ModelMaker

User Manual

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04/00

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E-mail support queries should be sent to support@modelkinetix.com.

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Contents

Installation and Licensing

ModelMaker can be installed as a 'desktop' or a 'network' version.

The desktop version is standard and should be chosen by most users. The network version is for installations where multiple linked workstations will be accessing the same data, and requires the purchase of more than one license.

Desktop installation

Installing ModelMaker

- Insert the ModelMaker CD into your CD-ROM drive

The installation routine should run automatically. If it does not, you must locate and run *autorun.exe*:

- Open *Windows Explorer* or *My Computer*
- Navigate to ***D:\*** (where ***D*** is the name of your CD drive)
- Locate and double click *autorun.exe* to run the installation

The ModelKinetix CD menu will open.

- Select Install ModelMaker 4

You will then be given 2 installation choices:

1. Install ModelMaker on your desktop
2. Install ModelMaker on your network

- Select option 1 and follow the on-screen instructions.

You must run the desktop version of ModelMaker from your local drive, *e.g.* C:\. By default, the installer suggests the directory:

C:\Program Files\Cherwell Scientific\ModelMaker 4

Registering and licensing ModelMaker

When ModelMaker is first run following installation, it runs as a fully functioning demo that will expire after 30 days. You must register your copy of ModelMaker with Cherwell Scientific in order to continue using it after 30 days. ModelMaker can be registered at any time during the demo or even after the demo has expired.

- Select Help | About ModelMaker to open the About ModelMaker dialog box

- Click *User Details* to open the User Details dialog

- Enter your User Name, Organization name and your ModelMaker Serial Number

Note that if you do not have a ModelMaker Serial Number this entry can be left blank.

- Click *OK*

- Click *Licensing* to open the Licensing dialog and note the settings in the following table:

Serial Number	
User Name	
Organization	
User Code 1	
User Code 2	

To complete your license registration, you must contact Cherwell Scientific to obtain your Activation Codes:

- Open the modelkinetix.com web site: **http://www.modelkinetix.com**

- Navigate to *Support* and follow the on-line instructions

Alternatively, you can e-mail us (**licensing@modelkinetix.com**) or, if you don't have internet access, telephone our UK office.

When you have obtained your Activation Codes:

- Enter the 2 Activation Codes in the License Control dialog box

- Click OK

Your copy of ModelMaker will now be fully licensed.

Network installation

This installation should only be attempted by network administrators. Both the server and client installations require administrator privileges.

It is important to follow the correct installation sequence:

A. Install ModelMaker on your server

B. Install ModelMaker on your client workstations

C. Run ModelMaker from one of the client workstations (NOT the server) and activate licensing

Installing ModelMaker

- Insert the ModelMaker CD and run *autorun.exe* as described for a desktop version

- Select Install ModelMaker 4

You will be given 2 installation choices:

1. Install ModelMaker on your desktop

2. Install ModelMaker on your network

- Select option 2 to install the network version of ModelMaker

You will be given 2 further choices:

1. Install ModelMaker on your network server

2. Install ModelMaker shortcuts and drivers on a network workstation

- Select option 1 to install ModelMaker to your desired network directory

- Run option 2 on every client workstation that will run ModelMaker over the network

When ModelMaker is first run following installation, it must be run from a client workstation. It will detect that it is being invoked from a network client and set itself up as a network version. The network license is then enabled which allows ModelMaker to be run from any workstation on your network.

Note that the installation will fail if ModelMaker is first run from the server.

Registering and licensing ModelMaker

- Register and license your network copy of ModelMaker as described for a desktop version

This information will be stored in the network license file and will be retrieved by whichever workstation is running the application.

Extra licenses can be bought at any stage for additional client workstations.

About this Manual

This manual will guide you through ModelMaker's comprehensive range of features. The accompanying Reference Manual contains mathematical theory and additional reference information.

Chapter 1 is a brief introduction to model design and will be of interest to users with little or no previous experience of creating and using models.

Chapter 2 is a tutorial, for users who are new to ModelMaker. In this chapter, we describe the layout of the interface, the construction of a simple model and some basic ModelMaker functions.

Chapters 3 to 16 make up the bulk of the manual and explain how ModelMaker's tools and features work – running the application, using the interface, model building and running, graphs, tables and analysis techniques.

Conventions used in this manual

- Program menu commands are referred to as File | Open, for example, meaning select Open from the File menu.

- Angled brackets are used to refer to keyboard characters. For example, <Esc> means press the Escape key, <Ctrl+C> means hold down the Control key whilst pressing C, <Alt, F,O> means press the Alt key followed by F then O.

- LMB refers to the Left Mouse Button and RMB refers to the Right Mouse Button menu. For example, RMB | Parameters means click the right mouse button within the Model Viewer panel and select Parameters from the menu.

In ModelMaker, there are typically several ways to access dialog boxes and features. These methods include toolbars, program menus, the Right Mouse Button (shortcut) menu and keyboard shortcuts. In general, only toolbar icons and program menus have been documented in this manual. However, the shortcut menu will also access many ModelMaker functions. Note that the appearance of the shortcut menu depends on the area or component that is clicked. See the *ModelMaker Reference Manual* for a list of keyboard shortcuts.

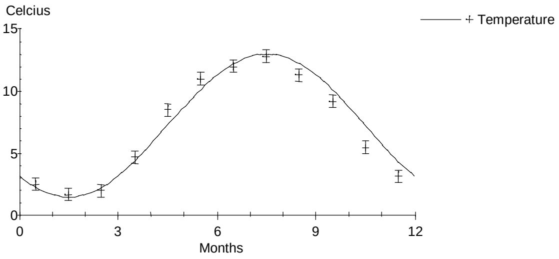
1. Introduction

A model is a quantitative description of a real-life process or system, and is typically composed of mathematical equations which give numerical answers. These answers can be substantiated against factual data to test the accuracy of a model. If a model is accurate, it can be used to make predictions.

In the next section, some of the important differences between empirical models and mechanistic or simulation models are discussed.

Empirical models

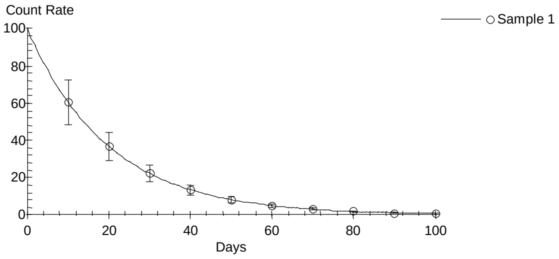
If you have some observed data for an event which shows how it varies in relation to another factor, then it is often possible to develop an empirical model which describes this variation. For example, in the temperate zone of the northern hemisphere, the mean monthly temperature varies during the year in a manner similar to that shown in the graph below:



The points on this graph provide some useful information, graphically summarizing the annual fluctuations. The data can be described further by ‘fitting’ a mathematical function using statistical methods, as shown in this case with a *sine* function. The *parameters* of the sine function are estimated by minimizing the deviations of the curve from the data points. This is often a useful exercise, as the resulting fitted equation can provide a useful summary of the data, although in many cases the nature of the equation has no *physical* meaning. In other words, the choice of function is quite arbitrary; we simply choose something of the right general shape. However, this is not always the case; sometimes the function used is dictated by some underlying theory whose parameters are unknown. In such cases, the fitting process takes on new meaning as we are estimating parameters which have some physical meaning based on theory. The 'goodness of fit' gives us some idea of how good the theory is. For example, radioactive decay is described by the equation:

$$N = N_0 \exp(- lt)$$

where N is the amount of radioactive material left at time t, if there was N_0 at time $t = 0$ and the *decay constant* of the radioactive material concerned is λ. This decay constant can be estimated by making observations of the count rate from the radioactive source at various times and then fitting the above equation to the data.



