Created in COMSOL Multiphysics 5.6

Aquifer Water Table Calculation

Introduction

This model demonstrates the application of COMSOL Multiphysics to a benchmark case of steady-state subsurface fluid flow and transient solute transport along a vertical cross section in an unconfined aquifer. Because of profound geologic heterogeneity, the model must estimate solute transport subject to highly irregular flow conditions with strong anisotropic dispersion. Van der Heijde (Ref. 1) classifies this case as “Level 2,” with enough potentially difficult parameter combinations to test a code’s ability to tackle realistic hydrological situations. Sudicky (Ref. 2) developed this problem to demonstrate a Laplace transform Galerkin code.

Model Definition

The hydrological setting for this problem is described in Figure 1, for groundwater flow at steady state. The aquifer is composed largely of fine-grained silty sand of hydraulic conductivity $K_1 = 5 \cdot 10^{-4}$ cm/s with lenses of relatively course material of hydraulic conductivity $K_2 = 1 \cdot 10^{-2}$ cm/s. Generally, groundwater moves from the upper surface of the saturated zone, the water table, to the outlet at $x = 250$ m. The water table is a free surface, that is, fluid pressure equals zero, across which there is vertical recharge, denoted by R, of 10 cm/a. The groundwater divide, a line of symmetry, occurs at $x = 0$. The base of the aquifer is impermeable.

Figure 2 shows conditions related to solute transport. The aquifer initially is pristine, and concentrations equal zero. For the first five years, a relative concentration of 1 is loaded over the interval 40 m < x < 80 m at the water table. The solute source is removed in year 5, and the concentration along this segment immediately drops to zero. The contaminant migrates within the aquifer via advection and dispersion. Throughout the domain, porosity, denoted by ε_p, is 0.35 as given by the benchmark, the longitudinal dispersivity, α_L, and transverse vertical dispersivity, α_T, are 0.5 m and 0.005 m, respectively. The effective molecular diffusion coefficient, D_m, is $1.34 \cdot 10^{-5}$ cm^2/s.

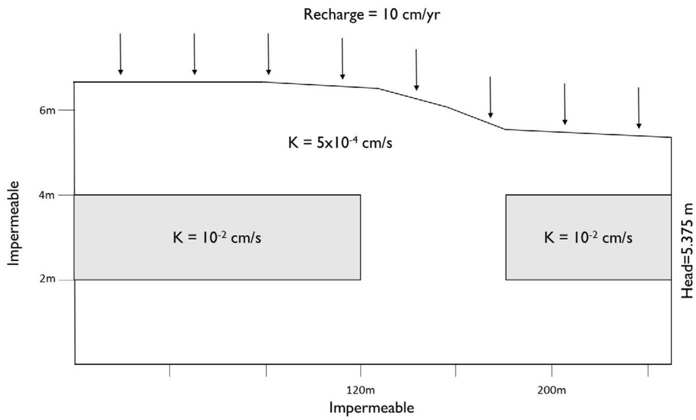


Figure 1: Settings for Darcy's Law.

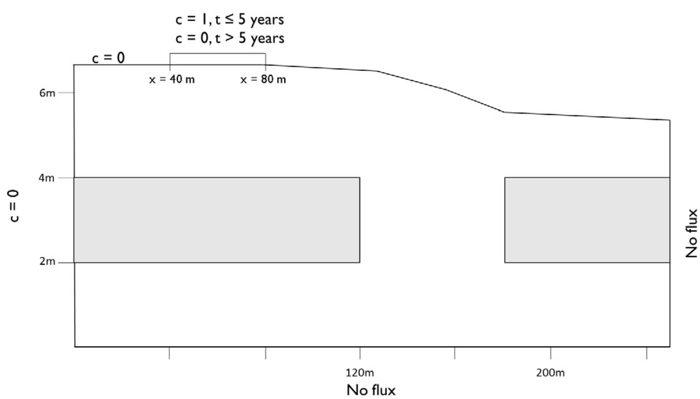


Figure 2: Definition of the transport problem.

FLUID FLOW

Steady groundwater flow generally is expressed with a Darcy's law for hydraulic head

$$\nabla \cdot (K \nabla H) = Q_{\mathrm{m}} \tag{1}$$

where K (m/s) is the hydraulic conductivity, Q_{m} (m^3/s) is the rate of recharge to water table per unit volume of aquifer, and H is the hydraulic head (m). Darcy's Law in

COMSOL is formulated with pressure p as the dependent variable. Hydraulic head and pressure are related by

$$p = \rho g(H - D)$$

where D (m) is the elevation.

