$$

where $b_1$ and $b_2$ are the thicknesses of each of the two cells.

The length of the horizontal component of the flow path (l) is given by:

$$l = \frac{\Delta x_1 + \Delta x_2}{2} \tag{14}$$

The mean density difference can be approximated from the difference between the harmonic mean of the fluid in each of the two cells and the reference fluid density:

$$\rho - \rho_0 = \frac{(\rho_1 - \rho_0)\,\Delta x_1 + (\rho_2 - \rho_0)\,\Delta x_2}{\Delta x_1 - \Delta x_2} \qquad (15)$$

The density dependent flow terms in equations 10 and 12 are not head dependent for confined model layers, so these terms must be placed on the right hand side (matrix RHS) of equation M.29, otherwise matrix [A] of equation M.29 would be rendered nonsymmetric.

## Viscosity Effects

The dynamic viscosity of the fluid in an aquifer can significantly alter the effective transmissivity of an aquifer. Dynamic viscosity is dependent on temperature, pressure and dissolved solids. Weiss (1982) has calculated the following empirical relationship between dynamic viscosity, dissolved solids concentration, and temperature:

$$\mu = \left( \frac{38.3432}{T_g^{1/2}} - \frac{14.621}{T_g^{1/4}} + 1.481 \right) \left( 1 + \frac{TDS}{300} \right) \qquad (16)$$

where $\mu$ = dynamic viscosity at node i,j,k in centipoise
$T_g$ = fluid temperature in °F
TDS = dissolved solids concentration, g/L

The reationship between temperature, TDS and viscosity is depicted graphically in figure 3.

The hydraulic conductivity values, and the values of parameters derived from conductivity values will be altered considerably if either:

i) the TDS of the fluid is high, and hence the viscosity of the fluid is high

or:

ii) the temperature of the fluid is high, and hence the viscosity of the fluid is low

If hydraulic conductivity or transmissivity values are determined from field measurements, then these values should be used as parameters in the hydrogeological model, provided that the fluid density does not change during the time period being modelled and between the time the measurements were

taken and the start of the time period being simulated. Care should be taken when extrapolating measured values of hydraulic conductivity parameters to other areas of the model where the fluid density is different, or where the temperature of the fluid varies.

