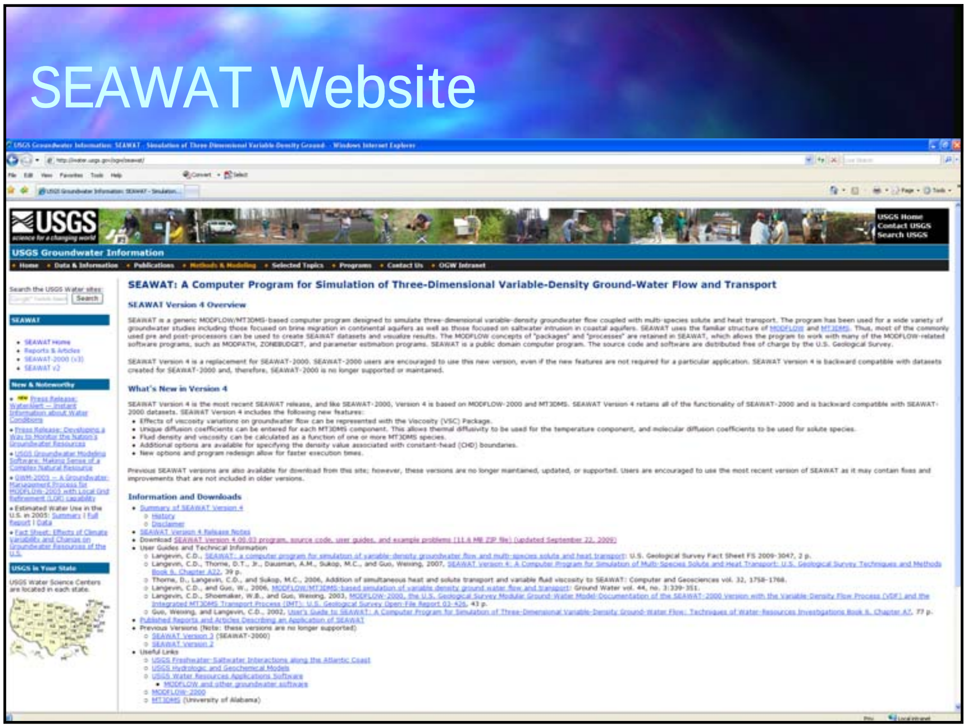
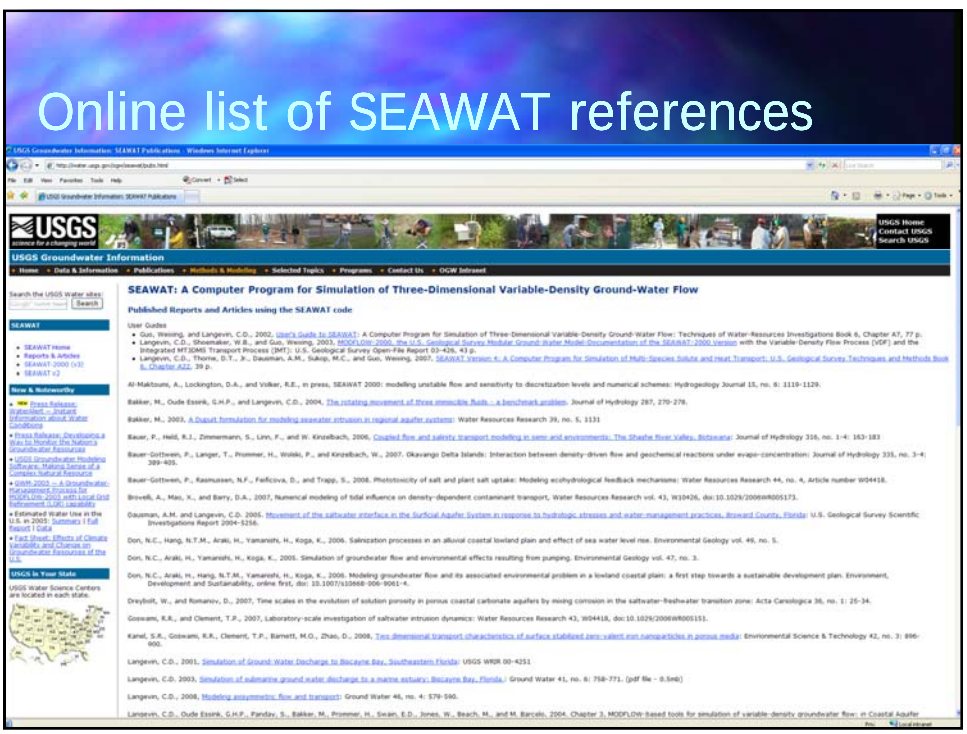
Presentation 11