The equations for groundwater flow and solute transport are linked by the average linear velocity:

$$\mathbf{u} = -\frac{K}{\rho g \varepsilon_{\mathrm{p}}}\nabla p \qquad (2)$$

where the porosity ε_{p} or the fraction of the aquifer containing water accounts for the fact that only a portion of a given aquifer block is available for flow.

The boundary conditions for the groundwater flow problem are shown in Figure 1 and stated below. No flow condition and symmetry condition are applied at $x = 0$ and $y = 0$. Both are mathematically the same:

$$-\mathbf{n} \cdot \rho \mathbf{u} = 0$$

Hydraulic head is specified at $x = 250$ m. To model the recharge of 10 cm/a this velocity is specified at the upper boundary.

SOLUTE TRANSPORT

Species transport typically is time dependent for geologic problems. The transport of a dissolved concentration c (mol/m^3) is described with the advection-dispersion equation:

$$\frac{\partial}{\partial t}(\varepsilon_{\mathrm{p}} c) + \mathbf{u} \cdot \nabla c = \nabla \cdot [(D_{\mathrm{D}} + D_{\mathrm{e}})\nabla c] \qquad (3)$$

where D_{D}(m^2/s) is the dispersion tensor and D_{e} (m^2/s) the effective diffusion; $\mathbf{u}$ is the velocity field; and t is time.

The dispersion tensor defines solute spreading by mechanical mixing and molecular diffusion. Typically, in porous media the spreading parallel to the flow (longitudinal dispersivity) exceeds the spreading perpendicular to the direction of flow (transverse dispersivity) by a multiple. This is an important aspect of the benchmark problem.

At the top boundary a space- and time-dependent function for the concentration is defined, according to

$$c = \begin{cases} 1, & 0 \le t \le 5\mathrm{a}; \quad 40\mathrm{m} \le x \le 80\mathrm{m} \\ 0, & \text{else} \end{cases} \tag{4}$$

At the left boundary the concentration is set to zero and a no flux condition is applied to the right and bottom boundary.

Results and Discussion

FLUID FLOW

Figure 3 provides hydraulic heads estimated with the COMSOL Multiphysics steady-state groundwater flow simulation. The hydraulic heads and streamlines correspond nicely to the benchmark results provided by Sudicky (Ref. 2). The water table geometry determined for the simulation nearly duplicates the benchmark geometry. The good match between the flow fields is expected because the initial water table geometry used with COMSOL Multiphysics was designed to closely resemble the benchmark geometry.

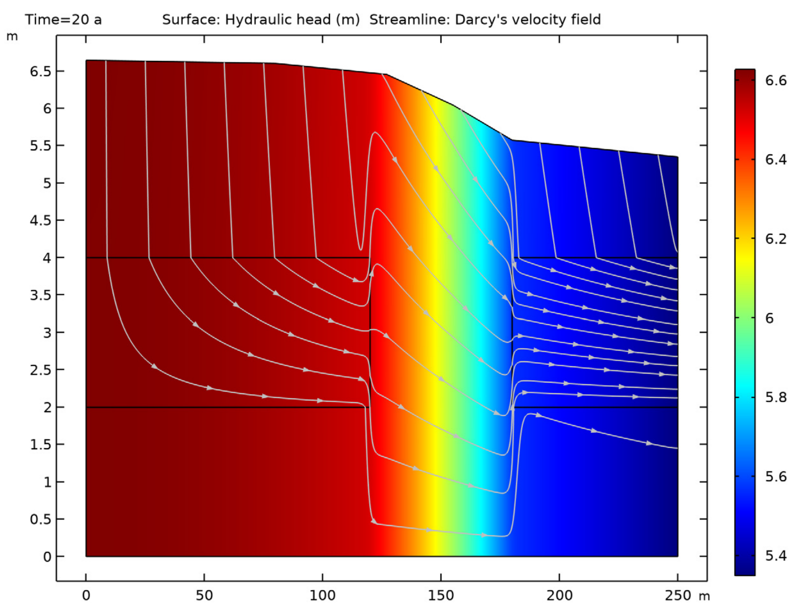
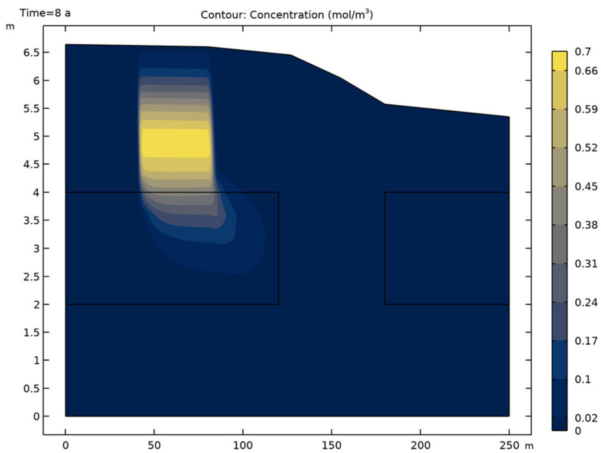
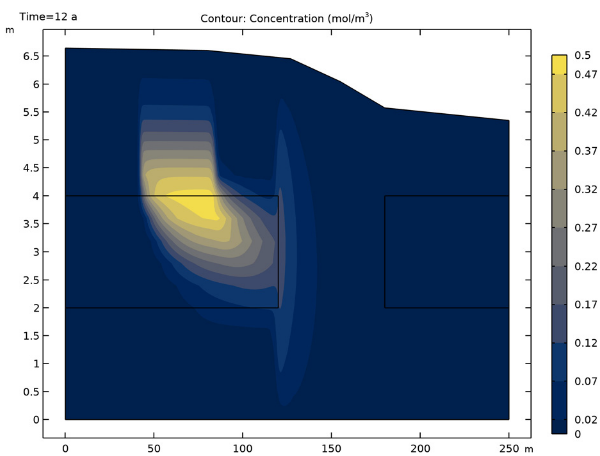


