Aquifer Characterization[1]

1. The formulation of this example is courtesy of Mr. Michael A. Cardiff and Prof. Peter K. Kitanidis of Stanford University, who have kindly made their own model version available (Ref. 1).

Introduction

This example illustrates how you can use COMSOL Multiphysics' Optimization interface in combination with a PDE or physics interface to solve inverse-modeling problems (sometimes referred to as parameter estimation or history-matching problems). The modeling techniques presented here in the context of flow in an aquifer with spatially variable hydraulic conductivity are generally applicable for solving underdetermined optimization problems with COMSOL Multiphysics.

Note: This model requires the Optimization Module.

INVERSE-MODELING BACKGROUND

Consider data consisting of the following components:

- A model — for example, a PDE — of a natural or engineered system with a set of unknown coefficients or parameters
- A set of measurements or observations with associated measurement errors

Inverse modeling is the practice of using data of this kind as input to estimate the unknown parameters of the example, which in this context is called the *forward model*. In particular, if the number of unknown parameters, n, is larger than the number of measurement values, m, the inverse problem is called *underdetermined*. This example belongs to this class of inverse problems.

When, as in this case, the forward model is a PDE and the unknown coefficient is a spatially varying random field, the number of unknown parameters is infinite. Even an ordinary finite element discretization typically gives too many unknown parameters by some orders of magnitude. Obtaining a tractable problem that can be solved numerically instead requires a separate *regularization*.

For underdetermined inverse problems, data fitting alone is not sufficient to single out an optimal solution; achieving this aim requires some additional criterion and an associated *penalty function* that ranks the solutions according how well they satisfy the criterion in question.

The objective function for an underdetermined inverse problem can thus be written as the sum of a fitness term and a penalty term:

$$L(\mathbf{y}, \mathbf{s}) = L_{\text{fitness}}(\mathbf{y}, \mathbf{s}) + L_{\text{penalty}}(\mathbf{s})$$

The fitness term

$$L_{\text{fitness}}(\mathbf{y},\mathbf{s}) = (\mathbf{y}-\mathbf{h}(\mathbf{s}))^T R^{-1}(\mathbf{y}-\mathbf{h}(\mathbf{s})) \quad (1)$$

measures how well the model fits with the observations. Here $\mathbf{y}$ denotes an m-dimensional row vector of measurement values; $\mathbf{s}$ is an n-dimensional row vector of parameter values; $\mathbf{h}: \mathbf{R}^n \to \mathbf{R}^m$ is the forward model, which maps from parameter values to expected measurements; and R is the m-by-m covariance matrix of measurement errors. Assuming, that the measurement errors are independent and identically distributed with variance $\sigma_R{}^2$, it follows that $R = \sigma_R{}^2 I$, where I denotes the m-by-m identity matrix.

The penalty term is relevant for problems where the number of parameters, n, exceeds the number of measurement values, m. It serves to discriminate between solutions with comparable fitness values. Through geostatistical reasoning, Kitanidis (Ref. 2) arrives at the penalty term

$$L_{\text{penalty}} = (\mathbf{s}-\mathbf{X}\beta)^T Q^{-1}(\mathbf{s}-\mathbf{X}\beta) \quad (2)$$

where Q^{-1} is the inverse of the spatial covariance matrix $Q \equiv E[(\mathbf{s}-\mathbf{X}\beta)(\mathbf{s}-\mathbf{X}\beta)^T]$, with $E[\ ]$ denoting the expectation operator, $\mathbf{X}$ being an n-dimensional row vector whose elements all equal 1, and β referring to the scalar constant mean of the parameter field.

The covariance Q is a symmetric n-b-n matrix, which must be estimated from the measurements or assumed known based on prior information about the process generating $\mathbf{s}$. It is typically assumed that $\mathbf{s}$ is a realization of a stationary and isotropic random field, such that elements of the covariance matrix are only a function of the distance between the corresponding points in space: $Q_{ij} = q(|\mathbf{x}_i - \mathbf{x}_j|)$. The dependence of $q(|\mathbf{x}_i - \mathbf{x}_j|)$ on distance is usually expressed as a *variogram* $\gamma(\mathbf{x}_i - \mathbf{x}_j|) = q(0) - q(|\mathbf{x}_i - \mathbf{x}_j|)$, which is in turn assumed to have a simple functional form with only a few parameters that can be fitted to the data.

Model Definition

FORWARD MODEL

Consider a square zone in a confined 2D aquifer of side $b = 100$ m and with spatially variable hydraulic conductivity, K_s (m/s), which is of interest for transport modeling or other purposes. In this simplified model, assume that the region of interest is surrounded by a practically infinite domain known to have roughly constant hydraulic conductivity, K_{s0}. Using *infinite elements*, you can accurately simulate the effect of the infinite exterior domain on the region of interest.

Neglecting any differences in elevation, the hydraulic potential governing the flow through the aquifer and its surroundings can be represented by the pressure head $H \equiv p/(\rho_f g)$ (m), where p is the fluid pressure (Pa), ρ_f (kg/m^3) is the (constant) fluid density, and g (m/s^2) is the acceleration due to gravity. The pressure head, or the hydraulic head, obeys Darcy's Law

$$\nabla \cdot (-K_s \nabla H) = Q_s$$

where Q_s (1/s) represents sources and sinks. At the modeling domain's boundary, on the outside of the infinite element zone, any effects of spatial inhomogeneities are negligible and you specify the condition $H = 0$ to complete the forward model. Note that this choice implies that the variable H refers to the *change* in hydraulic head from a reference state where no pumping occurs rather than the hydraulic head itself.

INVERSE MODEL

The inverse problem is to estimate the hydraulic-conductivity field in the aquifer using experimental data in the form of hydraulic-head measurements from four *dipole-pump tests*. More specifically, consider eight wells (represented as points) at the corners and midpoints of the zone being characterized. While injecting fluid at one point, fluid is extracted at the same rate at the opposite point on the rim across the aquifer, and the hydraulic-head values at the six remaining points are recorded. Repeating this procedure for the other three cross-aquifer point pairs, gives a total of 4 sets of 6 observations each. The hydraulic-head measurements are assumed to be independent and have an accuracy on the order of $\Delta H = 1$ cm, resulting in the fitness term (see Equation 1)

$$L_{\text{fitness}} = \frac{\|\mathbf{y} - \mathbf{h}(\mathbf{s})\|^2}{\Delta H^2} \tag{3}$$

To make use of the experimental data, you must reduce the infinite number of degrees of freedom in the hydraulic-conductivity field to a finite number of unknown parameters. To this end, decompose the quadratic aquifer domain into a 10-by-10 grid of squares of side $c = 10$ m, and assume that the hydraulic conductivity takes a constant value in each square. The number of parameters characterizing the aquifer is then 100, which gives a well-defined underdetermined inverse model that can be solved quickly as an example problem.