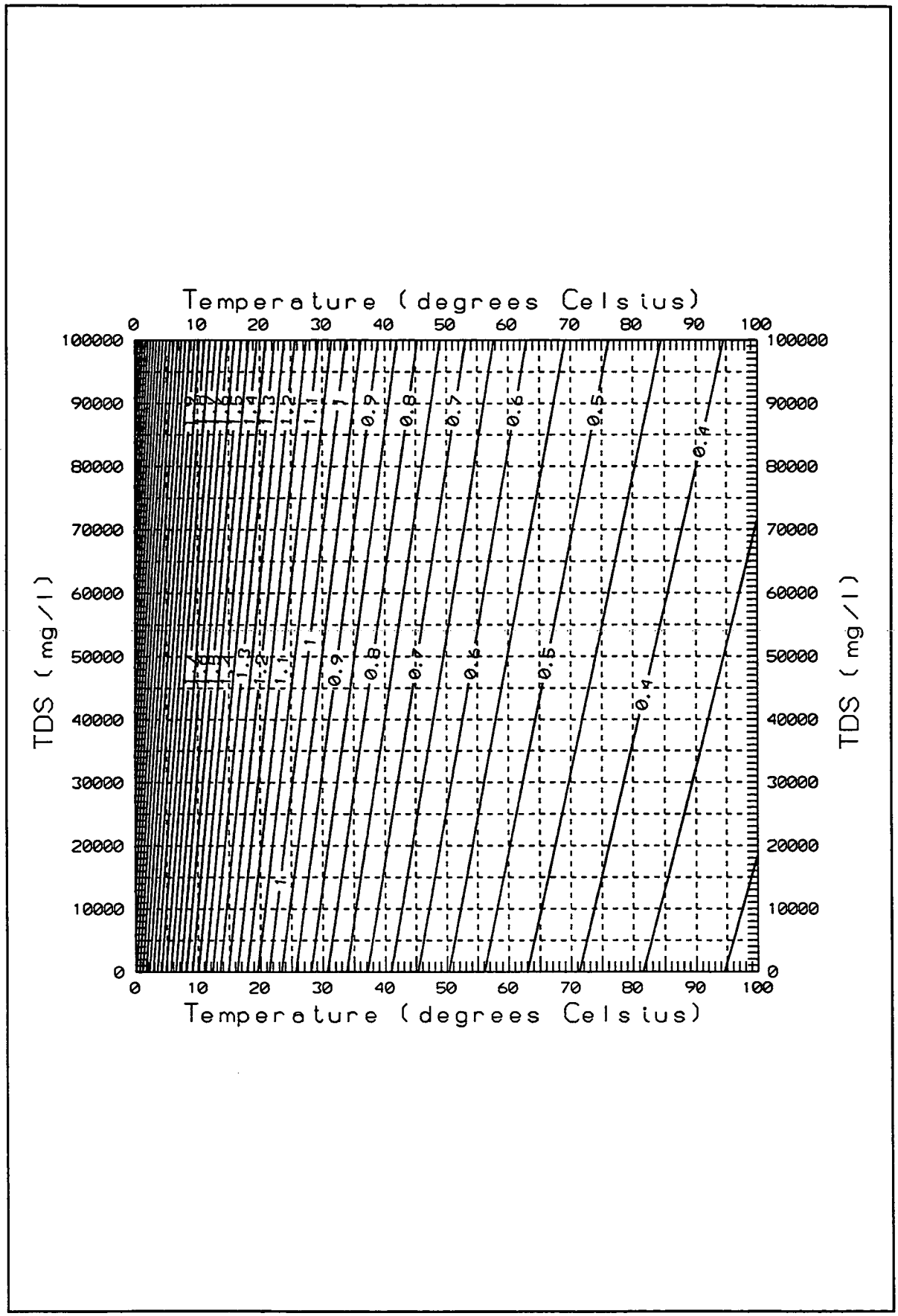


Figure 3: viscosity (centipoise) from temperature and total dissolved solids

CHAPTER 2

DENSITY PACKAGE

Conceptualisation and Implementation

The density package supports direct specification of the fluid density in each model cell, or alternatively, values for density can be calculated from the specified values of TDS (mg/litre), temperature (degrees celsius) and observed head at the centre of the cell (meters).

Calculation of Density from TDS, Temperature and Pressure

The density of the groundwater can be determined from temperature, pressure (as a head value) and TDS. The iterative method used is based on that of Kuiper (1985) and Kontis and Mandle (1987), and is based on the data of Potter and Brown (1977). The algorithm assumes that the solute in the groundwater sample is composed only of sodium chloride.

For the initial iteration of each density determination, the density of the groundwater sample is set to 1 gram/cc. The molality is then calculated from the following equation (Weiss, 1982):

$$MOL = \frac{TDS / 1000}{wt\left(\rho - \frac{TDS}{1,000,000}\right)} \qquad (17)$$

where: MOL = molality of groundwater, mol/kg
TDS = dissolved solids concentration of the groundwater, mg/l (at 20 °C and standard atmospheric pressure)
wt = gram molecular weight of sodium chloride (58.4428 g/mol)
$\rho$ = density of groundwater (gram/cc) (at 20 °C and standard atmospheric pressure)

The density ratio is then calculated (Potter and Brown, 1977, Kuiper, 1985) from:

$$\frac{\rho}{\rho_0} = \frac{1000 + wt\ MOL}{\frac{1000}{\rho_w/\rho_0} + A_0\ MOL + B_0\ MOL^{3/2} + C_0\ MOL^2} \qquad (18)$$

where: $\rho_w$ = density of pure water at the temperature and pressure of the groundwater sample
$A_0, B_0, C_0$ are constants for a given temperature, and determined by third order polynomial interpolation of known values of density and concentration of NaCl at 0, 25, 50 and 75 °C.

The pressure dependent density perturbation is calculated from (Kuiper, 1985):

$$\delta(P,MOL,T) = \begin{cases} \dfrac{a\ MOL + b}{10,000,000} P & ,0 \le P \le 10,000 kPa \\ \dfrac{a\ MOL+b}{1000} + \dfrac{.84(x-1)+3.75}{100,000}\left(\dfrac{P}{100}-100\right) & ,10,000 \le P \le 50,000 kPa \end{cases} \quad (19)$$

where: x = temperature / 25, with temperature in degrees celsius
a = -.75 (x - 1) + .25
b = 3.5 (x - 1) + 2
P = pressure, kPa

Pressure in the above equation is calculated from:

$$p = \rho g l' \quad (20)$$

where: $\rho$ = density of fluid in the cell
g = acceleration due to gravity
l' = observed head in cell

Because the pressure is density dependent, and the pressure perturbation in density is pressure dependent, the equations (19) and (20) are solved iteratively until the density pressure perturbation convergence criterion is satisfied.

When the new density value has been determined (with the pressure perturbation), the molality can then be recalculated with this most recent density value. Density and molality values are calculated iteratively until the density convergence criterion is satisfied.

The algorithm produces satisfactory results for temperatures in the range 0° C - 75° C, pressures between 0 and 10,000 kPa, and molalities less than 6 mol/kg.

## Density Package Input

Input for the density package is read from the unit specified in IUNIT(14).

FOR EACH SIMULATION

DEN1AL

1. Data: NDENOP IDENCB
   Format: I10 I10

DEN1RP

Density values or data sufficient to calculate density are read for each layer of the simulation in turn.

IF DENSITY IS TO BE ENTERED DIRECTLY

2. Data: DENS(NCOL,NROW)
   Module: U2DREL

IF DENSITY IS TO BE CALCULATED FROM TEMPERATURE, OBSERVED HYDRAULIC HEAD AND TDS

3. Data: TMPT(NCOL,NROW)
   Module: U2DREL

4. Data: TDS(NCOL,NROW)
   Module: U2DREL

5. Data: HDDN(NCOL,NROW)
   Module: U2DREL

### Explanation of Fields Used in the Input Instructions

NDENOP-- is the density calculation flag.

If NDENOP = 0, density values are input directly into the program.

If NDENOP = 1, density values are calculated from temperature, NaCl concentration, and starting head.

IDENCB-- is the density print out flag.

If IDENCB = 0, density values will not be printed.

If IDENCB = 1, density values will be printed.

DENS-- is the density of the fluid in the cell (kilograms/litre).
Read in directly if NDENOP is 0, or calculated from temperature, NaCl concentration and starting head if NDENOP is 1.

TMPT-- is the temperature in degrees celsius. Read in if NDENOP is 1.