Instructions for Using SEAWAT Version 4

Using SEAWAT Version 4

- Obtaining the program and current information
- Name (NAM) file
- Preparation of the VDF (and VSC) input file
- Considerations for MODFLOW packages
- Preparation of MT3DMS datasets
- Running SEAWAT_V4


SEAWAT Website
USGS
USGS Groundwater Information
SEAWAT: A Computer Program for Simulation of Three-Dimensional Variable-Density Ground-Water Flow and Transport
SEAWAT Version 4 Overview
What's New in Version 4
Information and Downloads


Online list of SEAWAT references
USGS
USGS Groundwater Information
SEAWAT: A Computer Program for Simulation of Three-Dimensional Variable-Density Ground-Water Flow
Published Reports and Articles using the SEAWAT code

Name File

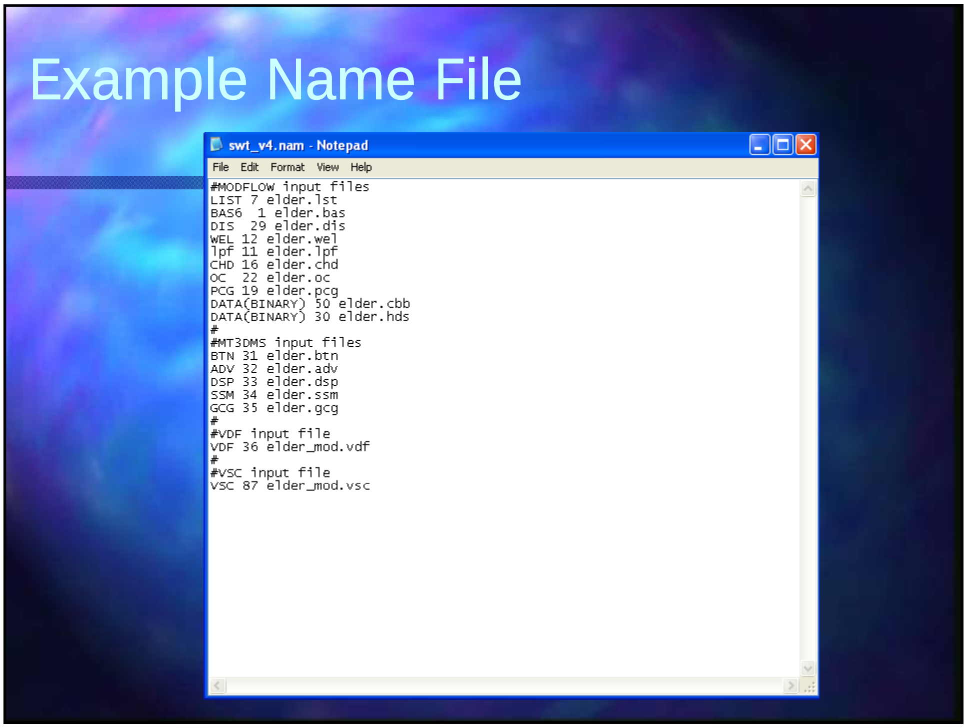
- Name file is requested when SEAWAT Version 4 runs
- Contains filetype, unit number, filename
- Contains file information for:
  - MODFLOW-2000 files
  - MT3DMS files
  - Variable-Density Flow (VDF) input file
  - Viscosity Package (VSC) input file [optional]
- Vistas creates valid SEAWAT Version 4 name file

