2D Example for **SUTRA**

Rocky2D and Rocky2D_irregular

(Clifford I. Voss, USGS)

This 2D example is presented in the **SUTRA** documentation (Voss and Provost, 2002, section 6.4, page 149). This exercise deals with simple modeling of constant-density flow and near-steady solute transport. It is a simple representation of ground-water flow and solute transport from a leaky contaminated waste pond at the Rocky Mountain Arsenal, Denver, Colorado, based on the detailed modeling of the system by Konikow (1977). Information is provided for two approaches to modeling the system. The *more-simplified representation* consists of an areal model of a rectangular alluvial aquifer with a constant transmissivity and two impermeable bedrock outcrops that influence groundwater flow, as shown in the **SUTRA** documentation. The second, *more realistic, representation* consists of an irregular model domain, and detailed steps for creating this with the **SutraGUI** are provided.

The first description follows for the *simplified representation*; it generally parallels the discussion in the **SUTRA** documentation where figures showing the model structure, mesh and results may also be found.

Regional flow is idealized as flow originating in a constant head region at the top of the rectangular model domain, and discharging to the river at the bottom of the rectangle, which also acts as a specified head region. Three wells pump from the aquifer (at a rate of Q_{OUT} each), and contamination enters the system through a leaking waste isolation pond (at a rate of Q_{IN}, with concentration, C^*). The natural background concentration of the contaminant is C_o. The desired solution is the steady-state distribution of hydraulic head and the near-steady evolution of concentration from the pond.

The main parameter values are:

α_L = 500. [ft]	Q_{IN} = 1.0 [ft^3/s]
α_T = 100. [ft]	C^* = 1000. [ppm]
ε = 0.2	C_o = 10. [ppm]
K = 2.5x10^{-4} [ft/s] (hydraulic conductivity)	Q_{OUT} = 0.2 [ft^3/s] (at each of three wells)
B = 40. ft	

Where the impermeable bedrock outcrop occurs, elements are assigned a conductivity value one millionth of the above aquifer value.

Boundary Conditions:

No flow occurs across any boundary except where constant head is specified at 250.0 [ft] at the top of the mesh and where constant head is specified as changing linearly between 17.5 [ft] at the bottom left corner, and 57.5 [ft] at the bottom right corner of the mesh. Inflow at the top of the mesh is at background concentration, C_o=10.0 [ppm]. A source is specified at the leaky pond node, and a sink is specified at each well node. The leaky pond is simulated as an injection of fluid (Q_{IN}, C^*) at a single node. Three wells pump from the aquifer (at a rate of Q_{OUT} each), each at a single node. A single value of constant head is specified along a portion of the top boundary, and a series of head values is specified along the bottom (river) boundary to represent changing elevation of the river.

Initial Conditions:

Initial pressures are arbitrary for steady-state simulation of pressure. Initial concentration is C_o=10.0 [ppm].

Mesh:

The rectangular mesh consists of 16 by 20 elements each of dimension 1000.0 [ft] by 1000.0 [ft] (NN=357, NE=320). Mesh thickness, B, is the actual aquifer thickness, assumed constant for the idealized model.

Simulation:

To obtain results in terms of hydraulic head and [ppm], the following must be specified in **SUTRA** input: ρ=1.0, $\partial\rho/\partial c$ =0.0, $|\underline{g}|$=0.0, μ=1.0. Hydraulic conductivities are entered in the permeability input data set. Head values in [ft] are entered in data sets for pressure. Concentrations in [ppm] are entered in data sets for mass fraction concentration. Sources and sinks are entered in units of volume [ft^3/s] per time.

One steady-state pressure solution is obtained and one concentration solution is obtained. The concentration solution is obtained after a single time step of 1000 years, which, for all practical purposes, brings the concentration distribution to a steady state. Although a steady state transport solution is also possible to run, the solute does not enter the bedrock islands in 1000 years (as it would in steady state), making the transient solution for concentration more interesting to view.

The run takes less than 1 second on a PC running Windows 2000 with a 2GHz Xeon processor; it uses less than 1 Mbyte of RAM.

