3D Example for **SUTRA**

Island3D

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This 3D example is presented in the **SUTRA** documentation (Voss and Provost, 2002, Version of June 2, 2008, section 6.8, page 174). It is intended for comparison with the 2D solution to the same problem, also described in the **SUTRA** documentation. It involves a transient saturated-unsaturated variable-density flow and transient solute transport simulation.

A circular island in the sea undergoes a prolonged drought, during which the water table declines to sea level, and all ground water beneath the island becomes saline. Then, renewed freshwater recharge finally restores the island's freshwater lens. This example concerns simulation of the post-drought recharge and restoration of the freshwater lens.

Following the drought, the water table is at sea level and both the saturated aquifer below sea level and the unsaturated zone above sea level contain only seawater. Fresh rainwater recharge to the surface of the island begins and continues at a constant rate, raising the water table on the island, flushing out seawater, and eventually establishing a stable freshwater lens and a diffuse saltwater-freshwater interface. The aquifer on the island is unconfined with both unsaturated and saturated zones and the material properties are generally homogeneous but permeability is anisotropic.

The problem may be simulated twice, using a 2D radial mesh (see the Island2D problem) and using a fully 3D mesh. The 3D steady-state solution may be compared with the 2D solution to verify that these give equivalent results. Although the solution is radially symmetric, the 3D simulation must arrive at this result using rectangular (x, y, z) (not radial) coordinates and a finite-element mesh that does not inherently favor a radially symmetric solution. To reduce the size of the simulation, the 3D mesh represents only one fourth of the entire island, taking some advantage of radial symmetry of the 3D solution.

This description follows the discussion in the **SUTRA** documentation where figures showing the mesh and results may also be found.

The main parameter values are:

$\alpha = 1.0 \times 10^{-8}$ [m·s²/kg] $\beta = 4.47 \times 10^{-10}$ [m·s²/kg]
(The α and β values imply that $S_{op} = 9.0447 \times 10^{-9}$ [m·s²/kg].)

$k_H = 5.0 \times 10^{-12}$ [m²] $\varepsilon = 0.1$

$k_V = 5.0 \times 10^{-13}$ [m²] $\mu = 1.0 \times 10^{-3}$ [kg/m·s]

$|\underline{g}| = 9.81$ [m/s²] $\sigma_w = 1.0 \times 10^{-9}$ [m²/s]

$\rho_0 = 1000.$ [kg/m³]

$$C_{sea} = 0.0357 \left[\frac{(\text{kg dissolved solids})}{(\text{kg seawater})}\right]$$

$\rho_{sea} = 1024.99$ [kg/m³]

$$\frac{\partial\rho}{\partial C} = 700. \left[\frac{(\text{kg seawater})/\text{m}^3}{(\text{kg dissolved solids})}\right]$$

$$\alpha_L = \begin{cases} 10. & \text{for horizontal flow} \\ 2.5 & \text{for vertical flow} \end{cases} \quad [\text{m}]$$

$D_m = 1.0 \times 10^{-9}$ [m²/s] $\alpha_T = 0.1$ [m]

$Q_{IN} = 2.3766\text{x}10^{-5}$ [kg/(m² of horizontally projected land surface area)·s] on land
(equivalent to 75. [cm/yr] of recharge)

$$C_{IN} = 0. \left[\frac{(\text{kg dissolved solids})}{(\text{kg seawater})}\right]$$

$$\left.\begin{aligned} S_w &= \begin{cases} 1 & \text{for } p \ge 0 \\ 0.3 + 0.7\left[1 + \left(5 \times 10^{-5}\, p\right)^2\right]^{-0.5} & \text{for } p < 0 \end{cases} \\ k_r &= \left(\frac{S_w - 0.3}{0.7}\right)^{0.5}\left(1 - \left\{1 - \left(\frac{S_w - 0.3}{0.7}\right)^2\right\}^{0.5}\right)^2 \end{aligned}\right\}$$

Unsaturated properties functions of Van Genuchten (1980) with $S_{wres} = 0.3$, $a = 5 \times 10^{-5}$ [m·s²/kg], and n = 2.
(See eqns. 2.8 and 2.21 in SUTRA documentation.)

Boundary Conditions:

In the 3D model, no flow crosses the bottom boundary (z = -100 m) and no flow crosses the planes of symmetry (x = 0 and y = 0). Specified pressure is set at hydrostatic seawater pressure along the vertical outer boundary (r = 800 m). Along the top boundary, nodes above sea level (r ≤ 500 [m]) receive freshwater recharge (equivalent to 75.0 cm/yr) totaling 18.665651 kg/s of recharge for the entire circular island. (All 3D boundary conditions are directly analogous to those in the 2D formulation.) At nodes below sea level along the top and the vertical outer boundary, the pressure is specified to be hydrostatic seawater pressure. Any fluid that enters at points of specified pressure has the concentration of seawater. The value for the specified pressure boundary condition factor, GNUP, in 3D is 100.0.

Note: When 2D and 3D simulations are set up using the graphical preprocessor, **SutraGUI** (Winston and Voss, 2003), small discrepancies may be expected between these models in some parameters, such as recharge to the top surface. However, despite the obvious differences in spatial discretization, according to the fluid budgets output by SUTRA, the total recharge to the top surface of the entire island in 2D and 3D representations matches to five significant figures: 18.665773 kg/s in 2D and 18.665651 kg/s in 3D.

Initial Conditions:

Seawater concentration and natural steady-state pressures are initially set everywhere in the aquifer. The natural initial pressure values are obtained through an extra initial simulation that calculates steady pressures for the conditions of seawater concentration throughout, zero recharge at the surface of the island, and specified hydrostatic pressures along the sea bottom and the outer boundary.