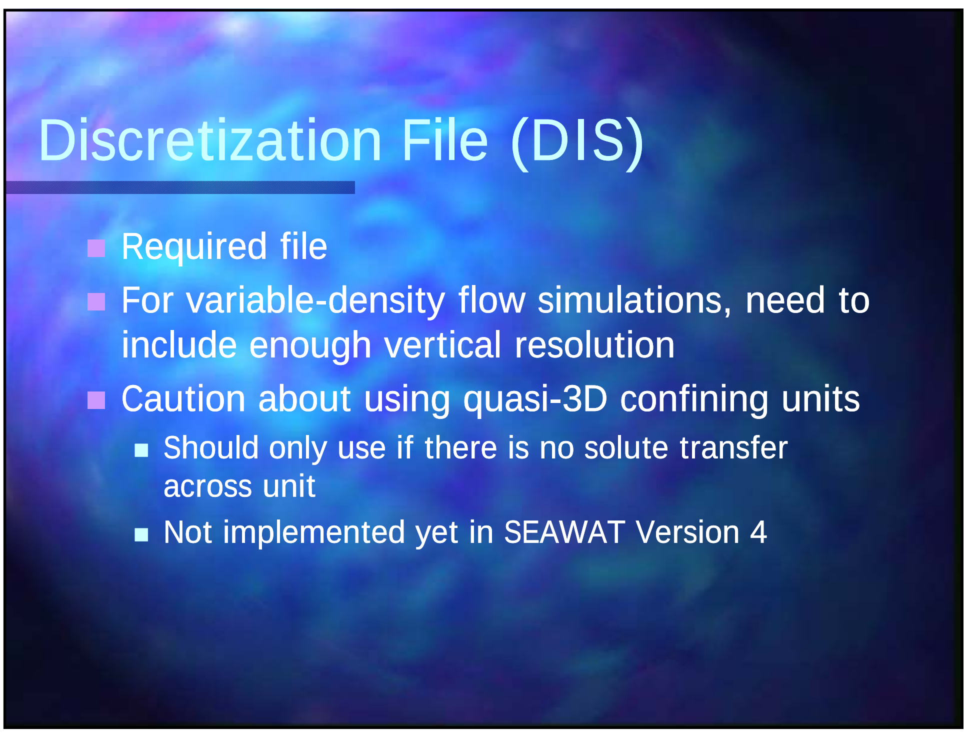
List of Packages and Input Files

Process	Package or file name	File type
GLO	[1]Global	GLOBAL
	[1]List	LIST
	[1]Discretization	DIS
	[1]Multiplier	MULT
	[1]Zone	ZONE
VDF	Variable-Density Flow	VDF
	[1,2]Basic	BAS6
	[1,2]Block-Centered Flow	BCF6
	[1]Layer-Property Flow	LPF
	[3]Hydrogeologic-Unit Flow	HUF
	[1,4]Hydraulic Flow Barrier	HFB6
	[1,2]Drain	DRN
	[1,2]River	RIV
	[1,2]General-Head Boundary	GHB
	[1,2]Evapotranspiration	EVT
	[1,2]Well	WEL
	[1,2]Recharge	RCH
	[1,5]Time-Variant Constant Head	CHD
	[1,2]Strongly Implicit Procedure	SIP
	[1,2]Slice-Successive Overrelaxation	SOR
	[1,6]Preconditioned Conjugate Gradient	PCG
	[1,7]Direct Solver	DE4
	[8]Link-AMG	LMG
	[9]Linkage with MT3DMS	LMT6
IMT	[10]Basic Transport	BTN
	[10]Advection	ADV
	[10]Dispersion	DSP
	[10]Source-Sink Mixing	SSM
	[10]Reaction	RCT
	[10]Generalized Conjugate Gradient	GCG
OBS	[11]Observation	OBS
	[11]Hydraulic-Head Observation	HOB
	[11]General-Head Boundary Observation	GHOB
	[11]Drain Observation	DROB
	[11]River Observation	RVOB
	[11]Constant-Head Flow Observation	CHOB

[1]Harbaugh and others (2000)
[2]McDonald and Harbaugh (1988)
[3]Anderman and Hill (2000)
[4]Hsieh and Freckleton (1993
[5]Leake and Prudic (1991)
[6]Hill (1990)
[7]Harbaugh (1995)
[8]Mehl and Hill (2001)
[9]Zheng and others (2001)
[10]Zheng and Wang (1999)
[11]Hill and others (2000)