Both of these empirically derived examples are simple 'models'. They provide a quantitative description of a process. They could be used to predict the amount of radioactive material remaining at times in the future, or to predict the temperature at various times next year. Of course the predictions may not be perfect as they depend on the accuracy of the model. In the case of radioactive decay, the model is good and we could be confident of its predictions. Predicting meteorological factors like temperature, however, is much harder and the sine model is probably only good at describing overall long term trends.

Simulation models

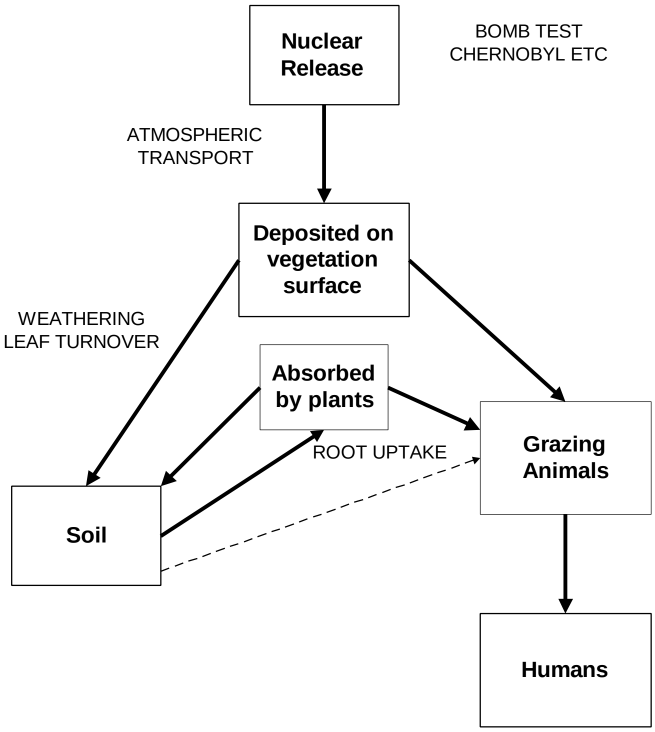
Simulation models, sometimes called mechanistic models, describe a number of sub-processes which can be combined to represent the behavior of a larger more complex system. Often the sub-process descriptions are empirical in nature, rather like those described in the previous section, but they are combined in a realistic way. For example, we might try to model how radioactive fallout is adsorbed by plants. The rate of uptake may be assumed to depend on the rate of plant growth, which in turn will depend upon temperature, so the model will have a temperature sub-process similar to the previous sine model. Our model will also have to account for the radioactive decay of the fallout, so we will also have a decay sub-model as described previously. These sub-processes would be combined with other relevant considerations to produce a model which simulates the overall system.

ModelMaker is intended primarily for developing simulation-type models rather than more statistically oriented empirical models.

Developing a ModelMaker model

Step 1: Your conceptual model

The first step in model development is to plan your model. Let's consider the important stages involved in the transfer of radiocaesium from grazing systems to the human food chain. A diagram is a good way to understand this process:



In this example, the major components of the system are shown as boxes and radiocaesium transfer is represented by arrows. In fact each of the boxes represents a complex system in its own right and it may be appropriate to further divide some of them into sub-components.

The next step is to identify the real-life processes at work. For example, radiocaesium deposited on the leaves of vegetation will be transferred to the soil via two real-life processes – weathering where radiocaesium is washed off by rain, and leaf turnover where leaves die and fall to the ground.

Step 2: Developing mathematical relationships

Each component will require an equation in terms of other components within the model, or externally input data and parameters. The equations needn't be very complicated, but generally require some consideration of the physical processes at work. Consider the example of radiocaesium weathering from a leaf surface, a process that must be dependent on rainfall. A simple first assumption might be that it is proportional to rainfall:

$$weathering \propto rainfall$$

As such, this equation can't be implemented in ModelMaker, so a weathering coefficient could be introduced to turn the proportionality into an equation:

$$weathering = W \times rainfall$$

The value of W can be estimated from our knowledge of the weathering process, and adjusted in relation to observed data. It may also be appropriate to undertake experimental work to estimate W directly.

In developing this relationship, two new factors have been introduced to the model - the parameter W and rainfall. Rainfall may be calculated in the model but is more likely to be input from external data. It is often the case that new relationships can only be added to the model if new components are also introduced.

The implementation of mathematical relationships is a very thorough process in which every system in your model must be quantified. In some cases the relationships may be well established, and come straight from a textbook. Often, as in the example used here, the processes are only poorly understood meaning that highly empirical relationships have to be used.

Step 3: Implementing your model

ModelMaker is designed to mimic the process of conceptual model development as much as possible. The first step involves constructing a diagram on the screen which represents the various model parts. This diagram is composed of a series of ModelMaker components, each of which is intended for a different type of mathematical operation. Each component has a definition which can be edited to insert its equation and any other appropriate information.

The next steps

Once your model has been implemented, it can be run; the equations are solved, generating results that can be interpreted in graphs or tables. Validation of your model may involve checking the model results against observed data to test its predictive power. ModelMaker provides a series of facilities to make this as straightforward as possible.

In practice model development is often very iterative. Having tested the model you are likely to find that some changes are required.

2. ModelMaker Tutorial

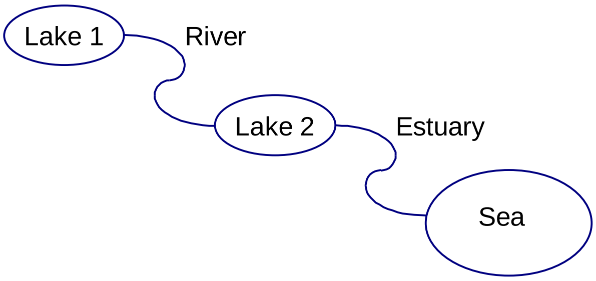
This tutorial will introduce you to ModelMaker's interface and to many of its main features. The step-by-step instructions will take you through the construction of a simple illustrative example – the flow of chemical contaminants through a water system.

ModelMaker opens with an empty model window called *noname00.mod*. ModelMaker's interface is divided into two panels – the Model Explorer on the left and the Model View on the right. The Model Explorer presents a tree view of the many views that make up a model, and provides an easy way to navigate your model.

noname00.mod opens with only one active view – the Diagram view (*Main*) where models are created and defined. More views are added to the Model Explorer as a model is built and analyzed.

Step 1: Planning your model

We are going to construct a model that represents the flow of pollutants through a simple water system that consists of two lakes connected to the sea by a river and an estuary.



We shall make the following assumptions:

1. The water level in the lakes is at equilibrium, so the effects of pollutant dilution can be ignored.
2. The amount of pollutant flowing through the river and the estuary is proportional to the amount of pollutant in the lake at their source:

- The flow of pollutant in the river = 0.1 × the amount of pollutant in the top lake.
- The flow of pollutant in the estuary = 0.05 × the amount of pollutant in the bottom lake.

3. 1000 units of pollutant are dumped in the top lake at time (*t*) = 0.

Step 2: Adding compartments

We shall start the model by adding compartments to the Diagram view (*Main*). A compartment is a container in a model and is defined in terms of what is entering and leaving it. See *Chapter 6: Components – Compartments, Flows, Variables and Defined Values.* Compartments appear in model diagrams as rectangular boxes.

- Click the Compartment icon on the toolbar
- Add a compartment (*C1*) by moving the cursor to the desired location in the model diagram and clicking with the Left Mouse Button (LMB)
- Repeat the above steps to add two more compartments (*C2* and *C3*)

The three compartments are filled with blue lines, indicating that the compartment equations are undefined.

The properties of a model component are defined in its component definition dialog box.