A common assumption in the geological sciences is that spatially distributed parameters follow a geostatistical distribution defined by some parameterized variogram. This COMSOL model uses an exponential variogram of the form

$$\gamma = \sigma^2(1 - e^{-h/r}) \tag{4}$$

with variance $\sigma^2 = 1$ (the *sill* parameter) and correlation length $r = 50$ m (the *range*). For the purpose of this modeling example, assume that the parameters σ and r are known; Kitanidis (Ref. 2) gives methods for estimating their values in the case where they are unknown. Since the covariance must approach zero as the distance between samples increases, this implies a simple covariance function $q(|\mathbf{x}_i - \mathbf{x}_j|) = q(h) = e^{-h/r}$.

Thus, for the penalty term, the elements of the covariance matrix Q are easy to evaluate. Computing the inverse, Q^{-1}, would be unnecessarily expensive. Instead, split Equation 2 in two, introducing an auxiliary vector $\mathbf{u}$ of the same length as the unknown parameter vector $\mathbf{s}$:

$$\begin{aligned} L_{\text{penalty}} &= (\mathbf{s} - \mathbf{X}\beta)^T\mathbf{u} \\ \mathbf{u} &= Q^{-1}(\mathbf{s} - \mathbf{X}\beta) \end{aligned} \tag{5}$$

Solving the linear system $Q\mathbf{u} = \mathbf{s} - \mathbf{X}\beta$ for the value of u is in general cheaper than inverting Q.

In Figure 1, the eight points on the rim of the area being characterized are numbered pairwise as 1±, 2±, 3±, 4±, with plus and minus signs denoting injection wells and pumping wells, respectively.

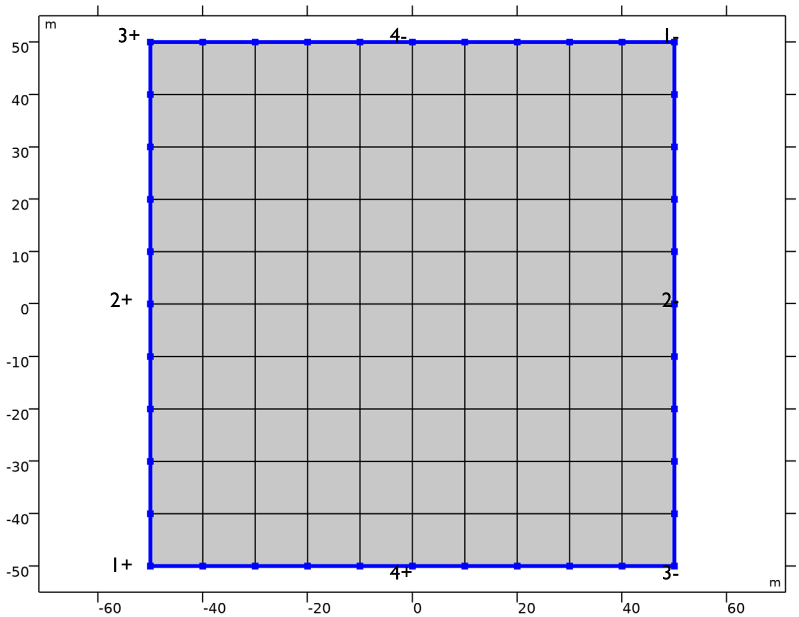


Figure 1: Discretization of the hydraulic-conductivity parameter field. Each 10 m-by-10 m square zone is associated with a degree of freedom encoding the constant $\log_{10} K_s$ *value in the zone. The numbers in blue, outside the square grid, are labels for the dipole-pump pairs ("+" for injection wells and "-" for pumping wells).*

MODEL DATA

The data required for setting up the example are supplied in text files included in your COMSOL installation:

- A text file with reference synthetically generated field data, containing the $\log_{10}$ values of the regularized hydraulic-conductivity parameter field that is used to generate fictitious hydraulic-head measurements. This allows you to evaluate the optimization solver's performance and accuracy, and to test and calibrate the inverse model. For example, you can try out different penalty terms in the objective function and investigate the solution's dependence on the number of observations used.

  The $\log_{10} K_s$ field for the reference model is visualized in Figure 2. It was generated with the exponential variogram, γ, given in Equation 4.

- Four CSV-files contain the hydraulic-head measurement data series. These datasets were generated by solving the reference forward model for the four different dipole-pump configurations.
- An auxiliary measurement data file containing a single zero value, to be used when implementing the penalty term formally on least-squares form.

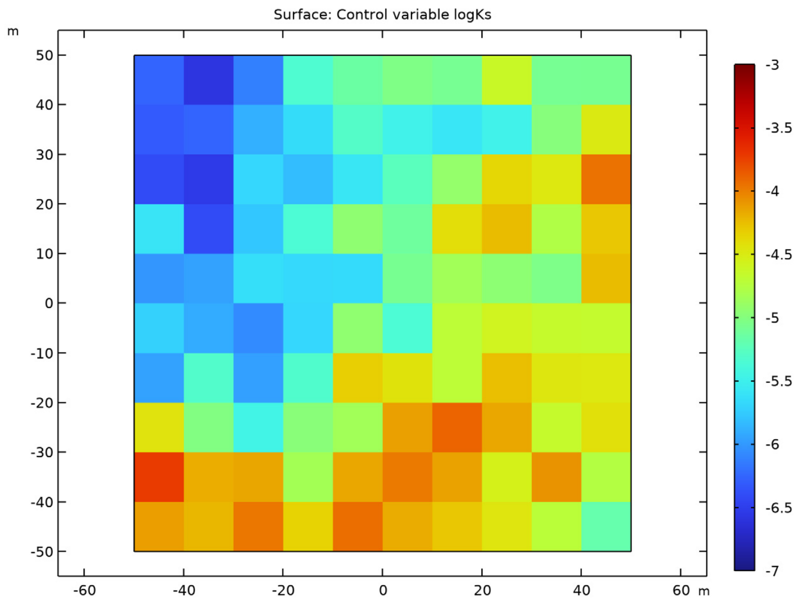


Figure 2: Discretized hydraulic-conductivity field for the reference forward model.

The four simulated dipole-pump tests for the reference forward model give the combined results listed in Table 1, here rounded off to the nearest millimeter; the example uses these numbers as fictitious measurement values.