Also includes:
HUF2
FHB
ETS
DRT
MNW
TOB


Example Name File
swt_v4.nam - Notepad
File Edit Format View Help
#MODFLOW input files
LIST 7 elder.lst
BAS6 1 elder.bas
DIS 29 elder.dis
WEL 12 elder.wel
lpf 11 elder.lpf
CHD 16 elder.chd
OC 22 elder.oc
PCG 19 elder.pcg
DATA(BINARY) 50 elder.cbb
DATA(BINARY) 30 elder.hds
#
#MT3DMS input files
BTN 31 elder.btn
ADV 32 elder.adv
DSP 33 elder.dsp
SSM 34 elder.ssm
GCG 35 elder.gcg
#
#VDF input file
VDF 36 elder_mod.vdf
#
#VSC input file
VSC 87 elder_mod.vsc


Discretization File (DIS)
Required file
For variable-density flow simulations, need to include enough vertical resolution
Caution about using quasi-3D confining units
Should only use if there is no solute transfer across unit
Not implemented yet in SEAWAT Version 4

VDF Input File

- By including in name file will activate the VDF process (otherwise GWF)
- Can have variable-density flow affected by one or more species
- VDF file is created by Groundwater Vistas

VDF File (cont.)

FOR EACH SIMULATION
0. [#Text]
Item 0 is optional and the symbol # must be in column 1. Item 0 can be repeated multiple times, but it cannot be used in the file after the first data record.
1. MT3DRHOFLG MFNADVFD NSWTCPL IWTABLE
2. DENSEMIN DENSEMAX
Read Item 3 if NSWTCPL > 1 or NSWTCPL = -1
3. DNSCRIT
Read Item 4 if MT3DRHOFLG ≥ 0
4. DENSEREF DRHODC(1)
Read Item 4a through 4c if MT3DRHOFLG = -1
4a. DENSEREF DRHODPRHD PRHDREF
4b. NSRHOEOS
4c. MTRHOSPEC(NSRHOEOS) DRHODC(NSRHOEOS) CRHOREF(NSRHOEOS)
Item 4c is read as a table, with one row representing each MT3DMS species to be included in the equation of state for fluid density. There is no requirement that this table be sorted by MTRHOSPEC.
5. FIRSTDT
FOR EACH STRESS PERIOD
Read Items 6 and 7 only if MT3DRHOFLG = 0
6. INDENSE
Read Item 7 only if INDENSE is greater than zero
7. [DENSE(NCOL,NROW)] – U2DREL
Item 7 is read for each layer in the grid.

VDF File (cont.)

Example VDF file

swt_v4.vdf - Notepad

File Edit Format View Help

```
        -1          1          0          0  MT3DRHOFLG MFNADVFD NSWTCPL IWTABLE
    0.0000     0.0000                        DENSEMIN DENSEMAX
 1000.0000     0.0000         0.             DENSEREF DRHODPRHD PRHDREF
         2                                   NSRHOEOS
         1     0.7000         0.             MTRHOSPEC(1) DRHODC(1) CRHOREF(1)
         2    -0.3750        25.             MTRHOSPEC(2) DRHODC(2) CRHOREF(2)
1.0000e-02                                   FIRSTDT
```

or

```
        -1          1         -1          0  MT3DRHOFLG   MFNADVFD   NSWTCPL   IWTABLE
    0.0000     0.0000                        DENSEMIN DENSEMAX
    0.0000                                   DNSCRIT
 1000.0000   4.46E-03         0.             DENSEREF DRHODPRHD PRHDREF
         2                                   NSRHOEOS
         1     0.7000         0.             MTRHOSPEC(1) DRHODC(1) CRHOREF(1)
         2    -0.3750        25.             MTRHOSPEC(2) DRHODC(2) CRHOREF(2)
1.0000e-02                                   FIRSTDT
```

DENSEREF and DENSESLP

Concentration		
units	freshwater	seawater
mg/L	0	35,000
g/L	0	35
lbs/ft³	0	2.188
relative	0	1

$$DENSESLP = \frac{\Delta\rho}{\Delta C}$$

Example:
use concentration in mg/L and density in kg/m³

$$DENSESLP = \frac{1025 - 1000 kg/m^3}{35000 - 0 mg/L} = 7.14x10^{-4}$$

Density		
units	Freshwater (DENSEREF)	seawater
g/cm³	1	1.025
kg/m³	1000	1025
lbs/ft³	62.42	63.98

Density length units must be same as length units used for model grid, hydraulic conductivity, etc.