- Double click *C1* with the LMB to open its definition dialog box
- Enter *Lake1* in the *Symbol* edit box and *1000* in the Initial Value edit box
- Click *OK* to close the dialog
- Double click *C2*
- Enter *Lake2* in the *Symbol* edit box
- Click *OK*

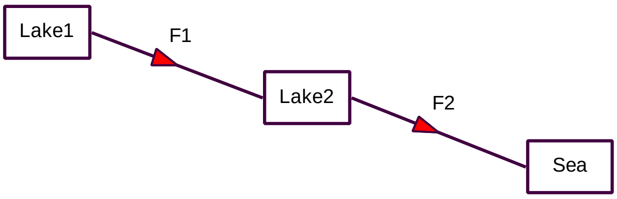
- Repeat for *C3*, entering *Sea* in the *Symbol* edit box

Step 3: Adding flows

Flows represent the transport of a quantity from one compartment to another, and are used in conjunction with compartments to build up systems of differential equations. See *Chapter 6: Components – Compartments, Flows, Variables and Defined Values.*

We shall add two flows to our model to represent the river and the estuary.

- Click the Flow icon on the toolbar
- Click *Lake1* with the LMB followed by *Lake2*
- Repeat to create a flow between *Lake2* and *Sea*



The equations of the compartments are automatically updated to reflect the presence of the flow. Thus, the blue shading of the compartments is removed, but now the flow is shaded red to indicate an equation error. This is because flow is defined as being proportional to the value of its source compartment:

$$F1 = ? * Lake1$$

$$F2 = ? * Lake2$$

? represents an as yet unknown value. We shall define *?* as a parameter and then complete the flow definition.

Step 4: Adding parameters

Parameters represent constant values within a model. Their values cannot be changed from within a model but can be adjusted during certain model analysis procedures. See *Chapter 10: Parameters.*

Parameters are added to a model from the Parameters view.

- Click the Parameters icon

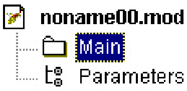
The Parameters view is created and activated. This view is divided into six columns – Name, Value, Optimize, Minimize, Monte Carlo and Dist Type.

- Click the Parameter icon on the Parameters toolbar

A new parameter, *p1*, is added to the Parameters view.

- Repeat to add a second parameter, *p2*
- Double click *p1* to open its definition dialog
- Enter *river_rate* in the *Symbol* edit box and *0.1* in the *Value* edit box
- Click *OK*
- Repeat for *p2*, entering *estuary_rate* and *0.05* in the *Symbol* and *Value* edit boxes

Now we can complete the flow definition:



- Activate the Diagram view (*Main*) by selecting it in the Model Explorer
- Double click *F1* to open its definition dialog box
- Enter *River* in the *Symbol* edit box and *river_rate * Lake1* in the *Equation* edit box (*i.e.* select *?* and double click *river_rate* in the *Available Components* list box)
- Click *OK*

- Repeat for *F2*, entering *Estuary* in the *Symbol* edit box and *estuary_rate* * *Lake2* in the *Equation* edit box

Once the flows have been updated, the model diagram should not contain any blue or red shading, indicating that ModelMaker can find no errors in the model definition and that the model is ready to run.

Step 5: Running your model

The model is now ready to run. This is the process of solving the equations over the desired range of the model’s independent variable. See *Chapter 11: Running Models*. By default, ModelMaker’s independent variable is time, *t*. All equations are solved over a range of values for *t*, and all equations are written with respect to *t*.

- Click the Integrate icon

The Run dialog box opens. ModelMaker runs a model from *t* = *0* to *t* = *100* by default, and calculates values 100 times during the model run.

- Click *OK*

The model is run with the default options. When the calculations are complete a message appears stating how long the calculation has taken. This simple model should only take a fraction of a second. Click OK to dismiss this dialog.

Step 6: Displaying tables

Tables provide access to the values calculated by ModelMaker during a model run. *See Chapter 13: Tables.* We shall create a table of *Lake1* and *Lake2* against time.

- Click the Table icon

The Table Selection dialog box opens.

- Select *Lake1* and *Lake2* in the *Components* list box (*i.e.* use <Ctrl> or <Shift> to make multiple component selections)

- Click >> to move *Lake1* and *Lake2* into the *Selected* list box

The independent variable, *t*, is selected by default.

- Click *OK*

The Results view is created and activated with a sub-view *Table1* which contains your model’s data. Tables can be customized using the Table Series dialog box. To open this dialog:

- Click the Series icon on the Tables toolbar

This dialog is used to change column titles and apply different numeric formats. Click OK to close the dialog.

Step 7: Displaying graphs

Graphs represent a useful way of examining data trends. See *Chapter 12: Graphs*. We shall plot a graph of *Lake1* and *Lake2* against time.

- Click the Graph icon

The Graph Selection dialog box opens.

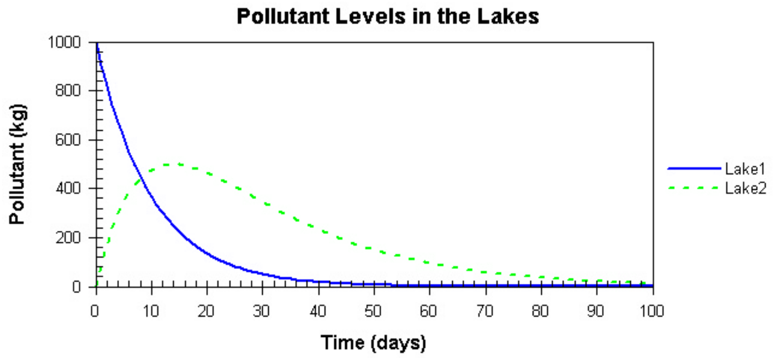
- Select *Lake1* and *Lake2* in the *Components* list box

- Click >> to move *Lake1* and *Lake2* into the *Vertical Axis* list box

By default, ModelMaker plots the graph against the independent variable.

- Click *OK*

The completed model up to this point is “tutor1.mod”



A new graph is added to the Results view as *Graph1*. Many of the graph’s properties can be customized in the Graph Series Options, Graph Attributes Configuration, X-Axis Configuration and Y-Axis Configuration dialog boxes. These dialogs can all be accessed from the Graph toolbar by clicking the Series, Attributes, X-Axis and Y-Axis icons respectively.

Step 8: Adding variables

We shall now assume that there is a continuous discharge of pollutant into *Lake1* in addition to the initial dumping incident. We will define the discharge as a variable component, where:

$$Discharge = 25 \times \sin\left(\frac{t \times p}{365}\right)$$

A variable is a value which is calculated as the model is run, according to its equation. See *Chapter 6: Components – Compartments, Flows, Variables and Defined Values.* Before adding the variable, we will add a new parameter, π (*pi*), to our model.

To follow this example load the model "tutor1.mod"

- Activate the Parameters view by selecting it in the Model Explorer
- Add a new parameter with the symbol *pi* and the approximate value *3.1415927*

Now we can define the variable, *Discharge*:

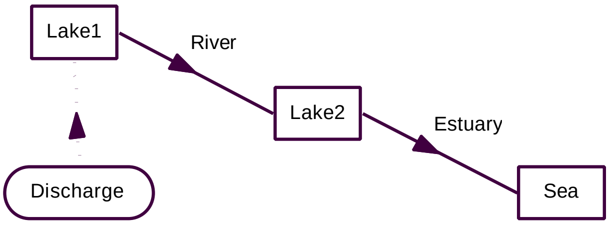
- Activate the Diagram view (*Main*) by selecting it in the Model Explorer
- Add a variable, *V1,* to your model
- Double click the variable to open the Variable Definition dialog box
- Enter *Discharge* in the *Symbol* edit box and *25*sin(t*pi/365*) in the *Equation* edit box
- Click *OK*

The next step in our model definition is to tell ModelMaker that *Lake1* will use the value of the *Discharge* variable. This is done by using an influence.