***SUTRA** files:*

input :
Rocky2D.inp, *Rocky2D.ics*, and SUTRA.FIL

output:
Rocky2D.smy, *Rocky2D.lst*, *Rocky2D.rst*, *Rocky2D.nod*, *Rocky2D.ele*, and *Rocky2D.obs*.

Preprocessing:

The ArgusONE setup file, *Rocky2D.mmb*, is included for use with **SutraGUI**. In **SutraGUI**, this problem uses a fishnet mesh with one block representing a rectangular model domain. Two islands of low hydraulic conductivity are specified to represent the bedrock islands. Line objects exactly along the top and bottom edges of the domain are the locations of specified head boundary conditions. The line object at the lower end of the domain, representing the river has a specified head that varies linearly along its extent. The pond and wells are represented by point sources exactly above nodes in the mesh.

Results:

A nearly steady-state solute plume for a conservative solute is obtained after a 1000-year time step. Just upstream of the plume envelope is a region in which concentration dips slightly below background levels. This is due to a numerical problem of insufficient spatial discretization in a region where the concentration must change sharply from fresh upstream values to contaminated plume values. Lower dispersivity values would exacerbate the problem in the upstream region, but minor upstream oscillations do not affect concentration values within the plume.

Postprocessing:

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

Spatial distributions of results may be viewed with **ArgusONE**, **SutraPlot** and **ModelViewer**.

For **ArgusONE**, the plot shows contours of concentration (250, 500 and 750 ppm) and flow vectors.

For **SutraPlot**, three setup files are provided: *Rocky2D_heads.spl*, *Rocky2D_concentrations.spl,* and *Rocky2D_velocities.spl*, these shows contours of hydraulic head, concentration and velocity vectors, respectively.

For **ModelViewer**, two setup files, *Rocky2D_head+velocity.mv* and *Rocky2D_head+velocity.mv* are provided for viewing the resultsThe first image of each shows the initial conditions. To see the end of the simulation, select Toolbox|Animation|Set to time: (select 1)|Set. **ModelViewer** can only visualize results from FishNet meshes in 2D, not from irregular meshes.

Reference:

Konikow, L.F., 1977, Modeling chloride movement in the alluvial aquifer at the Rocky Mountain Arsenal, Colorado: U.S. Geological Survey Water-Supply Paper 2044, 43 p.

Suggestions:

The user is encouraged to try simulation with steady-state solute transport and to compare results with that of the 1000-year time step, described above. In addition, the user can try to simulate transient transport with 6-month times steps for 20 years of plume growth.

More-Realistic AREAL MODELING OF SOLUTE TRANSPORT at the ROCKY MOUNTAIN ARSENAL with an Irregular Mesh

----

This second version of the Rocky example is more realistic, and requires use of a variety of boundary conditions, model options and simulation features.

The background is restated here. Liquid wastes containing a toxic chemical at a concentration of 1,000 mg/L were disposed of into an unlined basin at an industrial facility. The pond leaked water into the subsurface at a long-term average rate of 0.025 m^3/s. The geometry and boundaries of the system are provided in a digital map and the main aquifer properties are listed in Table 1. There is a river flowing to the west along the southern boundary of the alluvial aquifer system; bedrock adjacent to the alluvium on the east and west is essentially impermeable. The boundary at the north is dominated by a freshwater lake, which can be assumed to represent a fully penetrating constant-head boundary. The river acts as a constant-head boundary, and the river slopes to the west with head values decreasing in that direction. The alluvial aquifer is discontinuous where two bedrock highs interrupt the alluvium. The example determines the maximum extent of the plume by considering steady-state transport of a non-reactive solute through the aquifer from the leaking pond.

This modeling example is distinguished from the more-simplified example by:

1- Use of a digital map to initiate the project.
2- Use of an irregular finite element mesh (the other example uses a Fishnet mesh).
3- All units are MKS (the other example uses English units).
4- There are only 2 withdrawal wells (the other example uses 3 such wells).
5- The bedrock highs are modeled as holes in the irregular mesh (the other example places low-conductivity regions at these locations).
6- The pond is modeled as an areal source (the other example placed the pond at one node).