TABLE 1: HYDRAULIC HEAD (METERS) MEASURED AT WELLS FOR THE FOUR DIPOLE PUMP TESTS.

TEST	1+	1-	2+	2-	3+	3-	4+	4-
1	-	-	1.425	-0.718	-0.028	0.333	1.197	-1.330
2	0.568	-1.576	-	-	1.425	-1.176	-0.641	-0.689
3	-0.801	-0.439	1.187	-1.414	-	-	-1.565	0.958
4	1.636	-0.891	0.501	0.453	-1.272	1.251	-	-

Although the normalization of the fitness term (see Equation 3) assumes a measurement accuracy of 1 cm, this model (in contrast to Ref. 1) adds no random error component to the above data. This is because the primary aim here is to investigate the software's performance rather than the viability of the method for aquifer characterization.

Results and Discussion

Figure 3 and Figure 4 show the optimization results for the hydraulic conductivity obtained using only the first measurement series and all four measurement series, respectively. The corresponding values of the total mean square error are 0.318 (0.316) and 0.086 (0.087), where the values in parentheses are those obtained by Cardiff and Kitanidis (Ref. 1). Note that the error estimates are slightly different because Cardiff and Kitanidis include a synthetic measurement error of the order 1% in their observations. Figure 5 compares the results from four different inverse-modeling simulations, using 1, 2, 3, and 4 measurement series, respectively. As the figure shows, the improvement in accuracy is most marked when going from 1 to 2 pump tests (that is, from 6 to 12 observations). Including additional measurements appears to yield comparatively small benefits in accuracy. However, as discussed in Ref. 2, the posterior uncertainty in parameter estimates decreases as more measurements are added.

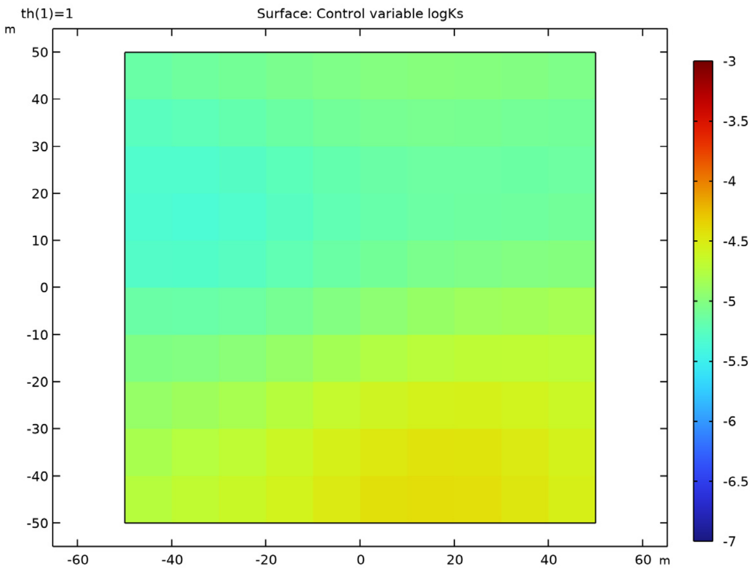


Figure 3: Inverse-modeling solution for the hydraulic conductivity logarithm parameter field obtained using only the first measurement series (dipole pair number 1).

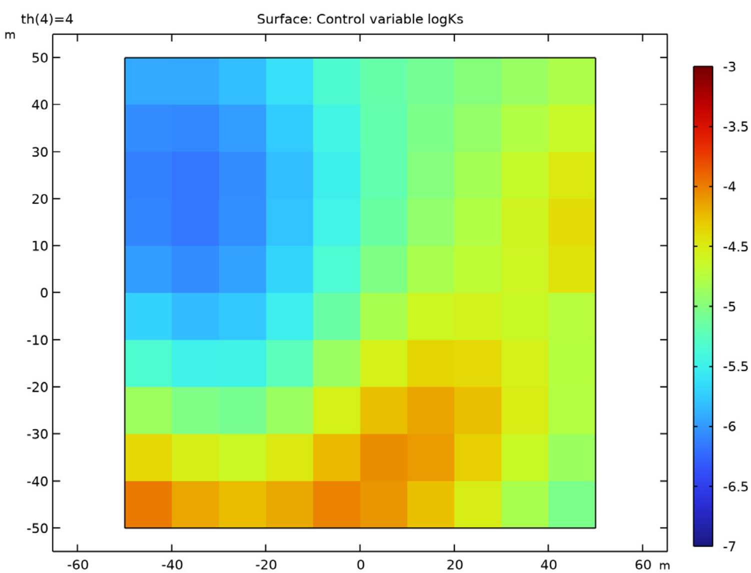


Figure 4: Hydraulic conductivity obtained by inverse modeling using 24 observations.

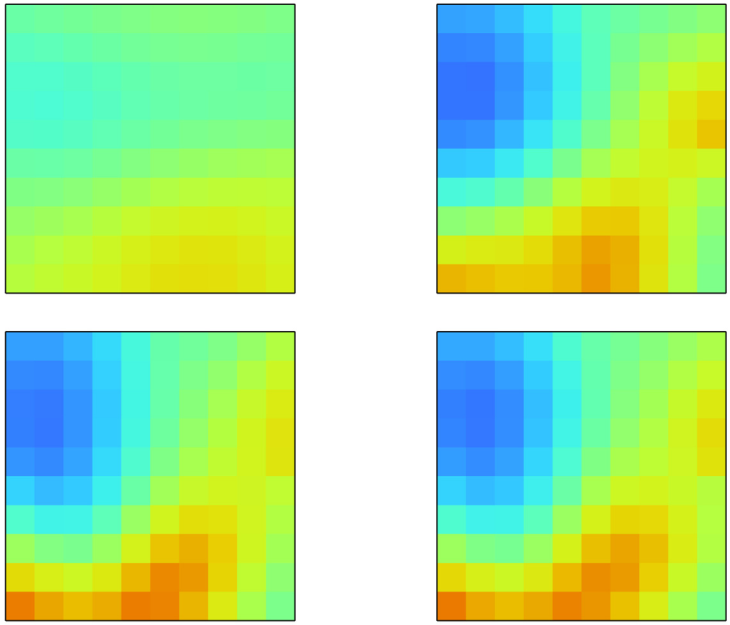


Figure 5: Inverse-modeling results for the hydraulic conductivity field with different numbers of hydraulic-head observations taken into account: 6 (upper left), 12 (upper right), 18 (lower left), and 24 (lower right). For a color-scale legend, see Figure 2.

