Presentation 9

SEAWAT Concepts

SEAWAT Concept

- Combine MODFLOW and MT3DMS into a single program
  - Insert MT3DMS into MODFLOW main program
- Modify MODFLOW routines to solve the variable-density groundwater flow equation

Programming Objectives

- Accurate
- Modular
- Minimal changes to existing MODFLOW and MT3D subroutines

SEAWAT Processes

- Global (GLO) Process
- Ground-Water Flow (GWF) Process
- **Variable-Density Flow (VDF) Process**
  - **Viscosity (VSC) Package**
- **Integrated MT3DMS Transport (IMT) Process**
- Observation (OBS) Process
- Sensitivity (SEN) Process
- Parameters Estimation (PES) Process

Global Process

- Not really a process (doesn't solve an equation)
- Simulation modes and process compatibility
- Program structure
- Discretization
  - Spatial
  - Temporal

Simulation Modes

	TRANSPORT EXCLUDED	TRANSPORT INCLUDED
CONSTANT-DENSITY GROUND-WATER FLOW	**A** GLO + GWF GLO + GWF (OBS) GLO + GWF (OBS + SEN) GLO + GWF (OBS + SEN + PES)	**B** GLO + GWF + IMT GLO + GWF (OBS) + IMT GLO + GWF (OBS + SEN) + IMT GLO + GWF (OBS + SEN + PES) + IMT
VARIABLE-DENSITY GROUND-WATER FLOW	**C** GLO + VDF GLO + VDF (OBS)	GLO + VDF + IMT GLO + VDF (OBS) + IMT **D** UNCOUPLED FLOW AND TRANSPORT GLO + VDF + IMT GLO + VDF (OBS) + IMT **E** COUPLED FLOW AND TRANSPORT

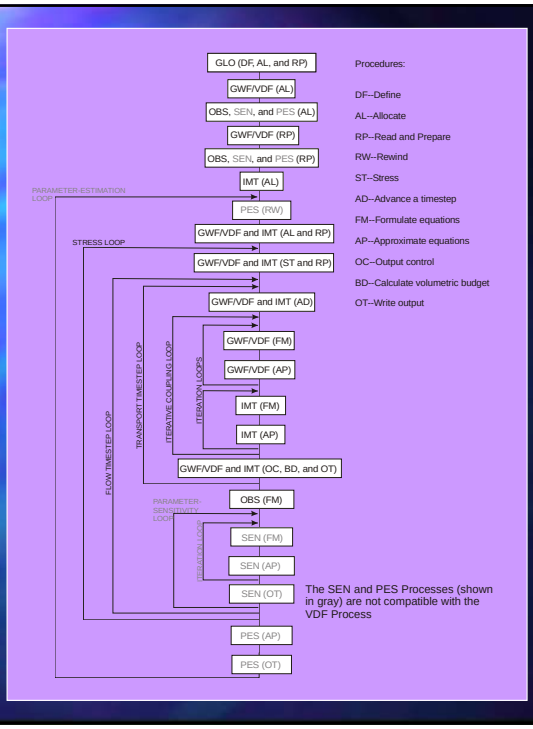
Optional Simulation Mode: VDF without Transport

- User enters 3D array of fluid density
- Caution—assumption is that fluid density will not change during the simulation period
- Advantage: simulations run quickly because not limited by stability requirements for transport equation

Process Compatibility

- VDF **not** compatible with SEN and PES
  - Cannot use in same simulation
- VDF **is** compatible with OBS
- IMT **not** compatible with OBS, SEN, and PES
  - Can be used during same simulation—do not interfere with each other

Program Structure

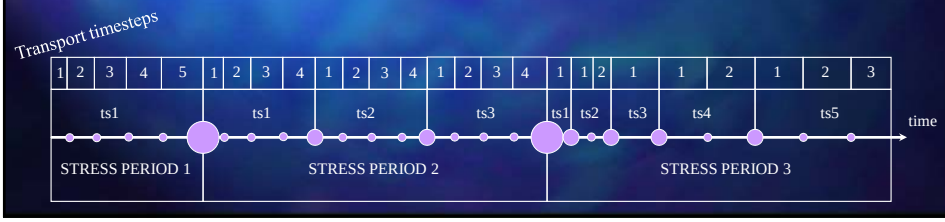


Spatial Discretization

- Information must be consistent between MODFLOW and MT3D
- Higher level of vertical discretization required for variable-density groundwater flow (rule of thumb—~10 layers per aquifer)

