# Presentation 10

Variable-Density Flow (VDF) Process in SEAWAT

## Variable-Density Flow (VDF) Process

- Alternative to GWF Process
- Uses modified and unmodified routines from GWF
- Compatible with GLO, IMT and OBS
- Not compatible with SEN or PES
- Activated when 'VDF' included in name file

# Groundwater Flow Equation

Constant density

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

Variable density

$$\frac{\partial}{\partial \alpha}\left[\rho K_{f\alpha}\left(\frac{\partial h_f}{\partial \alpha}+\frac{\rho-\rho_f}{\rho_f}\frac{\partial Z}{\partial \alpha}\right)\right]+\frac{\partial}{\partial \beta}\left[\rho K_{f\beta}\left(\frac{\partial h_f}{\partial \beta}+\frac{\rho-\rho_f}{\rho_f}\frac{\partial Z}{\partial \beta}\right)\right]$$
$$+\frac{\partial}{\partial \gamma}\left[\rho K_{f\gamma}\left(\frac{\partial h_f}{\partial \gamma}+\frac{\rho-\rho_f}{\rho_f}\frac{\partial Z}{\partial \gamma}\right)\right]=\rho S_f\frac{\partial h_f}{\partial t}+\theta\frac{\partial \rho}{\partial C}\frac{\partial C}{\partial t}-\rho_s q_s$$

Limitation: assumes viscosity not affected by concentration

# Finite-Difference Approximation

Constant density

$$CC\left(h^m_{i+1,j,k}-h^m_{i,j,k}\right)+CC\left(h^m_{i-1,j,k}-h^m_{i,j,k}\right)+CR\left(h^m_{i,j+1,k}-h^m_{f,i,j,k}\right)+CR\left(h^m_{i,j-1,k}-h^m_{i,j,k}\right)$$
$$+CV\left(h^m_{i,j,k+1}-h^m_{i,j,k}\right)+CV\left(h^m_{i,j,k-1}-h^m_{i,j,k}\right)+P_{i,j,k}h^m_{i,j,k}+Q_{i,j,k}=S_{i,j,k}V_{i,j,k}\frac{h^m_{i,j,k}-h^{m-1}_{i,j,k}}{t^m-t^{m-1}}$$

Variable density

$$\hat{\rho}_{i+1/2,j,k}CC\left(h^m_{f,i+1,j,k}-h^m_{f,i,j,k}\right)+\hat{\rho}_{i-1/2,j,k}CC\left(h^m_{f,i-1,j,k}-h^m_{f,i,j,k}\right)$$
$$+\hat{\rho}_{i,j+1/2,k}CR\left(h^m_{f,i,j+1,k}-h^m_{f,i,j,k}\right)+\hat{\rho}_{i,j-1/2,k}CR\left(h^m_{f,i,j-1,k}-h^m_{f,i,j,k}\right)$$
$$+\hat{\rho}_{i,j,k+1/2}CV\left(h^m_{f,i,j,k+1}-h^m_{f,i,j,k}\right)+\hat{\rho}_{i,j,k-1/2}CV\left(h^m_{f,i,j,k-1}-h^m_{f,i,j,k}\right)$$
$$+P_{i,j,k}h^m_{f,i,j,k}-\rho_{i,j,k}S_{f,i,j,k}V_{i,j,k}\frac{h^m_{f,i,j,k}}{t^m-t^{m-1}}$$
$$=\rho_{i,j,k}S_{f,i,j,k}V_{i,j,k}\frac{-h^{m-1}_{f,i,j,k}}{t^m-t^{m-1}}-Q_{i,j,k}-D_{i,j,k}+V_{i,j,k}R_{i,j,k}\theta$$

## Required and Optional Flow-Related Packages

- Basic Package (BAS6)
- Internodal Conductance Packages
- Time-Variant Constant-Head Package
- Source-Term Packages
- Solver Packages
- Link-MT3DMS Package (LMT)