Step 9: Adding influences

- Select the Influence icon
- Click *Discharge* followed by *Lake1*

The influence is inserted between the two components.

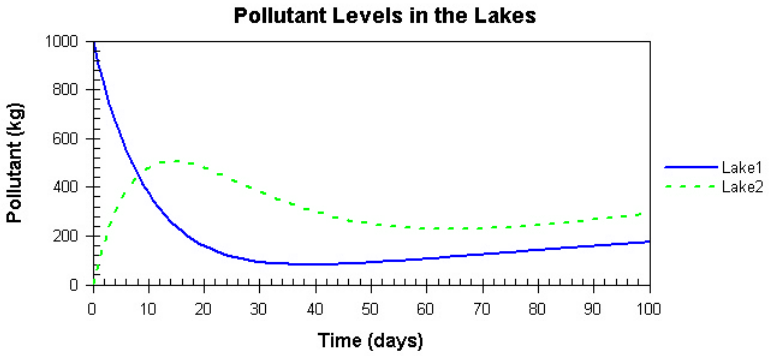


Next we must update the equation of the *Lake1* compartment to take account of the *Discharge* variable.

- Double click *Lake1* to open its definition dialog box
- Update the *Equation* edit box to read *Discharge – River*

Select the graph of *Lake1* and *Lake2* and re-run the model. The amount of pollutant now increases towards the end of the run, as the pollutant discharge increases.

The completed model up to this point is "tutor2.mod"



Step 10: Defining conditional components

Up to this point, all the components we have created have had only one equation, which has been evaluated throughout the model run. This is fine for most continuous models, but often things change as the model progresses.

For our model, for example, let's assume that when the level of pollutant in *Lake2* reaches 250 units, the discharge in the lake is reduced to a value given by the following equation:

$$Discharge = 10 \times \sin\left(\frac{t \times p}{365}\right)$$

To deal with this, we can make *Discharge* a conditional component. (See *Chapter 6: Components – Compartments, Flows, Variables and Defined Values*). Instead of having a single equation, a conditional component has a list of conditions with associated equations. ModelMaker evaluates each condition in turn until it finds a condition which is true and uses the associated equation to evaluate the component.

To follow this example load the model "tutor2.mod"

In our new model, the value of *Discharge* will be influenced by the value of *Lake2*, so we must insert a new influence between *Lake2* and *Discharge*.

- Add an influence from *Lake2* to *Discharge*

Now we can define *Discharge* as a conditional component.

- Double click *Discharge* to open its definition dialog box

- Click *Conditional...*

The Conditional Variable Definition dialog box opens. Initially, the conditional component is defined with a single default condition. Default or empty conditions are always defined as true.

- Click *New*

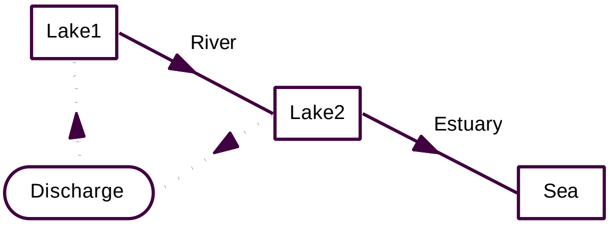
The Conditional Equation dialog box opens.

- Enter *Lake2>250* in the *Condition* edit box and *10*sin(t*pi/365)* in the *Equation* edit box

- Click *OK*

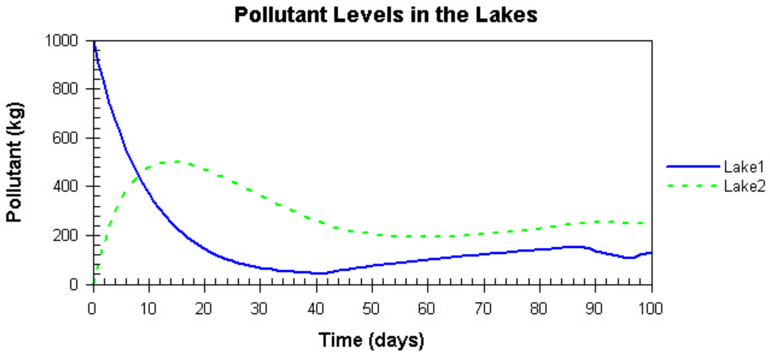
The new conditional equation is inserted into the *Condition* and *Equation* list boxes.

- Click *OK* to close the definition dialog box



Select the graph of *Lake1* and *Lake2* and re-run the model. The graph now shows the effect of switching the rate of discharge as the amount of pollutant in *Lake2* changes. Create a new graph of the value of *Discharge* to see how the conditional component changes during the model run.

The completed model up to this point is "tutor3.mod"



Step 11: Adding defined values and independent events

A defined value is calculated only at the start of a model run, or in response to the actions of an event. This means that they are very useful for holding values which do not change very often, or which change only in a discontinuous manner. See *Chapter 6: Components – Compartments, Flows, Variables and Defined Values.*

We shall use a defined value to hold the discharge level which is changed by an event.

ModelMaker provides two types of event to cater for discontinuous models – independent and component events; events can adjust model component values. See *Chapter 8 – Independent and Component Events.*

Let's assume that the pollutant discharge rate in our model follows a regular pattern: every week it switches between 25 kgd^{-1} and 10 kgd^{-1}. To model this behavior we will replace the variable *Discharge* with a defined value (also called *Discharge*) and an independent event.

To follow this example load the model "tutor3.mod"

- Select the *Discharge* variable and press <Delete>

Discharge and the influences connecting it to *Lake1* and *Lake2* are deleted.

- Add a defined value, *D1*
- Double click *D1* to open its definition dialog box
- Enter *Discharge* in the *Symbol* edit box and *25* in the *Equation* edit box
- Click *OK*
- Add an independent event, *E1*
- Insert three new influences between *Discharge* and *Lake1, Discharge* and *E1*, and *E1* and *Discharge*

Independent events are triggered at pre-determined values of the independent variable. Such triggers can be periodic or non-periodic.

- Double click *E1* to open its definition dialog box

- In the *Definition* tab, enter *Switch* in the *Symbol* edit box, set *Initial Status* to *Active* and set *Event Class* to *Reactivate*

- Select the *Triggers* tab

The Triggers tab defines when the event will be triggered.

- Select *Periodic Trigger*

- Enter *7* in the *Period* edit box and *7* in the *Starting At* edit box

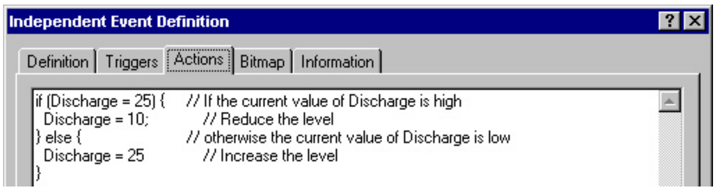
- Select the *Actions* tab

The Actions tab defines what will happen when the event is triggered. We want to say:

> *If the value of Discharge is 25*
> *Set Discharge to 10*
> *Otherwise*
> *Set Discharge to 25*

To define this action, we can use the *if... else* statement.