Mesh:

The 3D mesh is discretized vertically into 25 layers of elements, with 1,567 elements in each layer, giving NN=42,432 and NE=39,175. See Figures 6.22 and 6.23 in the **SUTRA** documentation. Vertical discretization in the unsaturated zone is relatively coarse because, in this problem, the intent is to approximately locate the water table and the details of the saturation distribution are of less interest. Symmetry is invoked to reduce the size of the problem while maintaining a fully 3D, logically rectangular mesh; only one quadrant of the island is simulated. The outer boundary approximates a circle of radius 800 m and is sufficiently distant from the island that it does not significantly influence the results.

Simulation:

For the steady-state pre-simulation, steady state is achieved by taking one extremely large time step. The CG solver is used with a convergence tolerance of 1×10^{-13}, requiring 76 solver iterations to obtain the p solution.

For the transient runs, for both pressure and concentration, the time step size is Δt = 6311520. s (0.2 yr). Because only the long-time (steady-state) behavior of the system is of interest, a single iteration for resolving nonlinearities is used per time step. The system essentially achieves a new steady state after 100 time steps (20 yr). The CG solver is used for p solutions, and the ORTHOMIN solver is used for C solutions, both with a convergence tolerance of 1×10^{-13}. Each p solution requires from 5 to 29 solver iterations, and each C solution requires from 5 to 17 iterations.

The transient run takes about 5 minutes on a PC running Windows XP with a 3.4 GHz Pentium 4 processor; it uses about 78 Mbytes of RAM.

***SUTRA** files:*

For initial run to obtain starting pressures

input :

Island3D_initial-p.inp, *Island3D_initial-p.ics*, and SUTRA.FIL

output:

Island3D_initial-p.smy, *Island3D_initial-p.lst*, *Island3D_initial-p.rst*, *Island3D_initial-p.nod*, and *Island3D_initial-p.ele*.

For transient run

input :

Island3D.inp, *Island3D.ics*, and SUTRA.FIL

output:

Island3D.smy, *Island3D.lst*, *Island3D.rst*, *Island3D.nod*, *Island3D.ele*, and *Island3D_Timed_Obs.obs*.

Preprocessing:

The ArgusONE setup files, *Island3D_initial-p.mmb* and *Island3D.mmb*, are included for use with **SutraGUI**. In **SutraGUI**, this problem uses a vertically-aligned mesh with two units. The top of the model represents the top of the island on land and the sea bottom below the sea. The top is assigned an elevation, given as a function of radius from the center of the island. The bottom of the upper unit is 5. m below the top, and the bottom of the model is at 100 m depth below sea level. Recharge is specified as a constant value on the land portion of the island on the top surface of the model with zero concentration of inflow. On the sea bottom, the pressure is specified as hydrostatic seawater. The outermost vertical side of the model is assigned a specified pressure of hydrostatic seawater in the information layer, Specified Pressure Sheets Vertical1. In the transient simulation, an observation well is placed on the island penetrating the entire vertical extent of the model.

> *Note:* To allow visualization of the top elevation while using ArgusONE, a parameter Z_element was added to the SUTRA Mesh layer that contains the value of top elevation for each element.

In order to begin the transient simulation with a natural pressure distribution, an initial steady-state simulation is done (using the ArgusONE setup file *Island3D_initial-p.mmb*) to determine the pressures in the model during the drought (when there is no recharge and all ground water is seawater). The pressures resulting from this simulation are used as the initial pressure condition for the transient simulation (that uses using the ArgusONE setup file *Island3D.mmb*). This is specified below "Select restart file:" on the Initial Conditions Controls page of the SUTRA Project Information dialog.

Results:

Results are reported 20 years after recharge begins, by which time the system has nearly reached a new steady state. (Note that more-exact steady-state solutions may be obtained by running longer simulations, e.g. 40 years or more.)

Postprocessing:

The match of specified and calculated pressures may be checked using **CheckMatchBC**.

> Start **CheckMatchBC**, click **Select Files**, then navigate to and open the files *Island3D.inp* and *Island3D.nod*.

Hydrographs of pressure, saturation and concentration at the observation nodes may be viewed using **GW_Chart**.

> Start **GW_Chart** and select **Chart type | Hydrographs**.
> Under "Data," click the **SUTRA** radio button.
> Under "SUTRA Data," click the radio button for the type of observation data you wish to plot (**Pressure**, **Concentration**, or **Saturation**).
> Click the **Read** button, then navigate to and open the SUTRA observations file *Island3D_Timed_Obs.obs*.
> In the list of observation nodes in the upper left, set the entry in the "Plot" column to **Yes** for any nodes for which you wish to plot results.

Spatial distributions of results may be viewed with **ModelViewer**. A setup file, *Island3D.mv*, is provided for viewing the results with a solid for concentration (10% to 90% seawater) and the finite element mesh on the rear surfaces. The first image shows the initial conditions, which has seawater concentration everywhere. To see the end of the simulation, select Toolbox|Animation|Set to time: (select 100)|Set. Vertical exaggeration is 4. The nodes on the island where recharge occurs (ones that have fluid sources) are marked with blue cubes.

NOTE: A version of **SutraPlot** that is compatible with **SUTRA** Version 2.1 is currently under development. Once it is completed, a setup file for plotting results from this simulation in **SutraPlot** will be provided. Please check the web site http://water.usgs.gov/nrp/gwsoftware/sutraplot/sutraplot.html for updates.

Suggestions:

Viewing the hydrographs of concentration and saturation using **GW_Chart**, it is apparent that some adjustment towards steady state conditions will still occur after the 20-year simulation described above. The user is encouraged to try this.

Spatial variations of hydrologic properties such as permeability may also be implemented, for example using **SutraGUI** to place low and high permeability lenses within the aquifer and the results examined.