TDS-(in mg/l measured at room temperature). Note that the algorithmn used to calculate density assumes that the solute is composed solely of NaCl. Read in if NDENOP is 1.

HDDN--is the observed hydraulic head at the centre of the cell (meters).
Read in if NDENOP is 1.

## Module Documentation for the Density Package

The density package has four primary modules and four sub-modules. The modules are:

### Primary Modules

DEN1AL Allocates space for data arrays used in the density package.

DEN1RP Reads all data needed by the package, invokes SDEN1CA to calculate density if required, SDEN1FH to calculate equivalent freshwater heads, and SDEN1SC to determine the saturated thickness of permanently saturated layers.

DEN1BD calculates mass budgets for density related gravity dependent flow.

DEN1RF calculates density related gravity dependent flow through the right face of cells.

DEN1RF calculates density related gravity dependent flow through the right face of each cell.

DEN1LF calculates density related gravity dependent flow through the lower face of each cell.

DEN1SH Calculates (and prints) hydraulic head from equivalent freshwater head, cell dimensions and saturated thickness.

DEN1SP saves current time step hydraulic heads as previous time step hydraulic heads.

DEN1FM Calculates the density related gravity dependent coefficients of the system of

equations. SDEN1ST is called to calculate the saturated thickness of unconfined layers.

DENCEN Calculates the centre of the saturated portion of a single cell from the layer type, bottom and hydraulic head or top of the cell.

Submodules

| | |
|---|---|
| SDEN1CA | Calculates (and prints) density for a layer from temperature, NaCl and observed hydraulic head at the centre of the cell. |
| SDEN1FH | Calculates (and prints) freshwater heads from hydraulic heads, density and cell dimensions. |
| SDEN1SC | Calculates the centre of the saturated portion of a cell from fresh water head and cell dimensions for permanently confined layers. |

Narrative for Module DEN1AL

This module allocates space for data arrays used in the density package. this is done in the following order. This is done in the following order:

1. Compute dimensions of arrays.

2. Print the message identifying the package.

3. If the density component of the model is not being used then set the hydraulic head array pointer to the freshwater head array pointer, initialise the density difference array values to 0, and return.

4. Read and print the density calculation flag (NDENOP), and the flag for printing the density values (IDENCB).

5. Compute the sizes of the arrays required to store density parameters, and allocate space for them, only allocate space for the TDS, observed head, and temperature arrays if they are needed.

6. Print the amount of space used by the density package.

7. Return.

Narrative for Module DEN1RP

This module reads all data needed by the density package, invokes SDEN1CA to calculate density if required, SDEN1FH to calculate equivalent freshwater heads, and SDEN1SC to determine the saturated thickness of permanently saturated layers. This is done in the following order:

1. Calculate the number of nodes in a layer.

2. For each layer, use utility module U2DREL to read the density parameters.

(a) Find the address of the array in the layer.

(b) If density is to be entered directly (NDENOP = 0), read in the density for the layer.

(c) If density is to be calculated (NDENOP = 1), read in the values of temperature (TMPT), TDS and observed heads (HDDN) for the layer.

(d) If density is to be calculated, call SDEN1CA to determine density from temperature, TDS and observed head.

3. Convert the density values in the DENS array to density difference values.

4. Calculate the freshwater equivalent head - saved in HOLD, and copy the values to HNEW (SDEN1FH). Convert the starting heads to freshwater equivalent heads (SDEN1FH).

5. Determine the cell centres of permanently saturated layers (SDEN1SC).

6. Return.

## Narrative for Module DENCEN

This module calculates the elevation of the centre of the saturated portion of a cell from the hydraulic head.

1. If the cell is permanently confined, the elevation of the centre of the saturated portion of the cell is midway between the top and bottom of the cell.

2. If the cell is permanently unconfined, the elevation of the centre of the saturated portion of the cell is midway between the water level in the cell and the bottom of the cell.

3. If the cell is convertible, the elevation of the centre of the saturated portion of the cell is midway between the top and bottom of the cell (if confined), or midway between the water level and the bottom of the cell (if unconfined).

4. Return.

Narrative for Module DEN1BD

This module calculates and prints mass budgets for density related gravity dependent flow. This is done by:

1. Initialise the density budget accumulators.

2. Set the cell by cell flow budget flag if cell by cell flow budget terms are required.

3. Clear the cell by cell flow budget array if cell by cell flow budget flag is set.

4. Process every cell in the model grid (5. - 11.)

5. Don't determine flow rates for cells that are not active.

6. If there is an active cell to the left of the current cell, determine the flow to or from that cell to the current cell.

7. If there is an active cell to the right of the current cell, determine the flow to or from that cell to the current cell.

8. If there is an active cell to the front of the current cell, determine the flow to or from that cell to the current cell.

9. If there is an active cell to the rear of the current cell, determine the flow to or from that cell to the current cell.

10. If there is an active cell above the current cell, determine the flow to or from that cell to the current cell.

11. If there is an active cell below the current cell, determine the flow to or from that cell to the current cell.

12. If cell by cell flow budgets are required, record the contents of the buffer.

13. Save the total of the density dependent flow rates.

14. Initialise the density mass budget print out titles.

## Narrative for Module DEN1RF

This module calculates density dependent flow through the right face of cells.

1. If there is only one column in the model, then return.

2. Process each cell in each layer (excepting the right most column), steps 3 - 4.

3. Only process density related gravity dependent flow between active cells and other active or constant head cells.

4. Calculate flow through the right face and add to the buffer.

5. Return.

## Narrative for Module DEN1FF

This module calculates density dependent flow through the front face of cells.