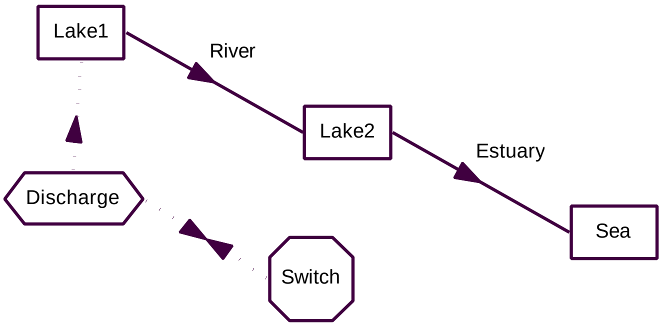
- Define the action as shown below:



```
if (Discharge = 25) {     // If the current value of Discharge is high
  Discharge = 10;           // Reduce the level
} else {                  // otherwise the current value of Discharge is low
  Discharge = 25            // Increase the level
}
```

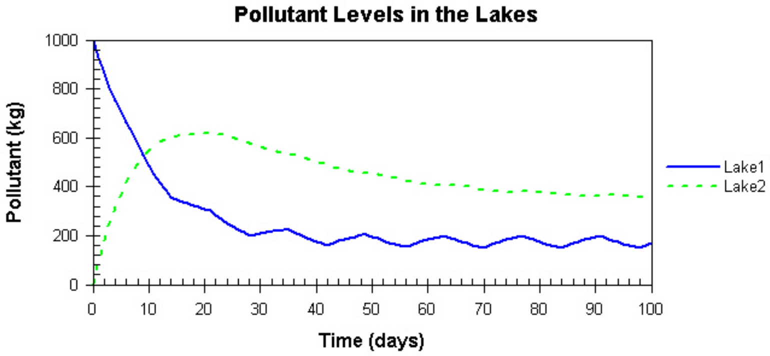
Everything to the right of a double slash '/ / 'is a comment and is ignored by ModelMaker.

- Click *OK* to close the dialog



This completes the definition of the independent event. Re-running the model results in a zigzag pattern of pollutant discharge as the initial dumping fades away.

The completed model up to this point is "tutor4.mod"



Step 12: Adding component events

Component events and independent events differ only in the way they are triggered. Component events are triggered when a defined condition becomes true. ModelMaker uses a tolerance value to ensure that component events are triggered correctly. See *Chapter 8 – Independent and Component Events.*

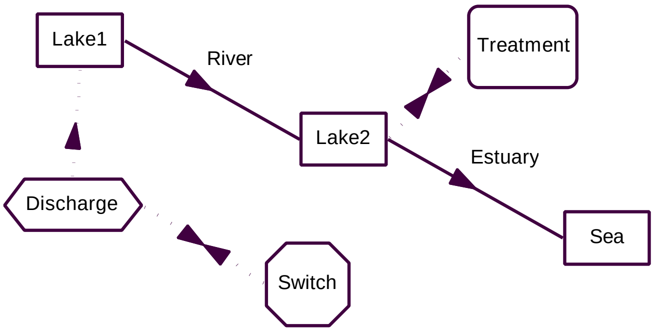
We shall now assume that when the pollutant level in our model reaches 400 kg, a chemical treatment is applied to the lake which removes 150 kg of pollutant from the water. This event will be triggered within one hour of the pollutant level becoming too high. The tolerance will therefore be set to 1/24 = 0.042.

To follow this example load the model "tutor4.mod"

The next stage in developing the model is to insert a new component event. The model also requires two new influences between *Lake2* and the event because the event both tests and adjusts the value of *Lake2*.

- Add a component event, *E1*

- Add two influences between *Lake2* and *E1*, and *E1* and *Lake2*



- Double click *E1* to open its definition dialog box

- In the *Definition* tab, enter *Treatment* in the *Symbol* edit box

- Select the *Trigger* tab

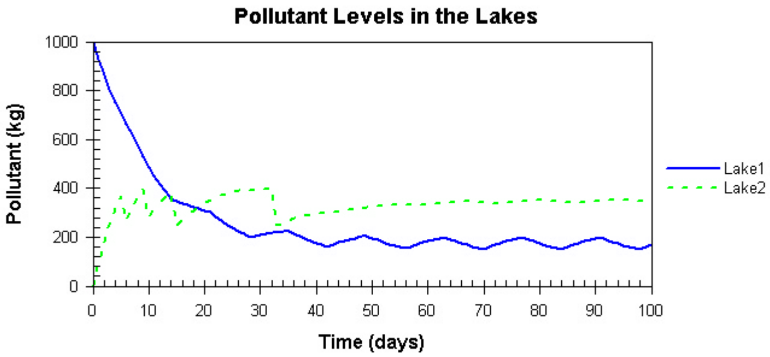
- Enter *Lake2>400* in the *Condition* edit box and *0.042* in the *Tolerance* edit box

- Select the *Actions* tab

- Enter *Lake2 = Lake2 – 150;* in the edit box

Re-run the model. The graph of *Lake2* shows the zigzag trace of the pollutant treatments.

The completed model up to this point is "tutor5.mod"



Step 13: Lookup tables

Suppose that somebody has actually gone out to Lake1 and measured the pollutant discharge rate on the first day of each week.

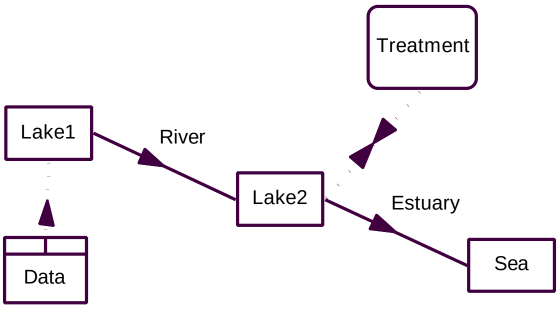
Instead of using the regular pattern of discharge assumed so far, we can use this new information to get a more accurate picture of what is going on. We will use a lookup table component (*Chapter 7: Components – Lookup Tables and Lookup Files*) to add the following table of data to our model:

To follow this example load the model "tutor5.mod"

Time (days)	Discharge rate (kgd^{-1})
0	25
7	12
14	30
21	20
28	50
35	4
42	65
49	15
56	20
63	3
70	45
77	17
84	21
91	10
98	8
105	2

- Delete the *Switch* event and the *Discharge* defined value

- Add a lookup table, *T1*
- Add an influence between *T1* and *Lake1*
- Double click *T1* to open its definition dialog box
- In the *Table* tab, enter *Data* in the *Symbol* edit box
- Select the *Series* tab



We must create a lookup series for every column of data in the table so that ModelMaker knows what the data represents. The first column of data contains observation times. We will define this column as a ‘control’ series because ModelMaker uses this column to control which value is drawn from the discharge rate column. We will define the second column as ‘controlled’ because it is controlled by time.

- Select *Series1* in the *Lookup Series* list box and enter *t* in the *Series Symbol* edit box

ModelMaker assumes that the first column is a control series.

- Click *Define* to complete the definition of the first series
- Select *Series2* in the *Lookup Series* list box and enter *Discharge* in the *Series Symbol* edit box

ModelMaker assumes that the second column is controlled by *t*.

There is not a data point for every day of the year, so if we want to know what the discharge rate is on day 65, for example, we must use interpolation. The default method is linear interpolation where the data takes a straight line between data points. In our model, we will assume that the discharge rate on day 65 is the same as on day 63, *i.e.* we will use start value interpolation.

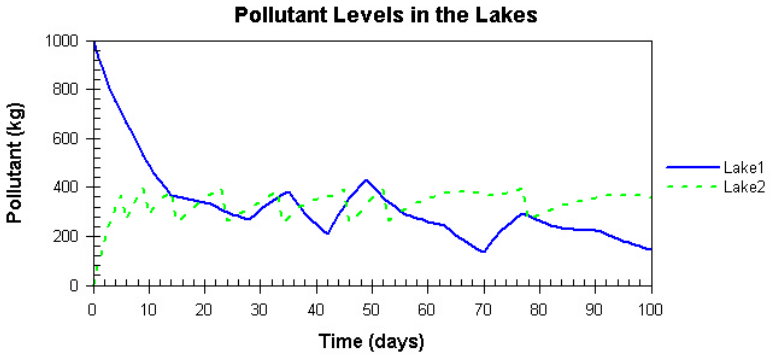
- Select the *Interval Start* interpolation method
- Click *Define* to complete the definition of the second series
- Click the *View Data* button

The Lookup Tables view is created and activated with the sub-view *Data*. *Data* contains an empty sheet called *Page 1* with the column headers *t* and *Discharge*. This is where the lookup table data are entered.