References

1. M. Cardiff and P.K. Kitanidis, “Efficient Solution of Nonlinear, Underdetermined Inverse Problems with a Generalized PDE Model,” *Computers & Geosciences*, vol. 34, pp. 1480–1491, 2008.

2. P.K. Kitanidis, “Quasi-linear Geostatistical Theory for Inversing,” *Water Resources Research*, vol. 31, no. 10, pp. 2411–2419, 1995.

Application Library path: `Subsurface_Flow_Module/Fluid_Flow/aquifer_characterization`

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 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Stationary**.

6 Click **Done**.

GEOMETRY 1

Square 1 (sq1)

1 In the **Geometry** toolbar, click **Square**.

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

3 In the **Side length** text field, type 100.

4 Locate the **Position** section. In the **x** text field, type -150.

5 In the **y** text field, type -150.

Array 1 (arr1)

1 In the **Geometry** toolbar, click **Transforms** and choose **Array**.

2 Select the object **sq1** only.

3 In the **Settings** window for **Array**, locate the **Size** section.

4 In the **x size** text field, type 3.

5 In the **y size** text field, type 3.

6 Locate the **Displacement** section. In the **x** text field, type 100.

7 In the **y** text field, type 100.

Point 1 (pt1)

1 In the **Geometry** toolbar, click **Point**.

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

3 In the **x** text field, type `-50,0,0,50`.

4 In the **y** text field, type `0,-50,50,0`.

5 In the **Geometry** toolbar, click **Build All**.

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

GLOBAL DEFINITIONS

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

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

3 In the table, enter the following settings:

Name	Expression	Description
`N0`	`0.1[kg/(m*s)]`	`Pump source strength`
`deltaH`	`1[cm]`	`Hydraulic head measurement error`
`logKs0`	`-5`	`Hydraulic conductivity, initial log10 value`
`th`	`1`	`Measurement-series index`
`sigma`	`1`	`Sill parameter`
`r`	`50[m]`	`Range parameter`
`elementTypeFactor`	`1`	`1 for quads, 0.5 for triangles`

As already mentioned, defining the model requires a number of external data files:

- The hydraulic-head measurement data series are stored in four separate CSV-files included in your COMSOL installation.
- A text file with the forward-model data for the log-transmittivity parameter field is provided to allow you to evaluate the optimization solver's performance and accuracy, and to test and calibrate the inverse model. For example, you can try out different penalty terms in the objective function and investigate the solution's dependence on the number of observations used.
- A dummy measurement file containing a single zero value, in order to implement the penalty term on the same form as a least-squares error term.

To make the data for the log-transmittivity field available in the model, create an interpolation function.

logKs Reference

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

2 In the **Settings** window for **Interpolation**, locate the **Definition** section.

3 From the **Data source** list, choose **File**.

4 Click **Browse**.

5 Browse to the model's Application Libraries folder and double-click the file `aquifer_characterization_logKs_ref.txt`.

6 From the **Data format** list, choose **Grid**.

7 Click **Import**.

8 In the **Label** text field, type `logKs Reference`.

9 Locate the **Definition** section. Find the **Functions** subsection. In the table, enter the following settings:

Function name	Position in file
logKs_ref	1

10 Locate the **Interpolation and Extrapolation** section. From the **Interpolation** list, choose **Nearest neighbor**.

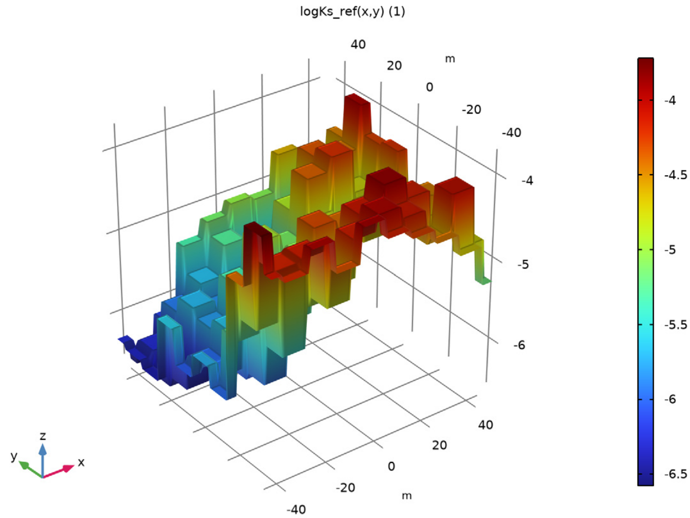
11 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
logKs_ref	1

12 In the **Argument** table, enter the following settings:

Argument	Unit
Argument 1	m
Argument 2	m

13 Click **Plot**.



DEFINITIONS

Define Infinite Element Domains for the outer squares.

Infinite Element Domain 1 (ie1)

1. In the **Definitions** toolbar, click **Infinite Element Domain**.
2. Select all rectangles except the one in the middle.

Variables 1

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

   For an initial evaluation of the forward model, use the reference solution's hydraulic conductivity field. Later, the control variable field for the Optimization interface will override this expression.
2. In the **Settings** window for **Variables**, locate the **Variables** section.
3. In the table, enter the following settings:

Name	Expression	Description
logKs	logKs_ref(x,y)	Hydraulic conductivity, log 10 value

MATERIALS

Assign water as the only domain material everywhere. Darcy's law in general requires separate specifications of the fluid and matrix material properties. In this case, the matrix conductivity is given first by an interpolation field, later by the Optimization interface. Darcy's Law for time-dependent problems also involves the porosity, but this model is stationary so you can safely ignore the warning about this property being undefined.

ADD MATERIAL

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

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

3 In the tree, select **Built-in>Water, liquid**.

4 Click **Add to Component** in the window toolbar.

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

DARCY'S LAW (DL)

Porous Matrix 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Darcy's Law (dl)> Porous Medium 1** click **Porous Matrix 1**.

2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.

3 From the **Permeability model** list, choose **Hydraulic conductivity**.

4 In the K text field, type `10^logKs0`. This is the conductivity that is applied to the **Infinite Element Domain**. The center domain is defined as follows:

Porous Medium 2

1 In the **Physics** toolbar, click **Domains** and choose **Porous Medium**.

2 Select Domain 5 only.

Porous Matrix 1

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

2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.