1. If there is only one row in the model, then return.

2. Process each cell in each layer (excepting the frontmost row), steps 3 - 4.

3. Only process density related gravity dependent flow between active cells and other active or constant head cells.

4. Calculate flow through the front face and add to the buffer.

5. Return.

## Narrative for Module DEN1LF

This module calculates density dependent flow through the lower face of cells.

1. If there is only one layer in the model, then return.

2. Process each cell in each layer (excepting the lower most layer) steps 3 - 4.

3. Only process density related gravity dependent flow between active cells and other active or constant head cells.

4. Calculate flow through the lower face and add to the buffer.

5. Return.

## Narrative for Module DEN1SH

This module calculates (and prints) hydraulic head from equivalent freshwater head, cell dimensions and saturated thickness. This is done in the following order:

1. For each active node in the simulation -

    (a) Calculate the center of the cell at the last iteration

    (b) Calculate the hydraulic head in the cell for the current time step.

    (c) Calculate the center of the cell for the current time step.

    (d) Calculate the freshwater head in the cell for the current time step.

2. Return.

## Narrative for Module DEN1SP

This module copies the hydraulic heads for the current time step into the array holding the hydraulic heads from the previous time step.

1. For each cell in the model grid, copy the hydraulic head for the current time step into the hydraulic head array for the previous time step if the cell is active. If the cell is not active, set the hydraulic head for the previous time step to zero.

2. Return.

## Narrative for Module DEN1FM

This module calculates the density related gravity dependent coefficients of the system of equations, and adds these coefficients to the right hand side array (RHS). SDEN1ST is called to calculate the saturated thickness of unconfined layers. This is done in the following order:

1. Calculate saturated height for potentially unconfined layers (SDEN1ST).

2. For each active node in the simulation :-

    (a) calculate density dependent flow to cell at left.

    (b) add density dependent flow to cell at left to RHS array.

    (c) calculate density dependent flow to cell in front.

    (d) add density dependent flow to cell in front to RHS array.

    (e) calculate density dependent flow to cell below.

    (f) add density dependent flow to cell below to RHS array.

3. Return.

Narrative for Module SDEN1CA

This module calculates (and prints) density from input temperature, NaCl and observed heads. This is done in the following order:

1. For each node in the simulation, perform steps 2 - 13

2. Set the density of inactive cells (IBOUND = 0) to zero, and process the next cell.

3. Get the TDS of the fluid in the cell.

4. Determine the molarity of the solution, assuming that the solution is composed water and sodium chloride, with a density of 1 gm/cc.

5. Determine the interpolation coefficients for the cell temperature.

6. Determine the density of pure water at the cell temperature.

7. Iteratively refine the density value by performing steps 9 - 12.

8. Save the latest molality value as the previous molality value, and determine molality using most recent density value.

9. Calculate density from most recent molality value and temperature.

10. Determine the constants for calculating the pressure perturbation.

11. Calculate the height of a column of groundwater fluid from the measurement point in the center of the cell.

12. Iteratively refine the pressure perturbation in density.

13. Save the density value in the density array.

14. Print the density values

15. Return.

Narrative for Module SDEN1FH

This module calculates (and prints) freshwater heads from hydraulic heads, density and cell dimensions. This is done in the following order:

1. For each active node in the simulation -

    (a) If the cell is inactive, set the freshwater head to zero.

    (b) Determine the center of the cell (DENCEN)

    (c) Determine the equivalent freshwater head from density, elevation of the cell bottom and hydraulic head.

2. Print the fresh water head of each node (ULAPRW).

3. Return.

Narrative for Module SDEN1SC

This module calculates the centre of the saturated portion of a cell from fresh water head and cell dimensions for permanently confined layers. This is done in the following manner:

1. For each active node in layers which are permanently confined

(a) calculate the saturated height from the elevation of the top of the cell.

(b) determine the elevation of the centre of the saturated portion of the cell from the saturated height of the cell and elevation of the base of the cell (DENCEN).

2. Return

Chapter 3

# BASIC PACKAGE

## Conceptualisation and Implementation

Minimal changes to the basic package have been made. It is now necessary to specify the input unit for the density package, this unit is held in the fourteenth element of the IUNIT array. Calls to the density package modules have been inserted into the main routine.

The starting heads must be specified as hydraulic heads rather than freshwater equivalent heads.

Chapter 4

# BLOCK CENTRED FLOW PACKAGE

## Conceptualisation and Implementation

The changes to the input format of the block centred flow package were prompted by the requirement that vertical cell dimensions be available to the algorithms of the density package, irrespective of whether the simulated layer is confined or unconfined. The tops and bottoms of all cells must be entered as model input parameters because:

i) density related gravity dependent flow between horizontally adjacent model cells is dependent on the difference in elevation between these model cells. Significant errors can result if density related gravity dependent flow components are ignored or poorly simulated (Davies, 1987).

ii) calculation of freshwater equivalent head and hydraulic head requires that the elevation of the center of the cell be known.