- Enter the lookup table data

We can now re-run the model. The new graph of *Lake2* shows that there is actually more pollutant reaching the bottom lake than we had assumed, and that the chemical treatment is being applied much more often.

The completed model up to this point is "tutor6.mod"



Step 14: Running sensitivity analysis

When developing or analyzing a model it is often useful to investigate the effect of altering aspects of the model. Sensitivity analysis allows the effect of systematic parameter adjustment on the values of selected components to be investigated. See *Chapter 11: Running Models*. In our model, we shall investigate the effect of adjusting *river_rate* from 0.05 to 0.09.

To follow this example load the model "tutor6.mod"

Sensitivity analysis is configured in the Run Options dialog box.

- Click the Integrate icon

The Run dialog box opens.

- Click the *Advanced...* button

The Run Options dialog box opens.

- Select the *Repeated Run* tab

- Enter *4* in the *Number of runs* edit box

- Double click *Lake1* in the *Components to include* list box

Lake1 is moved into the opposite list box. The values of *Lake1* will be saved as retained series.

- Select the *Repeated Run Setting*s tab

- Select the *Sensitivity analysis* option

- Select *river_rate* as the *Sensitivity Parameter*

- Enter *0.05* and *0.09* in the *Start Value* and *Stop Value* edit boxes

- Click *OK* in the Run Options dialog box

- Select *Repeated Run* in the Run dialog box

- Click *OK* in the Run dialog box

The model is run five times at *river_rate* values 0.05, 0.06, 0.07, 0.08 and 0.09. The resulting values of *Lake1* are saved as retained series which can be presented as a graph or table by accessing the Graph Selection or Table Selection dialog boxes.

We will replace the graph of *Lake1* and *Lake2* (Graph1) with a graph of the retained series.

- Activate *Graph1* by selecting it in the Model Explorer

- Click the Selection icon on the Graph toolbar

The Graph Selection dialog box opens.

- Select *Lake1* and *Lake2* in the *Vertical Axis* list box

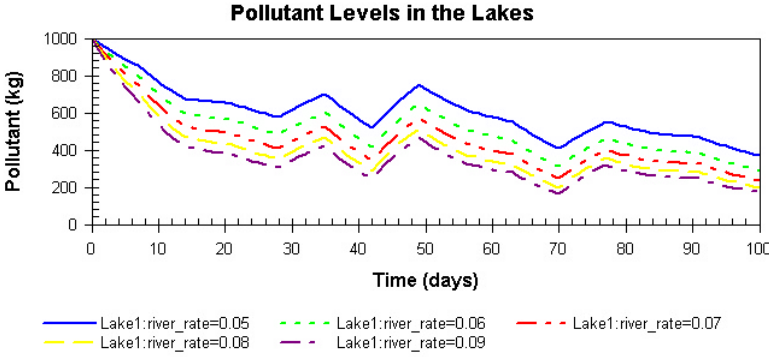
- Click << to move them into the *Components* list box

- Select *Lake1:river_rate=0.05, Lake1:river_rate=0.06, Lake1:river_rate=0.07, Lake1:river_rate=0.08, Lake1:river_rate=0.09* in the *Components* list box

- Click >> to move them into the *Vertical Axis* list box

- Click *OK* to plot the graph

The completed model up to this point is "tutor7.mod"



Step 15: Comparing the model with observed data

When a model of a ‘real’ system has been developed it is important to assess how well it is working by comparing the model's predictions with experimental data. We shall overlay some experimental data to a graph of our model's predictions.

For this example, we will reload tutor2.mod

To follow this example load the model "tutor2.mod"

Experimental data is configured in the Model Data view.

- Select View | Model Data

The Model Data view is created and activated with an empty sheet (*Page 1*). You need to enter the data.

- Enter the following experimental data:

Time (days)	**Pollutant Levels (kg)**	
	Lake1	**Lake2**
10	300	530
20	230	540
30	140	495
40	115	340
50	120	280
60	130	190
70	150	290
80	170	300
90	195	310
100	215	320

Each column of data must be configured and associated with a model component. One column must represent the independent variable (*t*) – this is assumed to be the first column by default.

- Click the Series icon on the Model Data toolbar

The Model Data Series Definition dialog box opens.

- Select the second series in the *Series* list box

- Change the series type to *Data Value* and select *Lake1* in the *Available Components* list box

- Click *Define* to complete the series definition

- Select the third series in the *Series* list box

- Change the series type to *Data Value* and select *Lake2* in the *Available Components* list box

- Click *OK* to complete the series definition and close the dialog

The model data values we have just configured are automatically added to the graph of *Lake1* and *Lake2* (unless otherwise configured in the Graph Series dialog box).

Error bars have also been calculated for the model data, based on the default optimization error which is configured in the Weighting tab of the Optimization Settings dialog box. We shall change the default error value to a more appropriate fractional error value of *0.25*:

- Select Model|Configure>Optimization

The Optimization Settings dialog box opens.

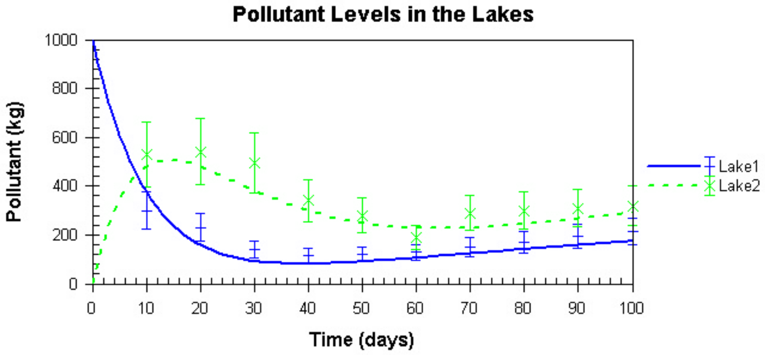
- Select the *Weighting* tab

- Check that *Fractional* is selected as the *Data Error* and enter *0.25* in the edit box

- Click *OK*

The graph of *Lake1* and *Lake2* is updated to reflect the new default error settings.

The completed model up to this point is "tutor8.mod"

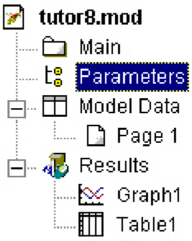


Step 16: Optimization

Once experimental data have been associated with a model, it is possible to improve the model so that it fits the experimental data more accurately. This is achieved by optimization, where selected model parameters are systematically adjusted to reduce the deviation between the model and experimental data. See *Chapter 14: Optimization.*

To follow this example load the model "tutor8.mod"

We are now in a position to optimize our example model with respect to the configured experimental data. We shall optimize the parameters *river_rate* and *estuary_rate* using the default optimization settings of Marquardt optimization and Ordinary least squares weighting.



tutor8.mod
Main
Parameters
Model Data
Page 1
Results
Graph1
Table1

- Activate the Parameters view by selecting it in the Model Explorer
- Select the *Optimize* check boxes for *river_rate* and *estuary_rate*

Optimization is now enabled.

- Click the Integrate icon arrow GO and select *Optimize* from the drop-down menu

The Optimization Run dialog box opens. Use this dialog to confirm the optimization method and parameter selection, and start the calculation.