Figure 3: Estimated hydraulic head and flow lines.

SOLUTE TRANSPORT

Solute transport solutions from the model are almost identical to the ones presented in Ref. 2. This is shown in the contour intervals for three times in Figure 4. In 1989, Sudicky concluded that the results illustrated in Ref. 2 are relatively free from numerical dispersion, as the low concentration contours closely follow the flow pattern. The surface plot for COMSOL also displays this property, in that even the lowest concentrations in Figure 4 still follow the irregular flow lines of Figure 3.





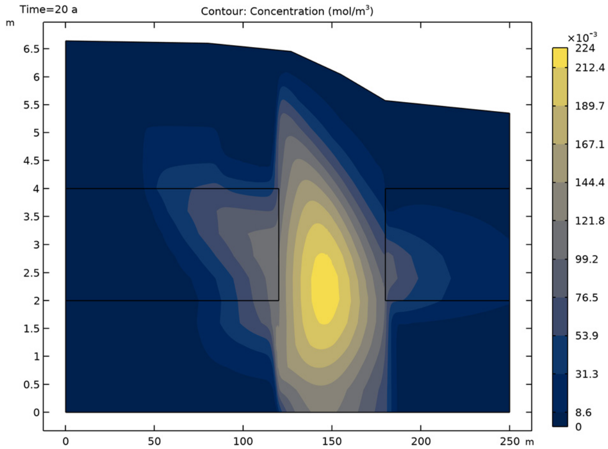


Figure 4: Solute concentration after 8, 12, and 20 years.

References

1. P.K.M. van der Heijde, "Model Testing: A Functionality Analysis, Performance Evaluation, and Applicability Assessment Protocol," *Groundwater Models for Resources Analysis and Management*, A.I. El-Kadi (ed.), CRC Press, Lewis Publishers, Boca Raton, FL, pp. 39–58, 1995.

2. E.A.Sudicky, "The Laplace Transform Galerkin Technique: A Time-Continuous Finite Element Theory and Application to Mass Transport in Groundwater," *Water Resources Research*, vol.25, No. 8, 1989.

Application Library path: `Subsurface_Flow_Module/Solute_Transport/aquifer_water_table`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.
2 In the **Select Physics** tree, select **Fluid Flow>Porous Media and Subsurface Flow>Darcy's Law (dl)**.
3 Click **Add**.
4 In the **Select Physics** tree, select **Chemical Species Transport>Transport of Diluted Species in Porous Media (tds)**.
5 Click **Add**.
6 Click **Study**.
7 In the **Select Study** tree, select **General Studies>Stationary**.
8 Click **Done**.

GEOMETRY 1

Polygon 1 (pol1)

1 In the **Geometry** toolbar, click **Polygon**.
2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.
3 In the table, enter the following settings:

x (m)	y (m)
0	0
250	0
250	5.35
180	5.575
155	6.045
127	6.455
80	6.603
0	6.645

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.
2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3 In the **Width** text field, type 120.
4 In the **Height** text field, type 2.
5 Locate the **Position** section. In the **y** text field, type 2.