Temporal Discretization

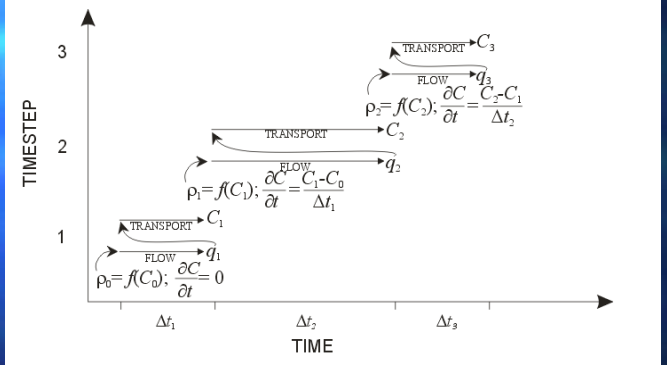
- Stress periods
- Flow timesteps
- Transport timesteps
- **Flow and transport equations solved for each transport timestep**



Options for Coupling Flow and Transport

- Explicit—one timestep lag
  - Works well for most problems
- Implicit—iterative coupling until convergence on fluid density
  - Can only be used if transport is solved using implicit finite difference
  - Can be time consuming and doesn't seem to help with accuracy for problems tested thus far

Explicit Coupling

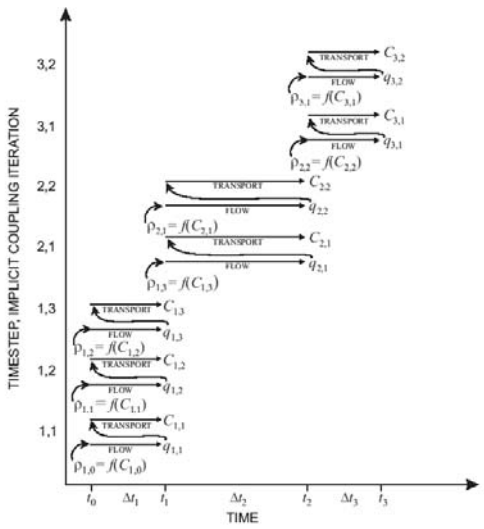


ρ_n Distribution of fluid density at end of timestep n [ML^{-3}]

C_n Distribution of solute concentration at end of timestep n [ML^{-3}]

q_n Field of specific discharge at end of timestep n [LT^{-1}]

Implicit Coupling



$\rho_{n,ncpl}$ Distribution of fluid density at end of timestep n and end of coupling iteration $ncpl$ [ML^{-3}]

$C_{n,ncpl}$ Distribution of solute concentration at end of timestep n and end of coupling iteration $ncpl$ [ML^{-3}]

$q_{n,ncpl}$ Field of specific discharge at end of timestep n and end of coupling iteration $ncpl$ [LT^{-1}]

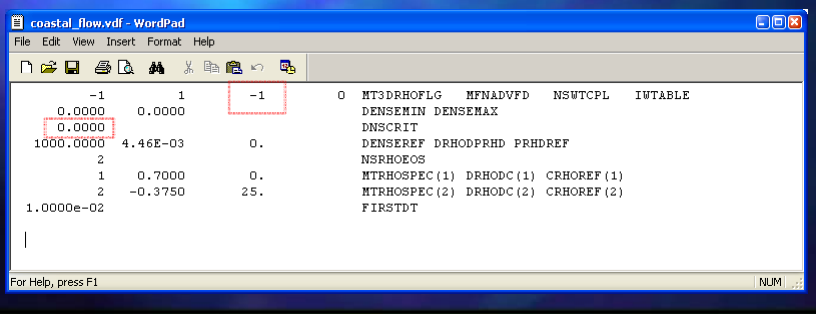
Flow Field Update Control

- Recalculate the flow field only if the density has changed by a user-specified density value
- May substantially improve computer runtimes
- Should probably avoid for sensitivity analyses and parameter estimation