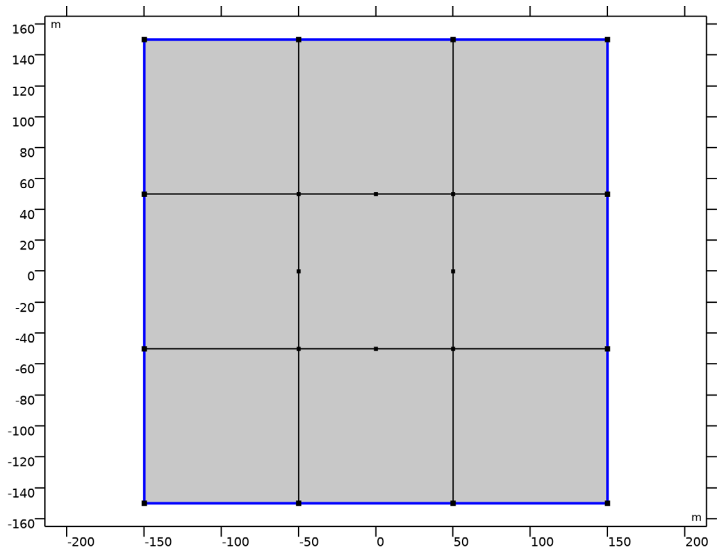
3 From the **Permeability model** list, choose **Hydraulic conductivity**.

4 In the K text field, type `10^logKs`.

Hydraulic Head 1

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

Select all outer boundaries.



Next, add the dipole pumps by using the **Line Mass Source** feature.

Line Mass Source 1

1 In the **Physics** toolbar, click **Points** and choose **Line Mass Source**.

2 Select Point 6 only.

3 In the **Settings** window for **Line Mass Source**, locate the **Line Mass Source** section.

4 In the N_0 text field, type `if(th==1,N0,0)`.

The conditional statement allows you to control which dipole pump to activate through the parameter `th`. Note that a value of zero is the default condition, so setting N_0 to zero has no effect on the model equations.

Line Mass Source 2-8

Proceed to create seven additional **Line Mass Source** features with the following settings:

Name	Selection	Expression
Line Mass Source 2	7	`if(th==2,N0,0)`
Line Mass Source 3	8	`if(th==3,N0,0)`
Line Mass Source 4	10	`if(th==4,N0,0)`

Name	Selection	Expression
Line Mass Source 5	11	`if(th==4,-N0,0)`
Line Mass Source 6	13	`if(th==3,-N0,0)`
Line Mass Source 7	14	`if(th==2,-N0,0)`
Line Mass Source 8	15	`if(th==1,-N0,0)`

MESH 1

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

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Size 1

1 In the **Model Builder** window, right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 5 only.

5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section.

7 Select the **Maximum element size** check box. In the associated text field, type `5`.

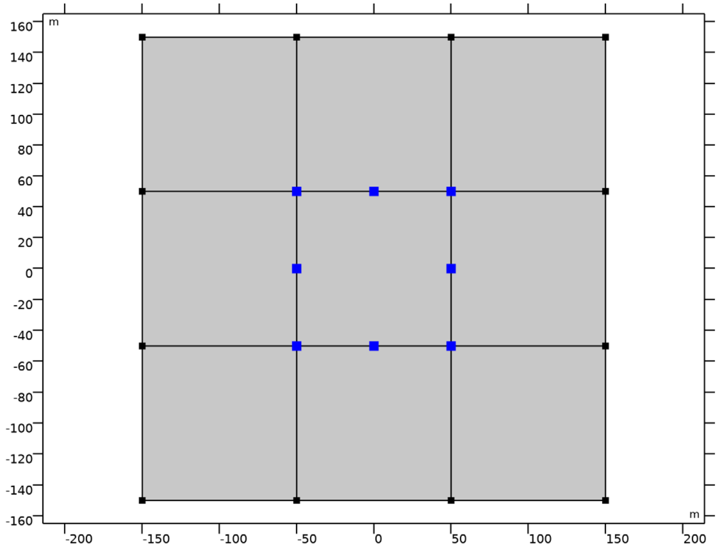
Size 2

1 Right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Points 6–8, 10, 11, and 13–15 only.

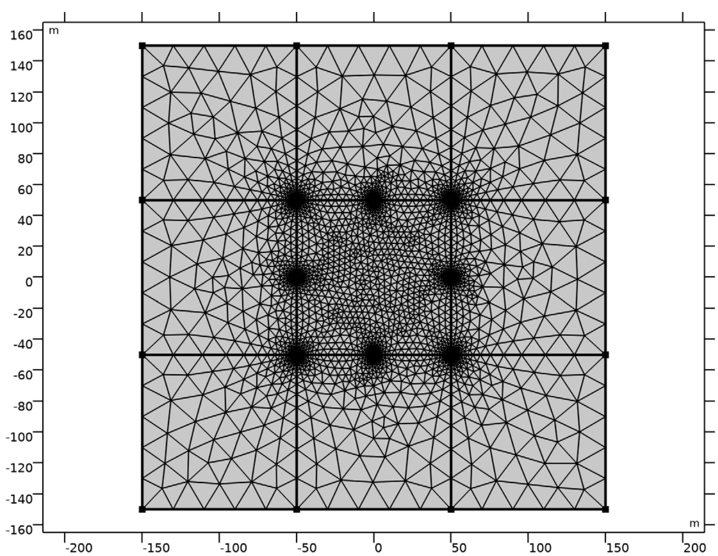


5 Locate the **Element Size** section. Click the **Custom** button.

6 Locate the **Element Size Parameters** section.

7 Select the **Maximum element size** check box. In the associated text field, type `0.1`.

8 Click **Build All**.



STUDY 1

Solve the forward problem to verify that you have implemented the physics correctly.

1 In the **Home** toolbar, click **Compute**.

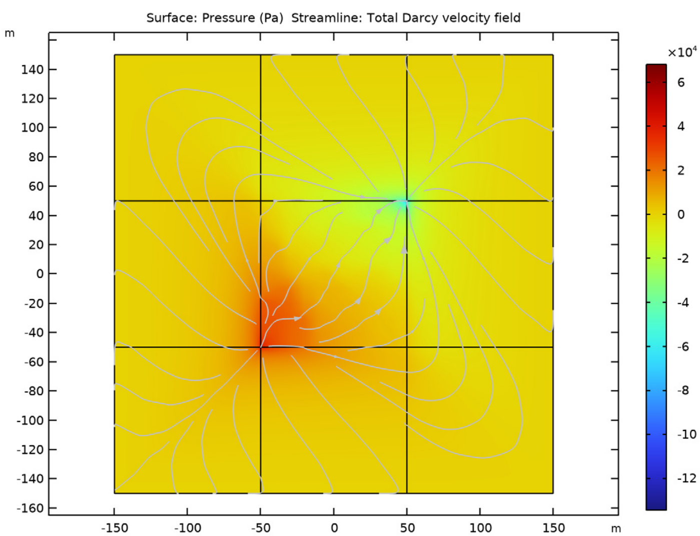
RESULTS

Pressure, Forward

The default plot shows the pressure distribution. Mark it with 'Forward' to be able to distinguish it from later solutions.