## Storage Term Conversion

Density dependent storage capacities can be calculated by multiplying the volumetric storage capacities by the density:

$$SC'_{i,j,k} = \rho_{i,j,k} \, SC_{i,j,k} \tag{21}$$

where $SC'_{i,j,k}$ = density dependent storage capacity for cell i,j,k
$SC_{i,j,k}$ = storage capacity for cell i,j,k
$\rho_{i,j,k}$ = density of fluid in cell i,j,k

The rate of accumulation of mass from storage is related to the rate of accumulation of fluid volume from storage by:

$$\frac{\Delta m}{\Delta t} = \rho \frac{\Delta V}{\Delta t} \tag{22}$$

Rate of accumulation of mass from unconfined storage is proportional to the change in hydraulic head (or water level) rather than the change in freshwater head (or pressure head), and is formulated as follows:

$$\frac{\Delta m}{\Delta t} = SCU'_{i,j,k} \cdot \frac{h^{m}_{i,j,k} - h^{m-1}_{i,j,k}}{t_m - t_{m-1}} \tag{23}$$

where $\Delta m/\Delta t$ = mass flow from storage
$SCU'_{i,j,k}$ = density dependent unconfined storage capacity
$t_m$ = time at start of time step
$t_{m-1}$ = time at end of time step

As the variable density version of MODFLOW uses freshwater heads to solve the simulation, the hydraulic head for the current time step in the previous equation must be expressed as a freshwater head:

$$\frac{\Delta m}{\Delta t} = SCU'_{i,j,k} \cdot \frac{\frac{h'^{m}_{i,j,k} - CEN^{m}_{i,j,k}}{\rho_{i,j,k}/\rho_0} + CEN^{m}_{i,j,k} - h_{i,j,k}}{t_m - t_{m-1}} \qquad (24)$$

Algebraic manipulation of equation (24) produces:

$$\frac{\Delta m}{\Delta t} = \frac{SCU'_{i,j,k}\, h'^{m}_{i,j,k}}{\rho_{i,j,k} / \rho_0 \; ( t_m - t_{m-1} )} + \frac{SCU'_{i,j,k} \cdot \left( CEN^{m}_{i,j,k} \left( 1 - \frac{1}{\rho_{i,j,k} / \rho_0} \right) - h^{m-1}_{i,j,k} \right)}{t_m - t_{m-1}} \qquad (25)$$

where the head for the current time step is expressed as a freshwater head. The coefficient of head (first term in equation (25)) is subtracted from the HCOF array, and the remaining two terms are added to the RHS array.

Rate of accumulation of mass from confined storage is dependent on the change in freshwater head (or pressure head), rather than hydraulic head (or water level), and is formulated as:

$$\frac{\Delta m}{\Delta t} = SCC'_{i,j,k} \cdot \frac{h'^{m}_{i,j,k} - h'^{m-1}_{i,j,k}}{t_m - t_{m-1}} \qquad (26)$$

where $\Delta m/\Delta t_{i,j,k}$ = mass flow from storage
$SCC'_{i,j,k}$ = density dependent confined storage capacity
$t_m$ = time at start of time step
$t_{m-1}$ = time at end of time step

Equation (27) can now be developed to describe the rate of accumulation of mass from storage

in a cell moving from a confined state to an unconfined state during a given time step:

$$\frac{\Delta m}{\Delta t} = \frac{SCU'_{i,j,k} \left( h^{m}_{i,j,k} - TOP_{i,j,k} \right) + SCC'_{i,j,k} \left( TOP'_{i,j,k} - h^{/m-1}_{i,j,k} \right)}{t_m - t_{m-1}} \qquad (27)$$

where $TOP'_{i,j,k}$ = freshwater head at the time the cell moves from a confined state to an unconfined state

If the hydraulic head during the current time step in equation (27) is expressed as a freshwater head, then:

$$\frac{m}{t} = \frac{SCU'_{i,j,k} \; h^{/m}_{i,j,k}}{\rho_{i,j,k} / \rho_0 \; ( t_m - t_{m-1} )} + \frac{SCU'_{i,j,k} \left( CEN^{m}_{i,j,k} \left(1 - \frac{1}{\rho_{i,j,k} / \rho_0}\right) - TOP_{i,j,k}\right) + SCC'_{i,j,k}\left(TOP'_{i,j,k} - h^{/m-1}_{i,j,k}\right)}{t_m - t_{m-1}} \qquad (28)$$

This equation can now be used in the variable density version of MODFLOW. The coefficient of head (first term on the right hand side of equation 6) is subtracted from the HCOF array, and the remaining two terms are added to the RHS array.

A similar equation can be derived for a cell moving from an unconfined state to a confined state:

$$\frac{\Delta m}{\Delta t} = \frac{SCC'_{i,j,k} \; h^{/m}_{i,j,k}}{t_m - t_{m-1}} + \frac{- SCC'_{i,j,k} \; TOP'_{i,j,k} + SCU'_{i,j,k} \; (TOP_{i,j,k} - h_{i,j,k})}{t_m - t_{m-1}} \qquad (29)$$

## Block Centred Flow Package Input

Input for the block centred flow package is read from the unit specified in IUNIT(1). Note that the confined and unconfined storage capacities in the input file have identical units to the U.S.G.S. version of MODFLOW, and are not adjusted for density effects.

FOR EACH SIMULATION

BCF1AL

1. Data: ISS IBCFCB
   Format: I10 I10

2. Data: LAYCON(NLAY) (Maximum of 80 layers)
   FORMAT: 40I2

   (If there are 40 or fewer layers, use 1 record; otherwise use two records.)