VSC Input File

- By including in name file will activate the VSC option
- VSC file is created by Groundwater Vistas
- Have multiple options from manual
  - Concentration
  - Temperature

VSC File

FOR EACH SIMULATION

0. [#Text]
   Item 0 is optional and the symbol # must be in column 1. Item 0 can be repeated multiple times.
1. MT3DMUFLG
2. VISCMIN VISCMAX
   Read item 3 if MT3DMUFLG ≥ 0
3. VISCREF DMUDC(1) CMUREF(1)
   Read item 3a through 3c if MT3DMUFLG = -1

3a. VISCREF
3b. NSMUEOS MUTEMPOPT
3c. MTMUSPEC(NSMUEOS) DMUDC(NSMUEOS) CMUREF(NSMUEOS)
Item 3c is read NSMUEOS times, once for each MT3DMS species to be included in the viscosity equation.
3d. MTMUTEMPSPEC AMUCOEFF(MUNCOEFF)
Item 3d is read if MUTEMPOPT > 0. The size of the AMUCOEFF coefficient array depends on the selected equation for viscosity.

FOR EACH STRESS PERIOD

Read items 4 and 5 only if MT3DMUFLG = 0

4. INVISC
   Read item 5 only if INVISC is greater than zero
5. [VISC(NCOL,NROW)] – U2DREL
   Item 5 is read for each layer in the grid.

VSC File (cont.)

Example VSC file

swt_v4.vsc - Notepad

File Edit Format View Help

```
#Viscosity Package
-1                                  MT3DMUFLG
0. 0.                               VISCMIN VISCMAX
8.904e-4                            VISCREF
1 1                                 NSMUEOS MUTEMPOPT
1 1.923e-6 0.                       MTMUSPEC(1) DMUDC(1) CMUREF(1)
2 239.4e-7 10. 248.37 133.15        MTMUTEMPSPEC A1 A2 A3 A4
```

VSC File (cont.)

$$\mu = \mu_T(T) + \sum_{k=1}^{NS} \frac{\partial \mu}{\partial C^k}\left(C^k - C_0^k\right)$$

- Viscosity as a function of temperature: 3 options

$$\mu_T(T) = A_1 \cdot A_2^{\left(\frac{A_3}{T+A_4}\right)}$$

$$\mu_T(T) = A_1 \cdot \left[A_2 + A_3\left(T + A_4\right)\right]^{A_5}$$

$$\mu_T(T) = A_1 \cdot T^{A_2}$$

Special Considerations for Packages

- All input and output is expressed in terms of head (not equivalent freshwater head)
- All storage and hydraulic properties must be represented in terms of equivalent freshwater values (or relative to the reference density)

Use of Auxiliary Variables for Flow Packages

Source-term package	**Auxiliary variable name**	**Description**	**Default value (if not entered using auxiliary variable)**
Well	WELDENS	Density of injection well fluid	DENSEREF
Drain	DRNBELEV	Drain bottom elevation	Cell center
River	RBDTHK	Thickness of riverbed sediments	Difference between river bottom elevation and cell center
River	RIVDEN	Density of river	Density of model cell
General-Head Boundary	GHBELEV	Elevation of the general-head boundary	Cell center
General-Head Boundary	GHBDENS	Density of general-head boundary fluid	Density of model cell

Solver Packages

- Variable-density simulations may require a smaller value for head convergence in order to calculate accurate vertical flow velocities
- Residual criterion for flow convergence (RCLOSE, in PCG) may be set larger than for a similar constant-density flow problem by a factor of the density

Running SEAWAT Version 4

- On a PC:

Double-click on swt_v4.bat in file manager

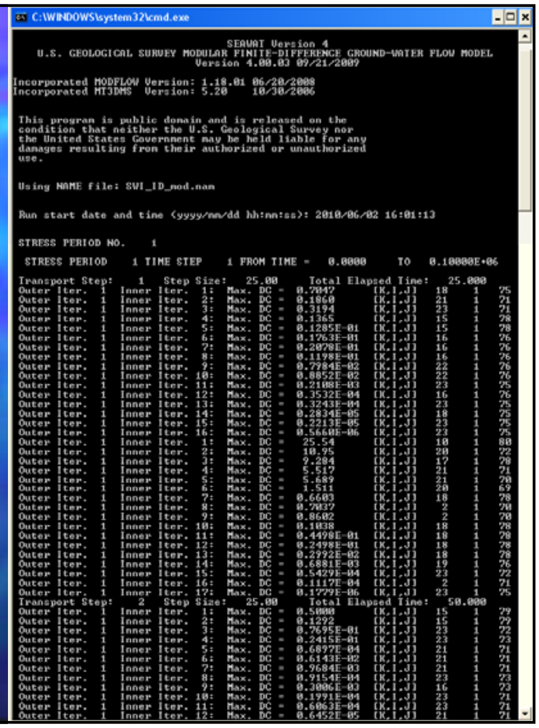
swt_v4.bat - Notepad

```
..\..\exe\swt_v4.exe swt_v4.nam
pause
```

swt_v4.nam - Notepad

```
#MODFLOW input files
LIST 7 elder.lst
BAS6  1 elder.bas
DIS  29 elder.dis
WEL 12 elder.wel
lpf 11 elder.lpf
CHD 16 elder.chd
OC  22 elder.oc
PCG 19 elder.pcg
DATA(BINARY) 50 elder.cbb
DATA(BINARY) 30 elder.hds
#
#MT3DMS input files
BTN 31 elder.btn
ADV 32 elder.adv
DSP 33 elder.dsp
SSM 34 elder.ssm
GCG 35 elder.gcg
#
#VDF input file
VDF 36 elder_mod.vdf
#
#VSC input file
VSC 87 elder_mod.vsc
```

Screen Output



Model Results of Interest

- Screen Output
- Listing Files
  - Flow budget
  - Solute mass budget
- Heads
- Flows
- Concentrations
  - Unformatted concentration file
  - Concentration observations
- Solute mass budget

Post Processing

- Groundwater Vistas
- Modelviewer
- Zone Budget
- MT3DMS
- MODPATH
- ETC...

Simultaneous Solute and Heat Transport Simulations

- Density and viscosity variations may be important
- Some MT3DMS input parameters must be entered as solute equivalents

Flow Equation

$$\nabla \cdot \left[\rho \frac{\mu_0}{\mu} \mathbf{K_0} \left(\nabla h_0 + \frac{\rho - \rho_0}{\rho_0} \nabla z \right) \right] = \rho S_{s,0} \frac{\partial h_0}{\partial t} + \theta \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} - \rho_s q'_s$$

What's different when including temperature effects?

•Prefer "reference" instead of "equivalent freshwater"

•density is a function of concentration and temperature

•viscosity variations may be more important

Transport Equations

sorption, advection, diffusion, mechanical dispersion, source/sink

$$\left(1 + \frac{\rho_b K_d}{\theta}\right) \frac{\partial (\theta C)}{\partial t} = -\nabla \cdot (\theta \mathbf{v} C) + \nabla \cdot \left[\theta \left(D^* + \boldsymbol{\alpha} \mathbf{v}\right) \cdot \nabla C \right] - q_s C_s$$

heat storage, convection, conduction, mechanical dispersion, source/sink

$$\left(1 + \frac{\rho_b K_d}{\theta}\right) \frac{\partial (\theta T)}{\partial t} = -\nabla \cdot (\theta \mathbf{v} T) + \nabla \cdot \left[\theta \left(D^* + \boldsymbol{\alpha} \mathbf{v}\right) \cdot \nabla T \right] - q_s T_s$$

$$K_d = \frac{1}{\rho} \frac{c_{P,solid}}{c_{P,fluid}} \qquad D^* = \frac{k_{T,bulk}}{\theta \rho c_{P,fluid}}$$