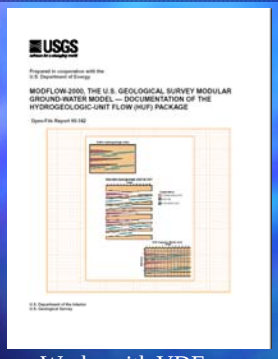
## Basic Package (BAS6)

- Required
- Reads heads and IBOUND array
- Initial heads read as h and converted to $h_f$ for use in the flow equation
- $h_f$ converted to h before being written to output files

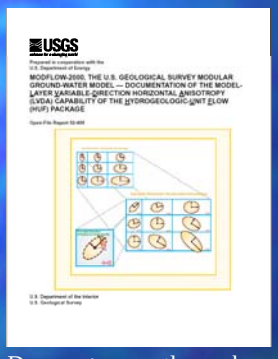
# Internodal Conductance Packages (compatible with VDF)

- At least one of the following three is required:
  - Block-centered flow (BCF6)
  - Layer-property flow (LPF)
  - Hydrogeologic unit flow (HUF)
- Horizontal flow barrier (HFB6)

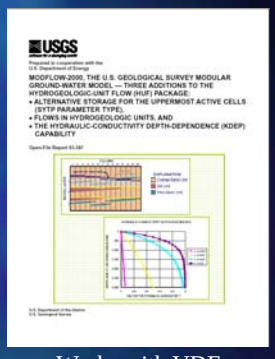
# Considerations for HUF2




Works with VDF




Does **not** currently work with VDF




Works with VDF

## Modifications to Internodal Conductance Packages to Work with VDF

- Relative density difference terms (come from variable-density form of Darcy's Law)
- Solute mass accumulation
- Conserve mass
- Use h instead of $h_f$
- Vertical leakage to partially saturated cell
- Variable-density flow for water-table case
- Effects of viscosity variations can be included

## Relative Density Difference Terms

Primary effect of variable-density flow

$$D_{i,j,k} = D_{i+1/2,j,k} + D_{i-1/2,j,k} + D_{i,j+1/2,k} + D_{i,j-1/2,k} + D_{i,j,k+1/2} + D_{i,j,k-1/2}$$

$$D_{i+1/2,j,k} = \hat{\rho}_{i+1/2,j,k} CC_{i+1/2,j,k} \left[ \frac{\rho_{i+1/2,j,k} - \rho_f}{\rho_f} \left( Z_{i+1,j,k} - Z_{i,j,k} \right) \right]$$

$$D_{i-1/2,j,k} = \hat{\rho}_{i-1/2,j,k} CC_{i-1/2,j,k} \left[ \frac{\rho_{i-1/2,j,k} - \rho_f}{\rho_f} \left( Z_{i-1,j,k} - Z_{i,j,k} \right) \right]$$

$$D_{i,j+1/2,k} = \hat{\rho}_{i,j+1/2,k} CR_{i,j+1/2,k} \left[ \frac{\rho_{i,j+1/2,k} - \rho_f}{\rho_f} \left( Z_{i,j+1,k} - Z_{i,j,k} \right) \right]$$

$$D_{i,j-1/2,k} = \hat{\rho}_{i,j-1/2,k} CR_{i,j-1/2,k} \left[ \frac{\rho_{i,j-1/2,k} - \rho_f}{\rho_f} \left( Z_{i,j-1,k} - Z_{i,j,k} \right) \right]$$

$$D_{i,j,k+1/2} = \hat{\rho}_{i,j,k+1/2} CV_{i,j,k+1/2} \left[ \frac{\rho_{i,j,k+1/2} - \rho_f}{\rho_f} \left( Z_{i,j,k+1} - Z_{i,j,k} \right) \right]$$

$$D_{i,j,k-1/2} = \hat{\rho}_{i,j,k-1/2} CV_{i,j,k-1/2} \left[ \frac{\rho_{i,j,k-1/2} - \rho_f}{\rho_f} \left( Z_{i,j,k-1} - Z_{i,j,k} \right) \right]$$

## Solute Mass Accumulation

- Explicit coupling between flow and transport

$$R_{i,j,k} = \frac{\rho\left(C_{i,j,k}^{m-1}\right) - \rho\left(C_{i,j,k}^{m-2}\right)}{t^{m-1} - t^{m-2}}$$