Rectangle 2 (r2)

1 In the **Geometry** toolbar, click **Rectangle**.
2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
3 In the **Width** text field, type `70`.
4 In the **Height** text field, type `2`.
5 Locate the **Position** section. In the **x** text field, type `180`.
6 In the **y** text field, type `2`.
7 Click **Build All Objects**.

The geometry is elongated. Define another **View** which scales the view in the **Graphics** window for easier set-up.

DEFINITIONS

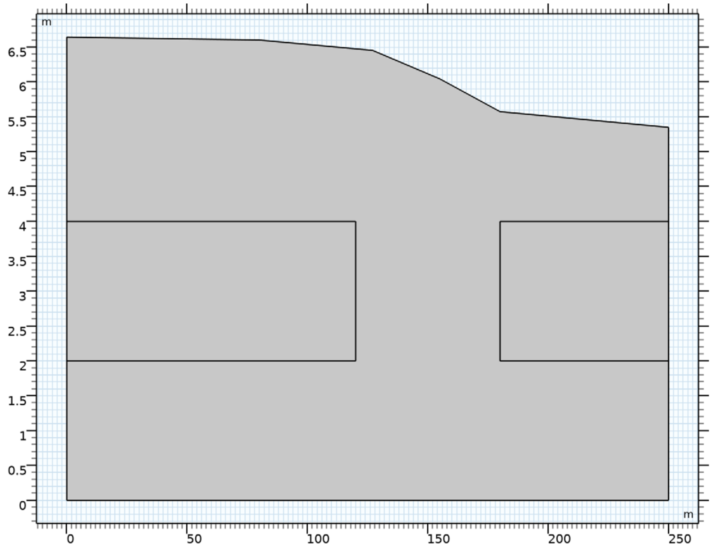
View 2

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **View**.

Axis

1 In the **Model Builder** window, expand the **View 2** node, then click **Axis**.
2 In the **Settings** window for **Axis**, locate the **Axis** section.
3 From the **View scale** list, choose **Automatic**.

4 Click **Update**.



DARCY'S LAW (DL)

Fluid and Matrix Properties 1

1. In the **Model Builder** window, under **Component 1 (comp1)>Darcy's Law (dl)** click **Fluid and Matrix Properties 1**.
2. In the **Settings** window for **Fluid and Matrix Properties**, locate the **Matrix Properties** section.
3. From the **Permeability model** list, choose **Hydraulic conductivity**.
4. In the K text field, type `5e-4[cm/s]`.

The rectangles have a higher hydraulic conductivity.

Fluid and Matrix Properties 2

1. Right-click **Component 1 (comp1)>Darcy's Law (dl)>Fluid and Matrix Properties 1** and choose **Duplicate**.
2. Select Domains 2 and 3 only.
3. In the **Settings** window for **Fluid and Matrix Properties**, locate the **Matrix Properties** section.
4. In the K text field, type `1e-2[cm/s]`.

   Next, set up the boundary conditions.

Inlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

2 Select Boundaries 7, 8, 10, 11, and 15 only. This corresponds to all upper boundaries.

3 In the **Settings** window for **Inlet**, locate the **Velocity** section.

4 In the U_0 text field, type `10[cm/a]`.

Hydraulic Head 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Hydraulic Head**.

2 Select Boundaries 16–18 only.

3 In the **Settings** window for **Hydraulic Head**, locate the **Hydraulic Head** section.

4 In the H_0 text field, type `5.3486`.

Symmetry 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.

2 Select Boundaries 1, 3, and 5 only.

Next, set up the transport equations. One important aspect of this benchmark problem is anisotropic dispersivity with a ratio of 100 between longitudinal and transverse dispersivity.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species in Porous Media (tds)>Porous Medium 1** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Convection** section.

3 From the $\mathbf{u}$ list, choose **Darcy's velocity field (dl)**.

4 Locate the **Diffusion** section. In the $D_{\mathrm{F,c}}$ text field, type `1.34e-5[cm^2/s]`.

Porous Medium 1

In the **Model Builder** window, click **Porous Medium 1**.

Dispersion 1

1 In the **Physics** toolbar, click **Attributes** and choose **Dispersion**.

2 In the **Settings** window for **Dispersion**, locate the **Dispersion** section.

3 From the **Dispersion tensor** list, choose **Dispersivity**.

4 In the α_{L} text field, type `0.5`.

5 In the α_{T} text field, type `0.005`.

The next step is to set up the boundary conditions. At the top boundary the concentration is 0 except for the first five years within 40 m and 80 m. Define a function that will help you setting up this boundary condition.