1 In the **Settings** window for **2D Plot Group**, type `Pressure, Forward` in the **Label** text field.

The result should look like that in the figure below.



ADD PREDEFINED PLOT

Add a Flownet plot which displays the hydraulic head and compare it with the figure below.

1 In the **Home** toolbar, click **Windows** and choose **Add Predefined Plot**.

2 Go to the **Add Predefined Plot** window.

3 In the tree, select **Study 1/Solution 1 (sol1)>Darcy's Law>Flownet (dl)**.

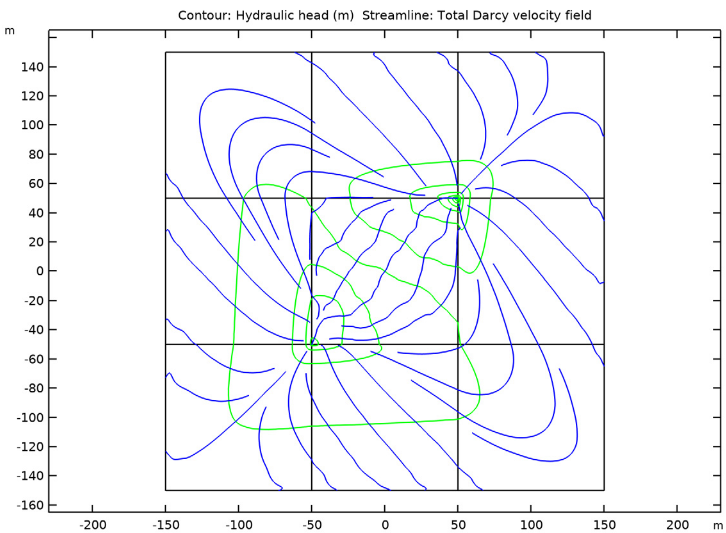
4 Click **Add Plot** in the window toolbar.

5 In the **Home** toolbar, click **Add Predefined Plot** to close the **Add Predefined Plot** window.

RESULTS

Flownet, Forward

1 In the **Settings** window for **2D Plot Group**, type `Flownet, Forward` in the **Label** text field.



ROOT

Next, set up the auxiliary model for the hydraulic conductivity control variable field and the help variable `u`.

ADD COMPONENT

In the **Model Builder** window, right-click the root node and choose **Add Component>2D**.

Next, create the auxiliary geometry on which the Optimization interface lives. This geometry is a copy of the aquifer domain, except that you do not need to include vertices at the positions of the sources and sinks.

ADD PHYSICS

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

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

3 In the tree, select **Mathematics>Optimization and Sensitivity>General Optimization (opt)**.

4 Click **Add to Component 2** in the window toolbar.

5 In the tree, select **Mathematics>ODE and DAE Interfaces>Domain ODEs and DAEs (dode)**.

6 Click **Add to Component 2** in the window toolbar.

7 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

ADD STUDY

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.

4 Click **Add Study** in the window toolbar.

5 In the **Model Builder** window, click the root node.

6 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

GEOMETRY 2

In the **Model Builder** window, under **Component 2 (comp2)** click **Geometry 2**.

Square 1 (sq1)

1 In the **Geometry** toolbar, click **Square**.

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

3 In the **Side length** text field, type 100.

4 Locate the **Position** section. From the **Base** list, choose **Center**.

DEFINITIONS (COMP2)

You will define the hydraulic conductivity control variable shortly. To make it available on the forward-model's geometry, use a General Extrusion operator.

General Extrusion 1 (genext1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **General Extrusion**.

2 In the **Settings** window for **General Extrusion**, locate the **Source Selection** section.

3 From the **Selection** list, choose **All domains**.

Define an operator for calculating the mean square error. Note that this is an area-weighted average.

Average 1 (aveop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Average**.

2 In the **Settings** window for **Average**, type `mean` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **All domains**.

To evaluate the penalty function, which is defined in terms of matrix-vector products with discrete control variable degrees of freedom, you need a way to compute a discrete sum over the mesh elements. This can be achieved using an Integration operator of order 0, together with appropriate compensation for the mesh element area.

Integration 1 (intop1)

1 In the **Definitions** toolbar, click **Nonlocal Couplings** and choose **Integration**.

2 In the **Settings** window for **Integration**, type `int0` in the **Operator name** text field.

3 Locate the **Source Selection** section. From the **Selection** list, choose **All domains**.

4 Locate the **Advanced** section. In the **Integration order** text field, type `0`.

Variables, Domain

1 In the **Definitions** toolbar, click a= **Local Variables**.

2 In the **Settings** window for **Variables**, type `Variables, Domain` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Domain**.

4 Select Domain 1 only.

5 Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Description
logKs_ref	logKs_ref(x,y)	Hydraulic conductivity, reference model
areaFactor	1/(elementTypeFactor*dvol)	Summation compensation factor
dist	sqrt((x-dest(x))^2+(y-dest(y))^2)	Distance between points inside summation

The `dest()` operator instructs the software to evaluate the enclosed argument at the destination point when evaluating an integral. The result of calling a nonlocal integration coupling with an argument containing the variable `dist` will therefore depend on where the integral is evaluated.

In this case, a nonlocal integration coupling is used to compute a discrete sum over elements. This is achieved using a single integration point per element and compensating for the corresponding integration point weight. The variable `dvol` is the volume scale factor that the software uses internally when mapping between dimensionless local element coordinates and the model geometry's global coordinate system shown in the user interface. The mesh-element volume in the local element coordinate system multiplied by `dvol` therefore gives the mesh-element volume in the global coordinates. In 2D, the mesh-element area in element coordinates is 1 for quadrilateral meshes and 1/2 for triangular meshes.

Variables, Global

1. In the **Definitions** toolbar, click a= **Local Variables**.

   Add variables for the mean squared error, the mean of the log conductivity and the penalty term.