Step-by-Step Instructions
for setting up steady-state SUTRA run

for Rocky Mtn. Arsenal example with *irregular* mesh

<u>Setup new SUTRA project:</u>

Start ArgusONE

PIEs|New SUTRA Project

Choose areal, saturated, solute transport, user-specified thickness, with irregular mesh.

Click **OK**. You will return to this dialog later

<u>Import a base map</u>

Activate **Map** layer

Import RMA map (**File|Import Map…**) *rma_map.dxf*

Imported objects extend out… **OK**

Click in image to unselect all objects.

Save the project.

<u>Create a domain outline for the model</u>

<u>Copy portions of map to the **Domain Outline** layer</u>

Select both bedrock islands and copy to clipboard.

Activate **Domain Outline layer** and paste in bedrock islands, then click outside of the contours to deselect them.

<u>Draw the external domain outline</u>

Draw a domain outline following left and right bedrock inside edges, lower edge of upper lake, and upper edge of river (use closed-contour drawing tool and double-click on last vertex to close the contour). Set the **element_size** to 100 in the **Contour Information dialog** that appears.

<u>Force nodes to occur at source/sink points</u>

Select the point contour drawing tool and place a point at each of the two withdrawal wells near the river, allowing to **element_size** to remain at *zero* in the **Contour Information dialog** that appears.

<u>Create mesh and optimize node numbering</u>

Select **Special|Preferences**

In the **Preferences** dialog, click on the second image (the one below the computer image) to select the **Meshing Preferences dialog**.

Deselect the last check box, "Ignore vertices on the Domain Outline that lie approximately on a straight line" and click **OK**.

Activate **SUTRA Mesh layer**, select magic wand and click inside domain to create mesh.

Optimize bandwidth by selecting **Special**, **Renumber…**, check **Optimize Bandwidth**, and **OK**.
Confirm that a node has been generated at each of the withdrawal well locations by activating the **Domain Outline** layer.

Save the project.

<u>Set boundary conditions for hydraulic head (Lake)</u>

Activate **Domain Outline** layer.
Select external domain outline (click on it).
Select lasso tool.
Encircle (lasso) the domain vertices along the lower edge of the lake along the top of the domain (these vertices become white).
Copy these to clipboard.
Activate **Specified Hydraulic Head** layer.
Paste in the copied object.
Double click the new open contour and in **Contour Information** dialog set **specified_hydraulic_head** to *75.* and **concentration** to *0.*

<u>Set boundary conditions for hydraulic head (River)</u>

Activate **Domain Outline** layer again and click outside of domain to deselect the white vertices, keeping the external domain selected (black vertices)
Select lasso tool.
Encircle (lasso) the domain vertices along the upper edge of the river (these vertices become white).
Copy these to clipboard.
Activate **Specified Hydraulic Head** layer.
Paste in the copied object.
Open **Layers** dialog by clicking on **Layers…** button in Layer List window.
Under Layer Parameters:, click on $\boldsymbol{f_x}$ to right of **specified_hydraulic_head** to open **Expression** window.
Specify a background function h(X) to obtain linear variation in head along river (e.g. 5.125E-3 * X() - 5.76) (find X under **functions: Mathematical**) and click **OK** in **Expression** window, and then **Done** in **Layers** dialog.
Double click the river contour and in **Contour Information** dialog delete the value of the **specified_hydraulic_head** (currently 100) and click on **concentration** (this automatically fills in a new value for **specified_hydraulic_head**).
Set concentration to 0, and click **OK** to exit the **Contour Information** dialog.

The two specified head boundary contours may be colored by selecting **Color** (by color bar) and then select **specified_hydraulic_head**.

Save the project.

<u>Set sources and sinks (Wells)</u>

Activate **Domain Outline** layer and click outside of domain twice to deselect all vertices.

Holding down the shift key, simultaneously select the two points (i.e. the two wells) and copy these to clipboard.
Activate **Sources of Fluid** layer and paste in the wells.
Double click on each of these in turn setting the **total_source** values to -0.001 (left well) and -0.002 (right well) and the **concentration_of_source** to 0 for both, and click **OK** each time.