- Click *OK* to run the optimization

The optimization eventually converges on the new parameter values of *river_rate* = 0.0968 and *estuary_rate* = 0.0431. The new parameter values are shown in the Parameter Results view which is a sub-view of Results. The Marquardt default optimization method also produces an estimate of the standard error associated with each optimized parameter value.

A summary of the optimization statistics is written to the Optimization Statistics view, which is also a sub-view of Results. The optimization process produces an excellent fit between the model and the experimental data, with an r^2 value of almost 0.9.

Updating the parameters

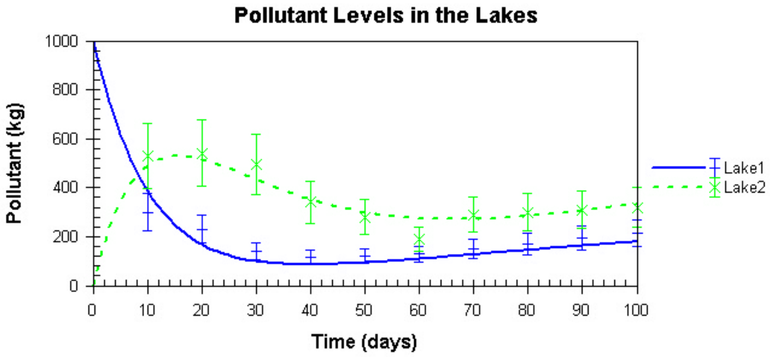
Now we can update the model with the optimized values of *river_rate* and *estuary_rate:*

- Activate the Parameter Results view
- Select *river_rate* and select RMB | Update parameter

- Repeat for *estuary_rate*

Now re-run the model with the optimized parameters to inspect the improved fit of the model to the experimental data.

The completed model up to this point is "tutor9.mod"



Step 17: Minimization

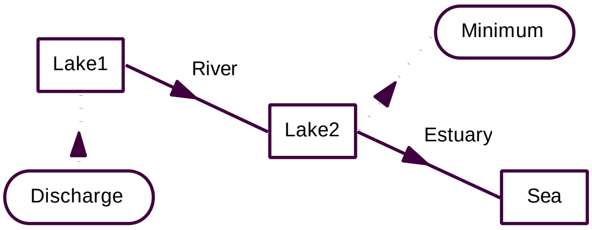
During minimization, the parameter values used in the model are systematically adjusted to find the smallest value of a particular component at a selected point in the model run. See *Chapter 15: Minimization.* However, by choosing the way in which the model component is defined, minimization can also be used to maximize another component value, or make it converge on a desired value.

In our model, let's assume that we want to force the amount of pollutant in *Lake2* to be 500 kg on day 20 of the model run. To do this, we shall add a new variable to the model.

For this example, we will reload tutor2.mod

To follow this example load the model "tutor2.mod"

- Add a variable, *V1*
- Add an influence between *Lake2* and *V1*
- Double click *V1* to open its definition dialog box
- Enter *Minimum* in the *Symbol* edit box and *abs(Lake2 – 500)* in the *Equation* edit box (abs is an absolute value)
- Click *OK* to close the dialog



Now the model definition is completed, we can set up the minimization options.

- Activate the Parameters view
- Select the *Minimize* check boxes for *river_rate* and *estuary_rate*

ModelMaker uses sample points to test the values of selected components at selected moments in time. Sample points are configured for minimization and Monte Carlo analysis in the Sample Points view.

- Click the Sample Points icon

The Sample Points view is created and activated. This view is divided into five columns – Name, Component, Time Point, Monte Carlo and Minimize.

- Click the Sample Point icon on the Sample Points toolbar

A new sample point, *SP1*, is created.

- Double click *SP1* to open the Sample Point Definition dialog box
- Enter *20* in the *Time Point* edit box and select *Minimum* in the *Component* list box
- Click *OK* to close the dialog
- Select the *Minimize* option button in the Sample Points view for *SP1*

The model is now ready to minimize.

- Click the Integrate icon arrow and select *Minimize* from the drop-down menu

The Start Minimization dialog box opens. This dialog summarizes the component, time point and parameter selection, and starts the calculation.

- Click *Advanced*

The Minimization Configuration dialog box opens.

- Enter *1* in the *Convergence Change* edit box and *25* in the *Convergence Steps* edit box
- Click OK to close the dialog
- Click OK to close the Start Minimization dialog and run the minimization

The completed model up to this point is "tutor10.mod"

ModelMaker runs the model many times, adjusting the values of *river_rate* and *estuary_rate*. When the process finishes, the new parameter values are displayed in the sub-view Parameter Results - *river_rate = 0.1048* and *estuary_rate = 0.0471*. Use the update command to adopt the minimize values in the model. Re-run the model and check a table of *Lake2* values to confirm that it contains 500 kg of pollutant on day 20.

Step 18: Monte Carlo analysis

Monte Carlo analysis enables model parameters to be specified as random distributions. A model is run for a specified number of times, and during each run the value of the parameter is taken from a specified probability distribution. In this way, the effect of varying parameters on a component value can be investigated. See *Chapter 16: Monte Carlo Analysis.*

In our model, we shall investigate what effect varying *estuary_rate* has on the value of *Lake2* on day 50 of the model run. We will specify that *estuary_rate* follows a normal distribution.

For this example, we will reload tutor6.mod

To follow this example load the model “tutor6.mod”

- Activate the Parameters view
- Select the *Monte Carlo* check box for *estuary_rate*
- Click the ... button in the in the *Dist Type* field for *estuary_rate*

The Distribution dialog box opens.

- Select *Normal* from the *Distribution* drop-down list
- Enter *0.05* in the *Mean* edit box and *0.02* in the *Standard deviation* edit box
- Click *OK*
- Click the Sample Points icon to activate the Sample Points view

As with minimization, Monte Carlo analysis uses sample points to test the values of selected components at selected moments in time.

- Add a sample point, *SP1*
- Double click *SP1* to open its definition dialog box
- Enter *50* in the *Time Point* edit box and select *Lake2* in the *Component* list box
- Click *OK*
- Select the Monte Carlo button in the Sample Points view for *SP1*

The Monte Carlo configuration is now complete and is ready to run.

- Click the Integrate icon arrow and select *Monte Carlo* from the drop-down menu

The Monte Carlo Run dialog box opens. This dialog summarizes the parameter and sample point configuration. We shall keep the default value of *100* trial runs.

- Click *OK* to run the analysis

Next we will display the Monte Carlo results as a histogram.

Histograms

- Click the Histogram icon

The Histogram Selection dialog box opens.

- Enter *15* in the *Number of Bins* edit box

The x-axis will be divided into 15 columns.

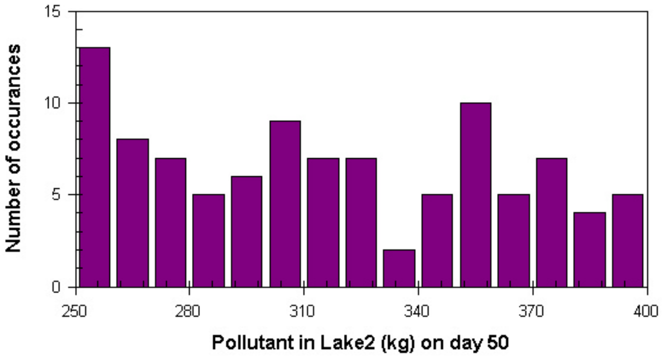
- Select *SP1* in the *Sample Points* list box and click >> to move it into the *Selected* list box

- Click *OK*

The histogram is added to the Results view as *Histo2.* The graph shows the frequency distribution of *Lake2* values (in 100 trials) if the *estuary_rate* fluctuates by a standard deviation of *0.02* around a normal distribution.

Like graphs, histograms can be customized in the Series, Attributes, X-axis and Y-axis dialogs which can be accessed from the Graph toolbar.