2. In the **Settings** window for **Variables**, type `Variables, Global` in the **Label** text field.
3. Locate the **Variables** section. In the table, enter the following settings:

Name	Expression	Description
MSE	mean((logKs-logKs_ref)^2)	Area-weighted mean squared error
logKs_mean	int0(logKs*areaFactor)/ int0(areaFactor)	Discrete control variable mean
L_penalty	int0((logKs-logKs_mean)*u* areaFactor)	Penalty function

Note that the penalty function is evaluated using the intermediate variable `u`, which is computed as the solution of an auxiliary equation. The integration operator `int0` together with `areaFactor` effectively computes the discrete scalar product between the vectors `logKs-logKs_mean` and `u`.
Furthermore, note that the model entry appears in red as `logKs` has not yet been defined in component 2. This will be done in the General Optimization settings.

Covariance function

1. In the **Definitions** toolbar, click f(x) **Analytic**.
2. In the **Settings** window for **Analytic**, type `Covariance function` in the **Label** text field.
3. In the **Function name** text field, type `Q`.
4. Locate the **Definition** section. In the **Expression** text field, type `sigma^2*exp(-x/r)`.
5. Locate the **Units** section. In the table, enter the following settings:

Argument	Unit
x	m

6. In the **Function** text field, type `1`.

GENERAL OPTIMIZATION (OPT)

In the **Model Builder** window, under **Component 2 (comp2)** click **General Optimization (opt)**.

Control Variable Field 1

1 In the **Physics** toolbar, click **Domains** and choose **Control Variable Field**.

2 In the **Settings** window for **Control Variable Field**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **All domains**.

4 Locate the **Control Variable** section. In the **Control variable name** text field, type `logKs`.

5 In the **Initial value** text field, type `logKs_ref`.

   This is just a temporary initial setting; after creating a plot of the reference solution you will change it to `logKs0`.

6 Locate the **Discretization** section. From the **Shape function type** list, choose **Discontinuous Lagrange**.

7 Find the **Base geometry** subsection. From the **Element order** list, choose **Constant**.

   This gives discontinuous elements of order zero for the control variable `logKs`, a choice that ensures that each auxiliary-geometry mesh element carries a single degree of freedom.

Global Least-Squares Objective 1

Here, use the measurement file `aquifer_characterization_zero.csv` to minimize a positive objective contribution that does not correspond to an actual measurement; you will add the real measurements shortly to the first model.

1 In the **Physics** toolbar, click **Global** and choose **Global Least-Squares Objective**.

2 In the **Settings** window for **Global Least-Squares Objective**, locate the **Experimental Data** section.

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `aquifer_characterization_zero.csv`.

To put the penalty term formally on least-squares format — something which is required by the Levenberg-Marquardt solver — enter the square root of the penalty value as a model expression to be compared with the dummy zero measurement.

Value Column 1

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

2 In the **Settings** window for **Value Column**, locate the **Value Column** section.

3 In the **Expression** text field, type `sqrt(L_penalty)`.

DOMAIN ODES AND DAES (DODE)

Set up the equation for the auxiliary vector `u`, which must use the same discretization as the control variable field `logKs`.

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Domain ODEs and DAEs (dode)**.
2 In the **Settings** window for **Domain ODEs and DAEs**, locate the **Units** section.
3 In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	1

4 Click to expand the **Discretization** section. From the **Element order** list, choose **Constant**.

Distributed ODE 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Domain ODEs and DAEs (dode)** click **Distributed ODE 1**.
2 In the **Settings** window for **Distributed ODE**, locate the **Source Term** section.
3 In the *f* text field, type `(logKs-logKs_mean-intO(u*Q(dist)*areaFactor))`.

MESH 2

Mapped 1

In the **Mesh** toolbar, click **Mapped**.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.
2 In the **Settings** window for **Distribution**, locate the **Boundary Selection** section.
3 From the **Selection** list, choose **All boundaries**.
4 Locate the **Distribution** section. In the **Number of elements** text field, type `10`.
5 Click **Build All**.

DEFINITIONS (COMP1)

Now return to **Component 1** and add an alternative definition of variable `logKs`, mapping the corresponding control variable field from **Component 2**.

Variables 1

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

Variables 4

1. In the **Model Builder** window, click **Variables 4**.
2. In the **Settings** window for **Variables**, locate the **Variables** section.
3. In the table, enter the following settings:

Name	Expression	Description
`logKs`	`comp2.genext1(comp2.logKs)`	`Hydraulic conductivity, log 10 value`

COMPONENT 1 (COMP1)

Because the measurements are to be compared with the solutions of **Component 1**, define the least-squares objective contributions in this model.

ADD PHYSICS

1. In the **Home** toolbar, click **Add Physics** to open the **Add Physics** window.
2. Go to the **Add Physics** window.
3. In the tree, select **Mathematics>Optimization and Sensitivity>General Optimization (opt)**.
4. Click **Add to Component 1** in the window toolbar.
5. In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

GENERAL OPTIMIZATION 2 (OPT2)

Least-Squares Objective 1

1. Right-click **Component 1 (comp1)>General Optimization 2 (opt2)** and choose the domain setting **Least-Squares Objective**.
2. Select Domain 5 only.
3. In the **Settings** window for **Least-Squares Objective**, locate the **Experimental Data** section.
4. Click **Browse**.
5. Browse to the model's Application Libraries folder and double-click the file `aquifer_characterization_H1.csv`.

   This file has three columns: the first two are coordinate columns defining the measurement location for the value found in the third column. The index `1` in the filename refers to the measurement series number. Thus, this feature contains the contribution from the first measurement series to the objective function, corresponding to the experimental parameter value `th=1`. Once you have set it up, you can duplicate it to conveniently add the contributions from the remaining three experiment series.
6. Locate the **Experimental Parameters** section. Click **Add**.

7 In the table, enter the following settings:

Name	Expression
th	1

Coordinate Column 1

In the **Physics** toolbar, click **Attributes** and choose **Coordinate Column**.

Least-Squares Objective 1

In the **Model Builder** window, click **Least-Squares Objective 1**.

Coordinate Column 2

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

2 In the **Settings** window for **Coordinate Column**, locate the **Coordinate Column** section.

3 From the **Coordinate** list, choose **y**.

Least-Squares Objective 1

In the **Model Builder** window, click **Least-Squares Objective 1**.

Value Column 1

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

2 In the **Settings** window for **Value Column**, locate the **Value Column** section.

3 In the **Expression** text field, type `comp1.dl.H`.

4 In the **Column contribution weight** text field, type `1/deltaH^2`.

The measurements are weighted by the inverse of the square of the measurement error.