BCF1RP

3. Data: TRPY(NLAY)
   Module: U1DREL

4. Data: DELR(NCOL)
   Module: U1DREL

5. Data: DELC(NCOL)
   Module: U1DREL

A subset of the following two dimensional arrays are used to describe each layer. The arrays needed for each layer depend on the layer type code (LAYCON) and whether the simulation is transient (ISS = 0) or steady state (ISS ≠ 0). If an array is not needed, it must be omitted. All of the arrays for layer 1 are read first; then all of the arrays for layer 2, etc.

FOR ALL LAYERS READ IN THE ELEVATION OF THE TOP OF EACH CELL

6. Data: TOPBOT(NCOL,NROW)
   Module: U2DREL

IF THE LAYER IS THE LOWERMOST, READ IN THE ELEVATION OF THE BOTTOM OF EACH CELL

7. Data: TOPBOT(NCOL,NROW)
   Module: U2DREL

FOR EVERY LAYER, READ IN THE HORIZONTAL HYDRAULIC CONDUCTIVITY

8. Data: HY(NCOL,NROW)
   Module: U2DREL

IF THE LAYER IS NOT THE LOWERMOST, READ IN VCONT (VERTICAL HYDRAULIC CONDUCTIVITY BETWEEN LAYERS DIVIDED BY THICKNESS)

9. Data: VCONT(NCOL,NROW)
Module: U2DREL

IF THE SIMULATION IS TRANSIENT

10.Data: SC1(NCOL,NROW)
Module: U2DREL

IF THE SIMULATION IS TRANSIENT, AND THE LAYER TYPE (LAYCON) IS 2 OR 3

11.Data: SC2(NCOL,NROW)
Module: U2DREL

All changes to the existing code have been bracketed with comments starting with "C AGT/BMR". Wherever reasonable, the pre-existing code has been retained as commented out sections.

BCF1AL has been modified to allocate storage for the new arrays used to save vertical and horizontal conductance. The array TOPBOT has been used to save top and bottom elevations of cells (the bottom elevation of a cell is the same as the elevation of the top of the cell below, the elevation of the bottom of the lowermost layer is entered explicitly). All references throughout the program to the previous TOP and BOT arrays have been replaced by references to the TOPBOT array.

BCF1RP has been modified to read the new input format for the BCF package.

SBCF1H now calculates conductance from saturated thickness and hydraulic conductivity.

BCFPRT is a debugging aid, and should not be useful in any other circumstance.

CHAPTER 5

# RIVER PACKAGE AND VARIABLE DENSITY GROUNDWATER FLOW

## Conceptualisation and Implementation

Rate of flow between a river and an aquifer is described in the constant density version of MODFLOW (M65) by the following two equations:

$$QRIV = \begin{cases} CRIV\ (HRIV - h_{i,j,k}) & , h_{i,j,k} > RBOT \\ CRIV\ (HRIV - RBOT) & , h_{i,j,k} \leq RBOT \end{cases} \qquad (30)$$

where QRIV = flow between the stream and the aquifer
CRIV = hydraulic conductance of the stream-aquifer connection
HRIV = head in the stream
$h_{i,j,k}$ = head in cell i,j,k
RBOT = elvation of river bottom

When the hydraulic head of the aquifer is above the base of the river, flow between the aquifer and the river is proportional to the difference between the freshwater head of the aquifer at the river bottom (which differs from the freshwater head at the centre of the aquifer) and the freshwater head of the river. Therefore, for a variable density model, the previous equation becomes:

$$QRIV' = \rho_0\ CRIV\ (\ HRIV' - h'_{Ri,j,k}\ ) \qquad (31)$$

where QRIV′ = mass flow into the cell from the river
HRIV′ = freshwater head in the river
$h'_{Ri,j,k}$ = freshwater head of the model cell at the elevation of the river bottom

As the variable density version of MODFLOW uses freshwater heads at the center of each cell to solve the simulation, the equivalent freshwater head in the model cell at the elevation of the river bottom must be expressed in terms of the equivalent freshwater head at the center of the model cell.

The relationship between the freshwater head of the aquifer at the base of the river ($h'_{Ri,j,k}$) and the freshwater head at the centre of the aquifer ($h'_{i,j,k}$) is given by:

$$\frac{h'_{Ri,j,k} - RBOT_{i,j,k}}{\rho_{i,j,k} / \rho_0} + RBOT_{i,j,k} = \frac{h'_{i,j,k} - CEN_{i,j,k}}{\rho_{i,j,k} / \rho_0} + CEN_{i,j,k} \qquad (32)$$

as the hydraulic head of the fluid within a cell is constant, irrespective of the position of the measuring point within the cell.

If the fluid in the river has a density greater than that of pure water, then the freshwater head of

$$HRIV' = ( HRIV - RBOT ) \frac{\rho_{RIV}}{\rho_0} + RBOT \qquad (33)$$

the river at the base of the river is given by:

where $\rho_{RIV}$ = density of the fluid in the river

The following formulation therefore describes flow between a river and an aquifer if the aquifer and/or river contain fluid with a density that is not equal to that of pure water:

$$RIV' = \begin{cases} \rho_0 \, CRIV \, (HRIV' - h'_{i,j,k} - (\rho_{i,j,k} / \rho_0 - 1)(CEN_{i,j,k} - RBOT)) & , h_{i,j,k} > RBOT \\ \rho_0 \, CRIV \, ( HRIV' - RBOT) & , h_{i,j,k} \leq RBOT \end{cases} \qquad (34)$$

The coefficient of the freshwater head (-CRIV) is added to the HCOF array if the hydraulic head in the aquifer is above the base of the river (RBOT), the remaining terms are subtracted from the RHS array.