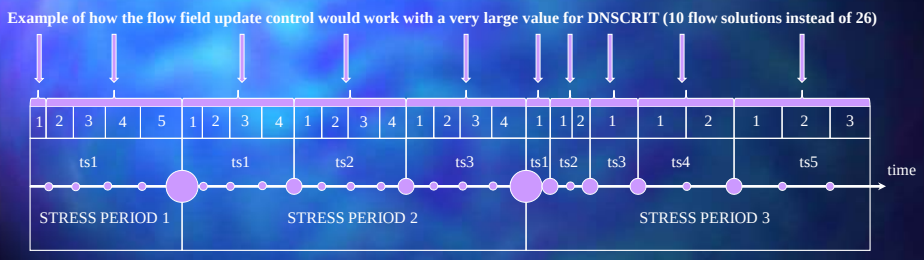
How it Works

Flow equation will be solved if:

- the density change since the last flow field update exceeds DNSCRIT
- it is the first transport timestep of the simulation
- it is the last transport timestep of a flow timestep



Example



Variable-Density Flow (VDF) Process

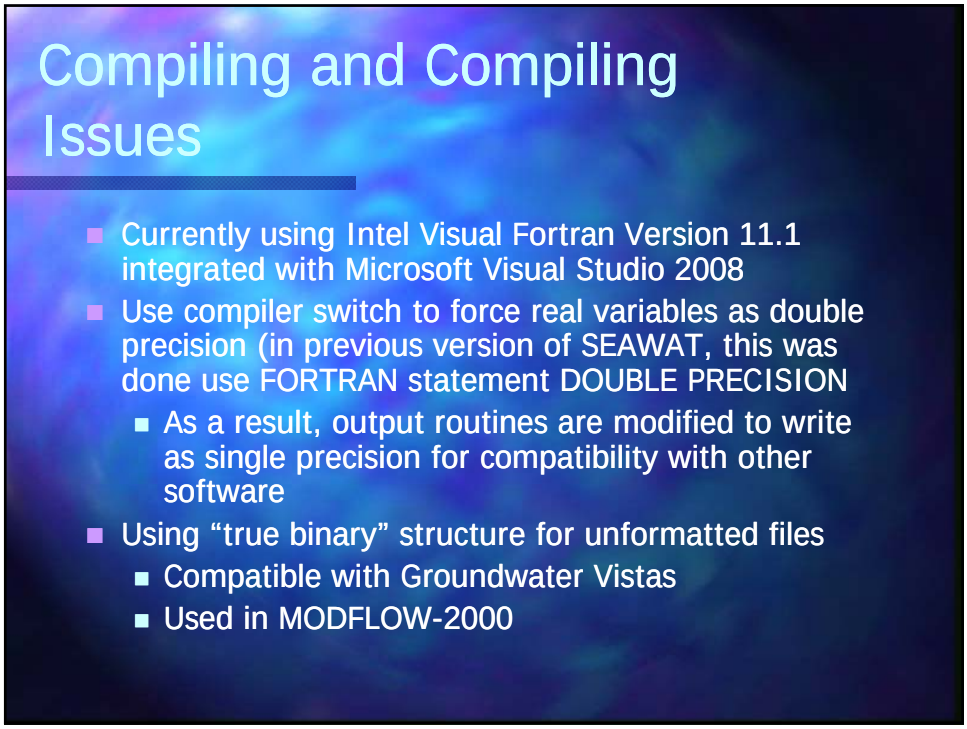
- Alternative to GWF Process
- Uses modified and unmodified routines from GWF
- Compatible with GLO, IMT and OBS
- Not compatible with SEN or PES

Integrated MT3DMS Transport (IMT) Process

- No substantial changes to original MT3DMS source code
- For variable-density simulations, transport equation should contain density gradient terms—these are **not** included in SEAWAT
  - Not a problem for simulations in range between freshwater and seawater
  - Could be important for brine transport

Observation Process (OBS)

- Variable-density form of Darcy's Law used to calculate simulated equivalents


Compiling and Compiling Issues
Currently using Intel Visual Fortran Version 11.1 integrated with Microsoft Visual Studio 2008
Use compiler switch to force real variables as double precision (in previous version of SEAWAT, this was done use FORTRAN statement DOUBLE PRECISION
As a result, output routines are modified to write as single precision for compatibility with other software
Using “true binary” structure for unformatted files
Compatible with Groundwater Vistas
Used in MODFLOW-2000