- Implicit coupling between flow and transport

$$R_{i,j,k} = \frac{\rho\left(C_{i,j,k}^{m*}\right) - \rho\left(C_{i,j,k}^{m-1}\right)}{t^{m} - t^{m-1}}$$

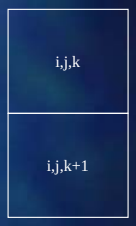
## Conservation of Mass

- All volumetric flow terms are multiplied by fluid density so that mass is conserved (rather than volume)
- ρQ conserved not Q

## Weighting Schemes for ρ

- Option 1—distance-weighted average

eg. $$\rho_{i,j,k+1/2} = \frac{\rho_{i,j,k}\left(Z_{i,j,k} - Z_{i,j,k+1/2}\right) + \rho_{i,j,k+1}\left(Z_{i,j,k+1/2} - Z_{i,j,k+1}\right)}{Z_{i,j,k} - Z_{i,j,k+1}}$$




- Option 2—upstream weighting

eg. $$If\ \_\ flow\ \_\ is\ \_\ down:$$
$$\rho_{i,j,k+1/2} = \rho_{i,j,k}$$
$$Else$$
$$\rho_{i,j,k+1/2} = \rho_{i,j,k+1}$$

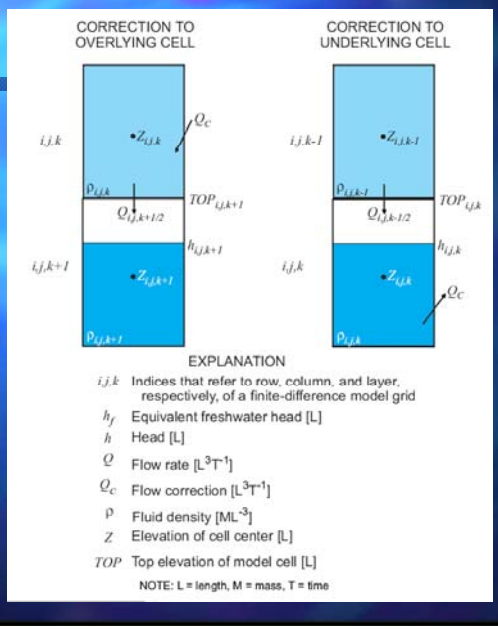
  - Note: this option is only available for density terms used to conserve fluid mass. All other density terms calculated using distance-weighted average

## Use of h Instead of $h_f$

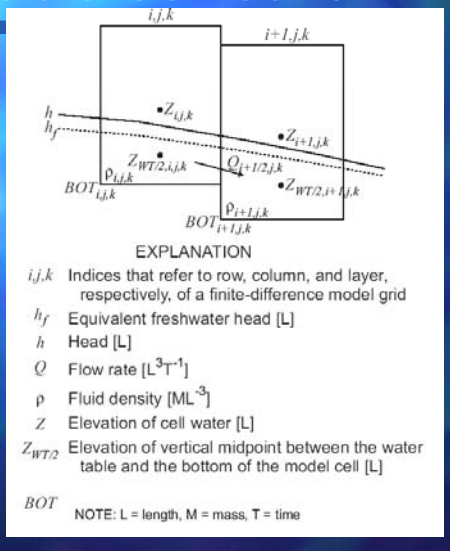
- Calculation of conductances
- Rewetting
- Conversion between confined and unconfined
- Evapotranspiration