## River Package Input

The formulation in the previous section requires that the density of the fluid in the river be specified in the river package input file. Input item 3 for the input file now becomes:

| 3. | Data: | Layer | Row | Column | Stage | Cond | Rbot | Rden |
|---|---|---|---|---|---|---|---|---|
| | Format: | I10 | I10 | I10 | F10.0 | F10.0 | F10.0 | F10.0 |

### Explanation of New or Modified Fields Used in the Input Instructions

Rden--is the density of the fluid in the river (kg/l)

CHAPTER 6

# RECHARGE PACKAGE AND VARIABLE DENSITY GROUNDWATER FLOW

## Conceptualisation and Implementation

Areal recharge in the constant density version of MODFLOW is modelled with the following equation:

$$Q_{Ri,j} = I_{i,j} * DELR_j * DELC_i \quad (35)$$

where $Q_{Ri,j}$ = recharge flow rate applied to the model at the horizontal cell location (i,j) (L*3/T)

$DELR_j * DELC_i$ = area of the cell

$I_{i,j}$ = recharge flux applied to the model cell (L/T)

The equivalent formula used for the variable density version of MODFLOW is:

$$Q'_{Ri,j} = I'_{i,j} * DELR_j * DELC_i \quad (36)$$

where $Q'_{Ri,j}$ = recharge mass flow rate applied to the model at the horizontal cell location (i,j) (M/T)

$DELR_j * DELC_i$ = area of the cell

$I'_{i,j}$ = recharge mass flux applied to the model cell (M/L*2/T)

As recharge is derived from rainfall (which by definition has a relative density of 1), the mass and volumetric recharge flux values in the two formulas are identical.

## Recharge Package Input

No changes have been made to the input file format for this module.

CHAPTER 7

WELL PACKAGE AND VARIABLE DENSITY GROUNDWATER FLOW

Conceptualisation and Implementation

The well recharge rate is now a mass recharge rate (M/T) rather than a volumetric recharge rate (L*3/T).

## Well Package Input

The mass recharge rate should now be specified in the well package input file rather than the volumetric recharge rate. Input item 3 of the well package input file becomes:

| | | | | | |
|---|---|---|---|---|---|
| 3. | DATA: | Layer | Row | Column | Q |
| | FORMAT: | I10 | I10 | I10 | F10.0 |

### Explanation of New or Modified Fields Used in the Input Instructions

Q--is now the mass recharge rate. A positive value indicates recharge and a negative value indicates discharge.

CHAPTER 8

# DRAIN PACKAGE AND VARIABLE DENSITY GROUNDWATER FLOW

## Conceptualisation and Implementation

Rate of flow between a drain and an aquifer is described in the constant density version of MODFLOW by the following equation:

$$QD_{i,j,k} = \begin{cases} CD_{i,j,k} \ (h_{i,j,k} - d_{i,j,k}) & , \ h_{i,j,k} > d_{i,j,k} \\ 0 & , \ h_{i,j,k} \leq d_{i,j,k} \end{cases} \qquad (37)$$

where $QD_{i,j,k}$ = discharge from aquifer to drain (L*3/T)
$CD_{i,j,k}$ = lumped hydraulic conductance of the drain-aquifer connection
$d_{i,j,k}$ = median drain elevation in cell i,j,k
$h_{i,j,k}$ = head in cell i,j,k

When the hydraulic head of the aquifer is above the median drain height, mass flow between the aquifer and the drain is proportional to the difference between the freshwater head of the aquifer at the median drain height and the freshwater head in the drain at the median drain height.

As the variable density version of MODFLOW uses freshwater heads to solve the simulation, the equivalent freshwater head in the model cell at the elevation of the drain must be expressed in terms of the freshwater head at the center of the model cell.

The relationship between the freshwater head of the aquifer at the elevation of the drain, and the freshwater head in the aquifer in the centre of the cell is (given that the hydraulic head within a cell is not dependent on elevation at which it is measured):

$$\frac{h'_{Di,j,k} - d_{i,j,k}}{\rho_{i,j,k} / \rho_0} + d_{i,j,k} = \frac{h'_{i,j,k} - CEN_{i,j,k}}{\rho_{i,j,k} / \rho_0} + CEN_{i,j,k} \qquad (38)$$

where $h'_{Di,j,k}$ = freshwater head at the elevation of the drain

Therefore the following equation describes mass flow between a drain and an aquifer:

$$QD'_{i,j,k} = \begin{cases} \rho_0 \, CD_{i,j,k}\left(h'_{i,j,k} + \left(\frac{\rho_{i,j,k}}{\rho_0} - 1\right)\left(CEN_{i,j,k} - d_{i,j,k}\right) - d_{i,j,k}\right) & , h_{i,j,k} > d_{i,j,k} \\ 0 & , h_{i,j,k} \le d_{i,j,k} \end{cases} \quad (39)$$

where $QD'_{i,j,k}$ = mass discharge from aquifer to drain (L*3/T)
$CD_{i,j,k}$ = lumped hydraulic conductance of the drain-aquifer connection
$d'_{i,j,k}$ = freshwater head at the median drain elevation
$h'_{i,j,k}$ = freshwater head in cell i,j,k

The coefficient of the freshwater head in the equation above is subtracted from the HCOF array, and the remaining terms are subtracted from the RHS array.