DSP Input File

```
$MultiDiffusion
         0     1.000(10E12.4)                    -1     DISPERSIVITY Layer   1
         0     1.000(10E12.4)                    -1     DISPERSIVITY Layer   2
(layers 3 through 99 not shown)
         0     1.000(10E12.4)                    -1     DISPERSIVITY Layer 100
         0     0.100(10E12.4)                    -1     HZ DISPERSIVITY RATIO
         0     0.100(10E12.4)                    -1     VT DISPERSIVITY RATIO
         0   1.0E-10                             -1     MOL DIFF SP 1 LAYER 001
         0   1.0E-10                             -1     MOL DIFF SP 1 LAYER 002
(layers 3 through 99 not shown)
         0   1.0E-10                             -1     MOL DIFF SP 1 LAYER 100
         0      0.15                             -1     MOL DIFF SP 2 LAYER 001
         0      0.15                             -1     MOL DIFF SP 2 LAYER 002
(layers 3 through 99 not shown)
         0      0.15                             -1     MOL DIFF SP 2 LAYER 100
```

$$D_{m\_temp} = \frac{k_{Tbulk}}{\theta \rho c_{Pfluid}}$$

$$k_{Tbulk} = \theta k_{Tfluid} + (1-\theta) k_{Tsolid}$$

RCT Input File

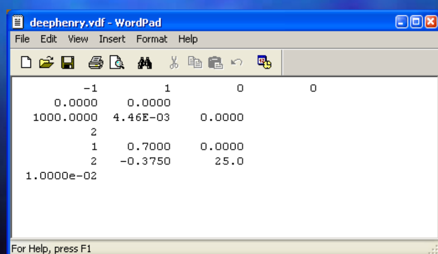
```
         1         0         2         0
         0  1760.000(10E12.4)                    -1     Blk Dnsty         Lay   1
         0  1760.000(10E12.4)                    -1     Blk Dnsty         Lay   2
(layers 3 through 99 not shown)
         0  1760.000(10E12.4)                    -1     Blk Dnsty         Lay 100
         00.0000e+00(10E12.4)                    -1     Kd Species 1      Lay   1
         00.0000e+00(10E12.4)                    -1     Kd Species 1      Lay   2
(layers 3 through 99 not shown)
         00.0000e+00(10E12.4)                    -1     Kd Species 1      Lay 100
         02.0000e-04(10E12.4)                    -1     Kd Species 2      Lay   1
         02.0000e-04(10E12.4)                    -1     Kd Species 2      Lay   2
(layers 3 through 99 not shown)
         02.0000e-04(10E12.4)                    -1     Kd Species 2      Lay 100
         00.0000e+00(10E12.4)                    -1     SP2 Sp 1 not used Lay   1
         00.0000e+00(10E12.4)                    -1     SP2 Sp 1 not used Lay   2
(layers 3 through 99 not shown)
         00.0000e+00(10E12.4)                    -1     SP2 Sp 1 not used Lay 100
         00.0000e+00(10E12.4)                    -1     SP2 Sp 2 not used Lay   1
         00.0000e+00(10E12.4)                    -1     SP2 Sp 2 not used Lay   2
(layers 3 through 99 not shown)
         00.0000e+00(10E12.4)                    -1     SP2 Sp 2 not used Lay 100
```

$$K_{d\_temp} = \frac{c_{Psolid}}{\rho c_{Pfliud}}$$

Density Equation of State

Multiple-species — Temperature — Water Compressibility

$$\rho = \rho_0 + \sum_{k=1}^{NS} \frac{\partial \rho}{\partial C^k}\left(C^k - C_0^k\right) + \frac{\partial \rho}{\partial T}\left(T - T_0\right) + \frac{\partial \rho}{\partial \ell}\left(\ell - \ell_0\right)$$




```
        -1          1          0          0
    0.0000     0.0000
 1000.0000  4.46E-03     0.0000
         2
         1     0.7000     0.0000
         2    -0.3750       25.0
1.0000e-02
```