$$h = \frac{\rho_f}{\rho} h_f + \frac{\rho - \rho_f}{\rho} Z$$

# Leakage to Partially Saturated Cell




# Water-Table Correction



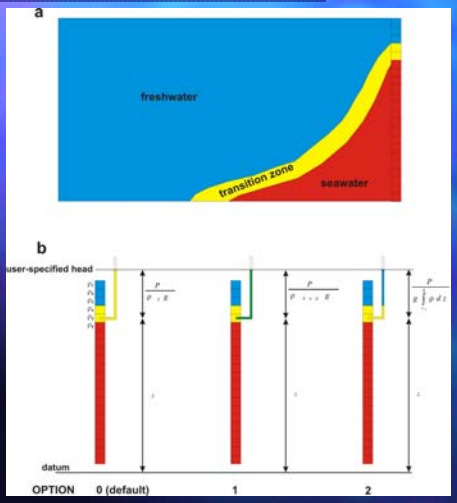
## Time-Variant Constant-Head Package

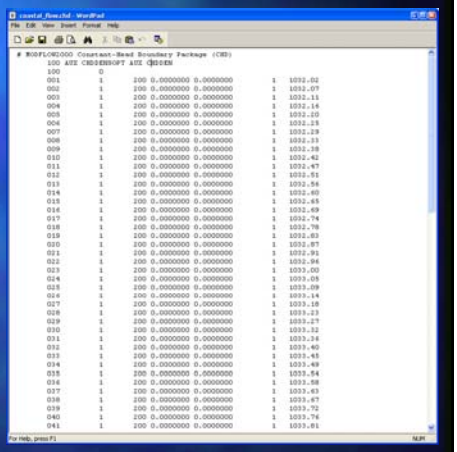
- Constant heads read as h and converted to $h_f$ for use in the flow equation
- Works same as for constant-density MODFLOW simulations

## Options for Specifying Constant Head Boundaries

- Set in BAS6
  - $h_f$ calculated from h and starting concentrations. $h_f$ held constant for simulation
  - Can't change h during simulation
- Set in CHD Package
  - $h_f$ calculated from temporally interpolated h and simulated concentration
  - Issue with MT3DMS boundary (ITYPE=1)

# Options for CHD Boundaries



# Source-Term Packages Compatible with VDF

- Packages modified to use variable-density form of Darcy's Law and to conserve fluid mass
  - Well (WEL)
  - Drain (DRN)
  - River (RIV)
  - General-head boundary (GHB)
  - Recharge (RCH)
  - Evapotranspiration (EVT)
  - Drain with Return Flow (DRT)
  - Segmented ET (ETS)
  - Multi-Node Well (MNW)
  - Flow and Head Boundary (FHB)

# Well Package (WEL)

$$mass\_flux = \rho_{well} Q_{well}$$

## Withdrawal

$\rho_{well} = \rho_{i,j,k}$

## Injection

Default $\rho_{well} = \rho_f$

If specified by user through auxiliary variable $\rho_{well} = \rho_{specified}$

For coupled variable-density flow (if IMT is linked with VDF) $\rho_{well} = \rho_f + \frac{\partial \rho}{\partial C} C_{well}$

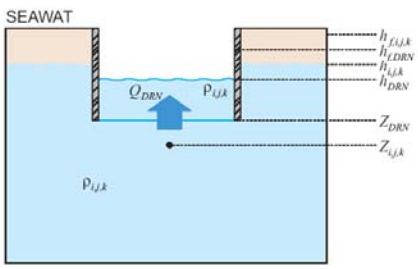
# Drain Package (DRN)

$$mass\_flux = \rho_{i,j,k} COND_{f,DRN} \left[ h_{f,DRN} - h_{f,i,j,k} - \frac{\rho_{i,j,k} - \rho_f}{\rho_f} \left( Z_{i,j,k} - Z_{DRN} \right) \right]$$

Always density of model cell

Not included in standard MODFLOW input files

Users can specify using an auxiliary variable. If not, then $Z_{DRN}$ set to $Z_{i,j,k}$




EXPLANATION

| | |
|---|---|
| $h_{i,j,k}$ | Head in the model cell [L] |
| $h_{DRN}$ | Head in the drain [L] |
| $h_{f,i,j,k}$ | Equivalent freshwater head in the model cell [L] |
| $h_{f,DRN}$ | Equivalent freshwater head in the drain [L] |
| $Z_{DRN}$ | Elevation of the drain bottom [L] |
| $Z_{i,j,k}$ | Elevation of the center of the model cell [L] |
| $\rho_{i,j,k}$ | Density of the water in the model cell [$ML^{-3}$] |
| $Q_{DRN}$ | Flux of water from the aquifer to the drain [$L^3T^{-1}$] |