<u>Set sources and sinks (Pond)</u>

Activate **Map** layer and click outside of the map to deselect any previously selected objects.
Select pond contour and copy to clipboard.
Activate **Sources of Fluid** layer and paste in the pond.
Double click the pond contour and in **Contour Information** dialog set **total_source** to 0.025 and **concentration** to 1000 and click **OK**. Click twice outside of domain to deselect the pond contour.

If contour value blocks view of the pond, select **View** and deselect **Show Contour Value**. If you would like to color the pond click **Color** (by color bar) and select **total_source**. To see an opaque pond, also click **Opaque Contours** under **View**.

Save the project.

<u>Set values of properties which are spatially constant</u>

Open **Layers** dialog by clicking on **Layers…** button in **Layer List** window.
Click in the line containing **Thickness** in the upper window and then under Layer Parameters, click on $\boldsymbol{f_x}$ to right of **thickness** to open the **Expression** window; type 12. and then click **OK**.
Repeat this for **Porosity**, **Hydraulic Conductivity**, and **Dispersivity**, setting the appropriate values for each (see Table 1). (For **Hydraulic Conductivity**, set both maximum and minimum to the same value, and for **Dispersivity**, set both longitudinal values to 30 and both transverse values to 3.)
Click **Done**.

Save the project.

PARAMETER	VALUE
HYDRAULIC CONDUCTIVITY	0.0001 m/s
POROSITY	0.20
SATURATED THICKNESS	12 m
LONGITUDINAL DISPERSIVITY	30 m
TRANSVERSE DISPERSIVITY	3 m
INITIAL CONCENTRATION	0 mg/L
Time Step Size	0.5 year

Table 1. Parameter values for Rocky Mountain Arsenal example.

Set values of non-spatial parameters

Under **PIEs**, select **Edit Project Info…**
In the **SUTRA Project Information** dialog that appears, check that *Steady flow - Steady transport* is selected on the **Simulation Modes** pane.
Click **OK** to exit.

Save the project.

Run steady-state flow and transport model

Activate **SUTRA Mesh** layer.
Under **PIEs**, select **Run SUTRA** and **OK**.
In the Root file name box, type *Rocky_irregular* as the desired prefix for the simulation files, and click **OK** and then **Save** in the **Save As** dialog that appears.
ArgusONE exports the **SUTRA** input files and then **SUTRA** runs in a black window.

Plot results

After **SUTRA** completes simulation, select **PIEs|Sutra 2D Post Proc…**
Select file, **Rocky_irregular.nod**, and click **OK.**
In the **Select SUTRA results to display** dialog that appears, in order to plot head, toggle "**no**" to "**yes**" below *Pressure* and click **OK**
Activate the **SUTRA Post Processing** layer that just appeared and turn off visibility of the **SUTRA Mesh** layer for a less cluttered view.
To change the number of contours, double-click the plot and change **minimum** to 4, **maximum** to 80 and **delta** to 2, and click **OK**.
To also plot concentration and velocity, begin again by selecting **PIEs|Sutra 2D Post Proc…**, toggle **Concentration** and **Velocity**, etc. To avoid overwriting the existing plot, select **Create a new layer with a different name**, each time when prompted.
Active the new plot layer, and then, to adjust concentration contours, double-click on the color bar to the right of the plot and choose a **minimum** contour of 50, **maximum** of 950, and **delta** of 50.

Rename plot data and plots

To save the plots and their underlying data for use later, enter the **Layers** dialog by clicking on **Layers…** button in **Layer List** window.
Click on the name, **SUTRA Post Processing Charts,** and change it to "SS head". Then click on the name, **SUTRA Post Processing Charts1,** and change it to " SS C_v PLOT ". Also change the name of the **nodal results** to "SS head node values", **nodal results1** to "SS Conc node values" and the **velocity results** layer to "SS velocity element values".

Save the project.

(Note that the results may also be viewed with **SutraPlot**.)