Least-Squares Objectives 2-4

Now add the three remaining measurement series, by duplicating the **Least-Squares Objective 1** node for each measurement. Make sure you end up with the following nodes and the correct settings:

Name	Filename	Parameter th
Least-Squares Objective 2	`aquifer_characterization_H2.csv`	2
Least-Squares Objective 3	`aquifer_characterization_H3.csv`	3
Least-Squares Objective 4	`aquifer_characterization_H4.csv`	4

STUDY 2

Step 1: Stationary

Before computing the inverse model, test the model setup by computing the forward-model solution corresponding to the reference hydraulic conductivity field mapped from **Component 2**. First, disable the original definition of the hydraulic conductivity for this study step.

1 In the **Model Builder** window, under **Study 2** click **Step 1: Stationary**.
2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.
3 Select the **Modify model configuration for study step** check box.
4 In the tree, select **Component 1 (comp1)>Definitions>Variables 1**.
5 Click **Disable**.
6 In the **Home** toolbar, click **Compute**.

RESULTS

For later comparison with the results of the inverse modeling runs, plot the reference solution for the hydraulic conductivity logarithm in a separate window. You can then let COMSOL Multiphysics update the **Graphics** window plot while solving.

Surface 1

1 In the **Model Builder** window, expand the **Results>General Optimization** node, then click **Surface 1**.
2 In the **Settings** window for **Surface**, click to expand the **Range** section.
3 Select the **Manual color range** check box.
4 In the **Minimum** text field, type `-7`.
5 In the **Maximum** text field, type `-3`.

By locking the color range in this way you ensure that the color legend is unaffected by changes in the maximum and minimum values for the control variable field.

6 Click to expand the **Quality** section. From the **Smoothing** list, choose **None**.

No smoothing is necessary because `logKs` is piecewise constant.

7 In the **General Optimization** toolbar, click **Plot**.

log Ks, 6 Obs.

1 In the **Model Builder** window, under **Results** click **General Optimization**.
2 In the **Settings** window for **2D Plot Group**, type `log Ks, 6 Obs.` in the **Label** text field.

3 In the **log Ks, 6 Obs.** toolbar, click **Plot In** and choose **New Window**.

This creates a static plot that is not updated when the solution dataset changes.

Now compute the inverse model for a single measurement series, but first set the initial solution for `logKs` to a constant value.

GENERAL OPTIMIZATION (OPT)

Control Variable Field 1

1 In the **Model Builder** window, under **Component 2 (comp2)>General Optimization (opt)** click **Control Variable Field 1**.

2 In the **Settings** window for **Control Variable Field**, locate the **Control Variable** section.

3 In the **Initial value** text field, type `logKs0`.

STUDY 2

Optimization

1 In the **Study** toolbar, click **Optimization** and choose **Optimization**.

2 In the **Settings** window for **Optimization**, locate the **Optimization Solver** section.

3 From the **Method** list, choose **Levenberg-Marquardt**.

4 In the **Optimality tolerance** text field, type `0.002`.

In order to see how the inverse model result improves as the number of measurements increases, begin by disabling the last three Least Squares Objective nodes.

5 Locate the **Objective Function** section. In the table, clear the **Active** check boxes for **General Optimization 2 (opt2)/Least-Squares Objective 2**, **General Optimization 2 (opt2)/Least-Squares Objective 3**, and **General Optimization 2 (opt2)/Least-Squares Objective 4**.

6 Locate the **Output While Solving** section. Select the **Plot** check box.

7 From the **Plot group** list, choose **log Ks, 6 Obs.**.

Disable table output of objective and constraint values.

8 Clear the **Keep objective values in table** check box.

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

RESULTS

Flownet, Forward

The solver converges after about 30 iterations and a solution time around 1 minute.

log Ks, 6 Obs.

Compare the plot with that shown in Figure 3.

Evaluate the mean square error as follows:

MSE, 6 obs.

1. In the **Model Builder** window, expand the **Results>Derived Values** node, then click **Global Evaluation 1**.
2. In the **Settings** window for **Global Evaluation**, type `MSE, 6 obs.` in the **Label** text field.
3. Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 2 (comp2)>Definitions>Variables>MSE - Area-weighted mean squared error - 1**.
4. Click **Evaluate**.

   The value should be close to 0.32.

TABLE 1

1. Go to the **Table 1** window.

   Finally, compute the inverse model including all four measurement series in a separate study.

   To keep the solution for 6 observations, you can either create a new study with the same settings as before or you create a copy of the current solution and modify **Study 2**. To do so, proceed as follows:

STUDY 2

Solver Configurations

In the **Study** toolbar, click **Create Solution Copy**.

Optimization

1. In the **Model Builder** window, click **Optimization**.
2. In the **Settings** window for **Optimization**, locate the **Objective Function** section.
3. In the table, select the **Active** check boxes for **General Optimization 2 (opt2)/Least-Squares Objective 2**, **General Optimization 2 (opt2)/Least-Squares Objective 3**, and **General Optimization 2 (opt2)/Least-Squares Objective 4**.

   Before hitting the **Compute** button, prepare the plots.

RESULTS

Domain ODEs and DAEs

Delete the plot group displaying the auxiliary variable `u`.

1 In the **Model Builder** window, under **Results** right-click **Domain ODEs and DAEs** and choose **Delete**.

2 Click **Yes** to confirm.

log Ks, 6 Obs.

1 In the **Model Builder** window, under **Results** click **log Ks, 6 Obs.**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 - Copy 1 (5) (sol3)**.

4 Right-click **Results>log Ks, 6 Obs.** and choose **Duplicate**.

log Ks, 24 Obs.

1 In the **Model Builder** window, under **Results** click **log Ks, 6 Obs. 1**.

2 In the **Settings** window for **2D Plot Group**, type `log Ks, 24 Obs.` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2/Solution 2 (3) (sol2)**.

MSE, 6 obs.

1 In the **Model Builder** window, under **Results>Derived Values** click **MSE, 6 obs.**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2/Solution 2 - Copy 1 (5) (sol3)**.

STUDY 2

Optimization

1 In the **Model Builder** window, under **Study 2** click **Optimization**.

2 In the **Settings** window for **Optimization**, locate the **Output While Solving** section.

3 From the **Plot group** list, choose **log Ks, 24 Obs.**.

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

RESULTS

log Ks, 24 Obs.

Now, compare the plot with that shown in Figure 4.

MSE, 24 obs.

1 In the **Model Builder** window, under **Results>Derived Values** click **Global Evaluation 2**.

2 In the **Settings** window for **Global Evaluation**, type `MSE, 24 obs.` in the **Label** text field.

3 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 2 (comp2)>Definitions>Variables>comp2.MSE - Area-weighted mean squared error - 1**.

4 Click **= Evaluate**.

The value should be approximately 0.086.