NOTE: L = length, M = mass, T = time

# River Package (RIV)

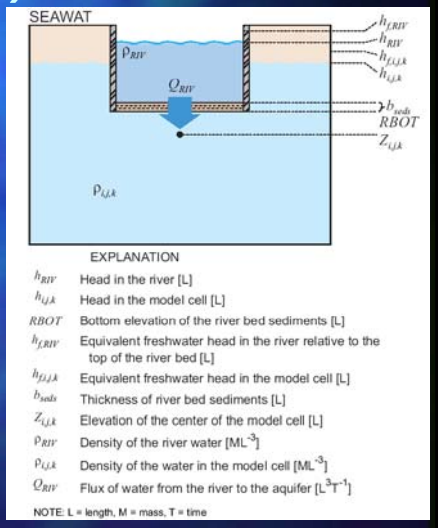
$$mass\_flux = \hat{\rho} \cdot COND_{f,RIV}\left[h_{f,RIV} - h_{f,i,j,k} - \frac{\rho_{i,j,k} - \rho_f}{\rho_f}\left(Z_{i,j,k} - Z_{RBOT}\right) + \frac{\overline{\rho} - \rho_f}{\rho_f} b_{seds}\right]$$

Flow into river: $\hat{\rho} = \rho_{i,j,k}$

Flow into aquifer: $\hat{\rho} = \rho_f$; $\hat{\rho} = \rho_{specified}$; $\hat{\rho} = \rho_f + \frac{\partial \rho}{\partial C} C_{RIV}$

Not included in standard MODFLOW input files

Users can specify using an auxiliary variable. If not, then $b_{seds}$ set to *abs*($Z_{i,j,k}$ – RBOT)




# General-Head Boundary Package (GHB)

$$mass\_flux = \hat{\rho} \cdot COND_{f,GHB}\left[h_{f,GHB} - h_{f,i,j,k} + \frac{\overline{\rho} - \rho_f}{\rho_f}\left(Z_{GHB} - Z_{i,j,k}\right)\right]$$

Flow into GHB: $\hat{\rho} = \rho_{i,j,k}$

Flow into aquifer:

Default: $\hat{\rho} = \rho_f$

If specified by user through auxiliary variable: $\hat{\rho} = \rho_{specified}$

For coupled variable-density flow (if IMT is linked with VDF): $\hat{\rho} = \rho_f + \frac{\partial \rho}{\partial C} C_{GHB}$

Not included in standard MODFLOW input files

Users can specify using an auxiliary variable. If not, then $Z_{GHB} = Z_{i,j,k}$

## Recharge Package (RCH)

$$mass\_flux = \hat{\rho} \cdot RECH \cdot \Delta x \cdot \Delta y$$

RECH < 0

$\hat{\rho} = \rho_{i,j,k}$

RECH > 0

Default $\hat{\rho} = \rho_f$

For coupled variable-density flow (if IMT is linked with VDF) $\hat{\rho} = \rho_f + \frac{\partial \rho}{\partial C} C_{RCH}$

## Evapotranspiration Package (EVT)

- ET equation reformulated to use head, instead of equivalent freshwater head
- For the density term used to conserve mass:
  - For coupled flow and transport, density calculated using concentration in source/sink mixing package
  - Otherwise, density is set to reference density

## Solver Packages

- No changes to solver packages themselves, but mass conductances are passed into solvers
- Current solver packages:
  - Strongly Implicit Procedure (SIP)
  - Slice-Successive Overrelaxation (SOR)
  - Preconditioned Conjugate-Gradient (PCG)
  - Direct Solver (DE4)
  - Algebraic Multi-Grid (LMG)
  - Geometric Multi-Grid (GMG)

## Link-MT3DMS (LMT) Package

- Modified to use variable-density forms of flux calculations
- Used internally in SEAWAT to pass flows from MODFLOW to MT3D
- Can be used to save a flow-transport link file for subsequent MT3DMS simulations