DEFINITIONS

Rectangle 1 (rect1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Parameters** section.

3 In the **Lower limit** text field, type `40`.

4 In the **Upper limit** text field, type `80`.

5 Click **Plot**.

This defines the local position of the concentration source.

TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)

Concentration 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Concentration**.

2 Select Boundaries 7, 8, 10, 11, and 15 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species c** check box.

5 In the $c_{0,c}$ text field, type `rect1(x[1/m])*(t<=5[a])`.

This expression calls the rectangle function width the argument x and gives the location of the species source. It is followed by a logic expression that applies the concentration for the first five years only. After that it remains 0.

Concentration 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Concentration**.

2 Select Boundaries 1, 3, and 5 only.

3 In the **Settings** window for **Concentration**, locate the **Concentration** section.

4 Select the **Species c** check box.

Outflow 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outflow**.

2 Select Boundaries 2 and 16–18 only.

Add a material and fill out the missing values for the porosity and density.

ADD MATERIAL

1 In the **Home** toolbar, click **Add Material** to open the **Add Material** window.

2 Go to the **Add Material** window.

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

3 In the **Settings** window for **Material**, locate the **Material Contents** section.

4 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	1000	kg/m³	Basic
Porosity	epsilon	0.35	1	Basic

MESH 1

A proper mesh resolution ensures smooth and accurate results. Restrict the maximum element size to prevent too large mesh elements.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Extremely fine**.

4 Locate the **Mesh Settings** section. From the **Sequence type** list, choose **User-controlled mesh**.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 Click the **Custom** button.

4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type `0.5`.

5 Click **Build All**.

STUDY 1

Now, set up the solver sequence. First calculate a stationary Darcy velocity field. Use this for the second time-dependent step which computes the transport of the species over 20 years.

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Transport of Diluted Species in Porous Media (tds)**.

Time Dependent

1 In the **Study** toolbar, click **Study Steps** and choose **Time Dependent>Time Dependent**.

Now, solve for the concentration only. The Darcy velocity field used to calculate the convective transport is known from the previous stationary step.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 In the table, clear the **Solve for** check box for **Darcy's Law (dl)**.

4 Locate the **Study Settings** section. From the **Time unit** list, choose **a**.

5 In the **Output times** text field, type `range(0,1,20)`.

These are the output time steps. The solver will choose the computational time steps according to a convergence criteria. When using time dependent functions it is often recommended to restrict the computational time steps. Otherwise, if the convergence of the time-dependent solver is good, it can happen that the solver overestimates the required time step size and hence the user-defined time dependent function is not resolved properly.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

4 From the **Steps taken by solver** list, choose **Strict**.

5 In the **Study** toolbar, click **Compute**.

RESULTS

Pressure (dl)

A surface plot of the pressure field and a surface plot of the species concentration is created per default. Modify the surface plot to show the hydraulic head and add streamlines to create the plot shown in Figure 3.

Surface

1 In the **Model Builder** window, expand the **Pressure (dl)** node, then click **Surface**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `dl.H`.

Streamline 1

1 In the **Model Builder** window, click **Streamline 1**.

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

3 From the **Positioning** list, choose **On selected boundaries**.

4 Locate the **Selection** section. Select the **Activate Selection** toggle button.

5 Select Boundaries 7, 8, 10, 11, and 15 only.

6 Locate the **Streamline Positioning** section. In the **Number** text field, type `15`.

7 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Arrow length** list, choose **Normalized**.

8 Select the **Scale factor** check box.

9 In the associated text field, type `3e7`.

10 In the **Pressure (dl)** toolbar, click **Plot**.

To create the concentration contour plots from Figure 4 proceed with the next steps.

Concentration Contours

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.

2 In the **Settings** window for **2D Plot Group**, type `Concentration Contours` in the **Label** text field.

Contour 1

1 Right-click **Concentration Contours** and choose **Contour**.

2 In the **Settings** window for **Contour**, locate the **Expression** section.

3 In the **Expression** text field, type `c`.

4 Locate the **Levels** section. In the **Total levels** text field, type `10`.

5 Locate the **Coloring and Style** section. From the **Contour type** list, choose **Filled**.

6 From the **Color table** list, choose **Cividis**.

7 Click the **Zoom Extents** button in the **Graphics** toolbar.

To get the plots for the other times select them from the **Time (a)** list in the **Data** section of this plot group.