This formulation does not require the user to specify the density of the fluid in the drain.

## Drain Package Input

The calculation of freshwater head at the median drain elevation is performed by the MODFLOW program (from the density of the fluid in the model cell and the median elevation of the drain), and therefore there is no change to the input file format for this package.

CHAPTER 9

EVAPOTRANSPIRATION PACKAGE AND VARIABLE DENSITY GROUNDWATER FLOW

Conceptualisation and Implementation

Rate of volumetric flow from an aquifer due to evapotranspiration losses is modelled in the constant density version of MODFLOW with the following equation:

$$Q_{ETi,j} = \begin{cases} Q_{ETMi,j} & , h_{i,j,k} > h_{si,j} \\ 0 & , h_{i,j,k} > h_{si,j} - d_{i,j} \\ Q_{ETMi,j}\left(\dfrac{h_{i,j,k} - (h_{si,j} - d_{i,j})}{d_{i,j}}\right) & , (h_{si,j} - d_{i,j}) \le h_{i,j,k} \le h_{si,j} \end{cases} \quad (40)$$

where $Q_{ETi,j}$ = rate of loss per unit surface area of water table due to evapotranspiration
$Q_{ETMij}$ = maximum possible value of RETi,j
$h_{i,j,k}$ = head in cell i,j,k
$h_{si,j,k}$ = ET surface elevation
$d_{i,j}$ = cutoff or extinction depth

Evapotranspiration removes pure water from aquifers, and so the mass flow rate and volumetric flow rates due to evapotranspiration are numerically identical. The equation above may be expressed in terms of freshwater head:

$$\begin{cases} Q'_{ETMi,j} & , h_{i,j,k} > h_{si,j} \\ 0 & , h_{i,j,k} > h_{si,j} - d_{i,j} \\ Q'_{ETMi,j}\left(\dfrac{h'_{i,j,k}}{\rho_{i,j,k}/\rho_0\, d_{i,j}} + \dfrac{CEN_{i,j,k}\left(1 - \dfrac{1}{\rho_{i,j,k}/\rho_0}\right) - (h_{si,j} - d_{i,j})}{d_{i,j}}\right) & , (h_{si,j} - d_{i,j}) \le h_{i,j,k} \le h_{si,j} \end{cases} \quad (41)$$

where $Q'_{ETi,j}$ = rate of loss per unit area surface area of water table due to evapotranspiration
$Q'_{ETMij}$ = maximum possible value of RETi,j
$h_{i,j,k}$ = head in cell i,j,k
$h_{si,j,k}$ = ET surface elevation
$d_{i,j}$ = cutoff or extinction depth

The coefficient of freshwater head in the equation above is subtracted from the HCOF array, and the remaining terms are added to the RHS array.

## Evapotranspiration Package Input

No changes have been made to the input file format for this module.

CHAPTER 10

# GENERAL HEAD BOUNDARY PACKAGE AND VARIABLE DENSITY GROUNDWATER FLOW

## Conceptualisation and Implementation

In the constant density version of MODFLOW, the relationship for flow between a cell and an external source/sink (i.e. general head boundary) is defined as:

$$Q_{bi,j,k} = C_{bi,j,k} \left( h_{bi,j,k} - h_{i,j,k} \right) \qquad (42)$$

where $Q_{bi,j,k}$ = volumetric flow into the cell from a source

$C_{bi,j,k}$ = conductance between the external source and the cell

$h_{bi,j,k}$ = head assigned to the external source

$h_{i,j,k}$ = head in cell i,j,k

The equivalent variable density formulation is:

$$Q'_{bi,j,k} = \rho_0 C_{bi,j,k} \left( h'_{bi,j,k} - h'_{i,j,k} \right) \qquad (43)$$

where $Q'_{bi,j,k}$ = mass flow into the cell from a source

$C_{bi,j,k}$ = conductance between the external source and the cell

$h'_{bi,j,k}$ = freshwater head assigned to the external source

$h'_{i,j,k}$ = freshwater head in cell i,j,k

The variable density formulation of MODFLOW takes the density of the fluid in the source/sink as being identical to the density of the fluid in the model cell.

## General Head Boundary Package Input

The freshwater head of the external source must now be entered, rather than the hydraulic head. Input item 3 now becomes:

| | | | | | Boundary | |
|---|---|---|---|---|---|---|
| 3. | Data: | Layer | Row | Column | Head | Cond |
| | Format: | I10 | I10 | I10 | F10.0 | F10.0 |

### Explanation of New or Modified Fields Used in Input Instructions

Boundary head--is the freshwater head on the boundary.

# CHAPTER 11

## OTHER CHANGES TO THE VARIABLE DENSITY MODFLOW PROGRAM

Several changes to the MODFLOW program that are unrelated to the simulation of variable density groundwater flow have been implemented by the Bureau of Mineral Resources. These changes are:

i) removal of output control codes for page and line formatting.

ii) default display of input and output arrays in strip rather than wrap format.

iii) display of the boundary array at the end of each time step.

iv) console messages describing the current MODFLOW activity.

v) a console message listing largest head change at the end of each iteration.

vi) support for interactive specification of input and output files.

vii) removal of the divide by zero error that occurs when total input and output to the modelled area are identical.

viii) removal of the floating point error that occurs in the SIP solver package when all the cells surrounding a single active cell are converted to a no-flow state.

ix) the output unit number has been reassigned from 6 to 55 to overcome a FORTRAN compiler implementation limitation.

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