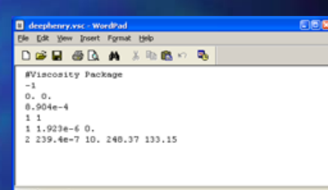
$$\frac{\partial \rho}{\partial \ell} = \rho_0^2 g \beta_P$$

Constitutive Relation for Viscosity

$$\mu = \mu_0 + \sum_{k=1}^{NS} \frac{\partial \mu}{\partial C^k}\left(C^k - C_0^k\right) + \frac{\partial \mu}{\partial T}\left(T - T_0\right)$$

or

$$\mu = \mu(T) + \sum_{k=1}^{NS} \frac{\partial \mu}{\partial C^k}\left(C^k - C_0^k\right)$$

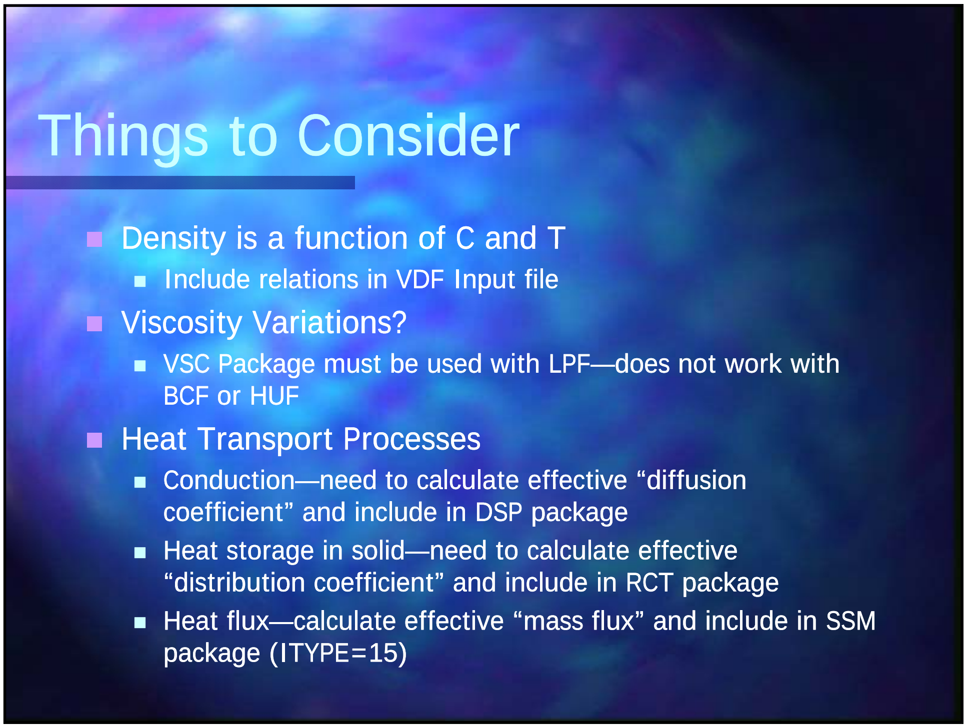



```
#Viscosity Package
-1
0. 0.
8.904e-4
1 1
1 1.923e-6 0.
2 239.4e-7 10. 248.37 133.15
```

	MUTEMPOPT
$\mu(T) = A_1 \cdot A_2^{\left(\frac{A_3}{T+A_4}\right)}$	1
$\mu(T) = A_1 \cdot \left[A_2 + A_3(T + A_4)\right]^{A_5}$	2
$\mu(T) = A_1 \cdot T^{A_2}$	3

e.g. SUTRA

$$\mu(T) = 239.4x10^{-7} \cdot 10^{\left(\frac{248.37}{T+133.15}\right)}$$


Things to Consider
Density is a function of C and T
Include relations in VDF Input file
Viscosity Variations?
VSC Package must be used with LPF—does not work with BCF or HUF
Heat Transport Processes
Conduction—need to calculate effective “diffusion coefficient” and include in DSP package
Heat storage in solid—need to calculate effective “distribution coefficient” and include in RCT package
Heat flux—calculate effective “mass flux” and include in SSM package (ITYPE=15)