Try adjusting the axis scaling until you are happy with the distribution.



Monte Carlo statistics

To view the statistics from the Monte Carlo analysis:

- Click the Series icon on the Graph toolbar

The Graph Series Options dialog box opens.

- Click *Series Statistics*

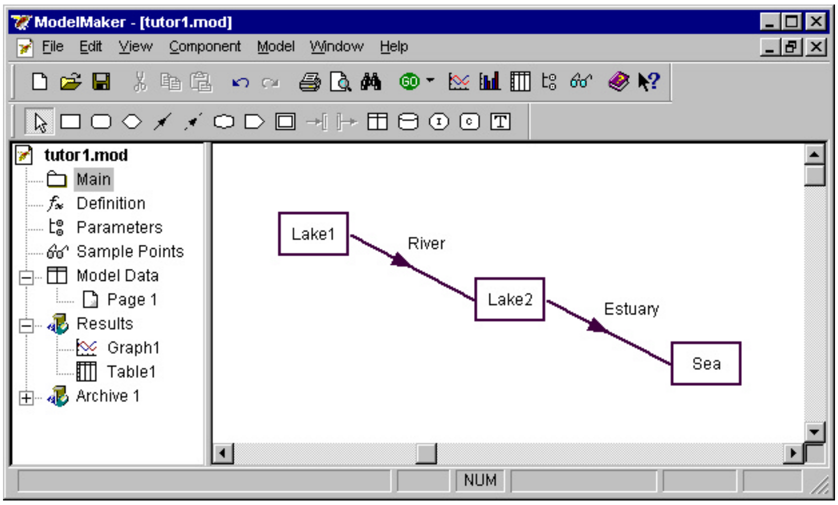
The completed model up to this point is "tutor11.mod"

The Global Sensitivity Results dialog box opens. This dialog summarizes the statistics for *SP1.* In our distribution, *Lake2* varies from *250.9* to *399.5* kg with a mean value of *317.2* kg.

3. Views and Toolbars

The Model Explorer

ModelMaker's interface is divided into two panels – the Model Explorer on the left and the Model View on the right. The Model Explorer organizes the many views that make up a model into a tree structure, with each branch representing a different view, and provides a simple way to navigate your model. Click a view in the Model Explorer to display its contents in the Model View. Expand and collapse branches by clicking the plus and minus icons.



When a new model is opened, only the Diagram view is represented in the Model Explorer. Additional views are added to the Model Explorer as a model grows in complexity.

Views

The Diagram view

The Diagram view contains the model diagram and is where models are created and defined. This view is displayed when a new model is opened and has the default name Main. Sub-models are stored under the Diagram view as sub-views called Sub1, Sub2 etc.

The Diagram toolbar, plus specific View menu, Component menu and RMB commands are active in the Diagram view. Components and model building are discussed in more detail in *Chapters 5, 6, 7, 8* and *9*.

The Definition view

The Definition view shows the definition of all model components. It provides a tree view of the structure of a model, with each branch representing a sub-model or set of component array elements. To create the Definition view:

- Select View | Definition

If the Definition view already exists, it becomes the active view.

The Model Definition view is an alphabetical text listing of the components of a model. When used in combination with the model diagram, it can speed the process of model development and debugging. Double click a component to open its definition dialog box directly from the Definition view.

The Parameter view

The Parameter view is used to create, view and manipulate parameters. It provides a tree view of a model's structure, with each branch representing a sub-model or parameter array range. To create the Parameter view:

- Click the Parameters icon

If the Parameter view already exists, it becomes the active view.

The Parameter toolbar, plus specific Component menu and RMB commands, are active in the Parameter view. Parameters and the Parameter view are discussed in more detail in *Chapter 10: Parameters*.

The Model Data view

The Model Data view is used to configure experimental data for optimization, when the fit between the model predictions and the configured data is improved. To create the Model Data view:

- Select View | Model Data

If the Model Data view already exists, it becomes the active view.

The Model Data toolbar, plus specific View menu and RMB commands are active in the Model Data view. The Model Data view is discussed in more detail in *Chapter 14: Optimization*.

The Results view

The Results view contains a set of working results where graphs, tables, minimization results and optimization results are stored as sub-views. The Results view is created when a graph or table is defined, or results are generated during an optimization or minimization calculation.

Graphs and histograms are stored under the Results view as Graph1, Graph2 or Histo1, Histo2 etc. The Graph toolbar, plus specific View menu and RMB commands are available in the graph sub-views. Graphs and histograms are discussed in more detail in *Chapter 12: Graphs* and *Chapter 16: Monte Carlo Analysis.*

Tables are stored under the Results view as Table1, Table2 etc. The Table toolbar, plus specific View menu and RMB commands are available in the table sub-views. Tables are discussed in more detail in *Chapter 13: Tables.*

The optimization and minimization parameter results are stored in the Parameter Results sub-view, and the statistics from the optimization calculation are stored in the Optimization Statistics sub-view. See *Chapter 14: Optimization* and *Chapter 15: Minimization.*

The Results view can be archived to a new view which is not updated as your model is changed. To archive the Results view:

- Click the Results view in the Model Explorer
- Select RMB | Archive

The Results view and a copy of the Definition view are archived to a view called Archive1. Additional results sets are archived as Archive2, Archive3 etc.

The Sample Points view

The Sample Points view is used to create sample points for minimization and Monte Carlo analysis. A sample point represents the value of a component at a particular moment in time. To create the Sample Points view:

- Click the Sample Points icon

If the Sample Points view already exists it becomes the active view. Sample points are discussed in more detail in *Chapter 15: Minimization* and *Chapter 16: Monte Carlo Analysis.*

The Lookup Tables view

The Lookup Tables view is created when a lookup table component is configured. All lookup table data are stored under this view. See *Chapter 7: Components – Lookup Tables and Lookup Files.*

Deleting and renaming views

To delete a view:

- Click the view to be deleted in the Model Explorer
- Select RMB | Delete View

To rename a view:

- Click the view to be renamed in the Model Explorer
- Select RMB | Rename View

The View Name dialog box opens.

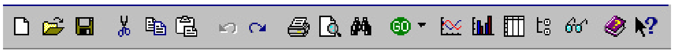
- Enter a name in the *View Name* edit box and click *OK*

Toolbars

By default ModelMaker displays two toolbars – the Main toolbar and the View toolbar. Pass the mouse cursor over an icon to display its ToolTip.

The Main toolbar cannot be customized and is always displayed. It displays the New, Open, Save, Cut, Copy, Paste, Undo, Redo, Print, Print Preview, Find Component, Integrate, Graph, Histogram, Table, Parameters, Sample Points, Contents and What's This? icons.

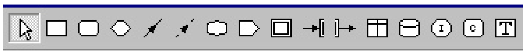
The Main toolbar



The View toolbar icon selection varies with each ModelMaker view. It ensures that the dialog boxes and features most relevant to a particular view are readily available.

For example, the Diagram toolbar is displayed when the Diagram view (*Main*) is active. It displays the Select, Compartment, Variable, Defined Value, Flow, Influence, Delay, DLL Function, Sub-model, Input, Output, Lookup Table, Lookup File, Independent Event, Component Event and Text Box icons.

The Diagram toolbar



To turn the View toolbar off or on:

- Select View | Toolbar>Display

To customize the View toolbar:

- Select View | Toolbar>Customize...

The Toolbar Customization dialog box opens.

Select the view toolbar to be customized in the View drop-down list. The toolbar icons available for selection are listed on the left-hand side of the dialog box, and the currently selected icons are listed on the right. Use >> and << to add or remove icons from the toolbar. The order in which the chosen icons are listed corresponds to the order in which they appear on the toolbar.

Use *Up* and *Down* to alter the relative position of icons. Use the *Separator* button to group icons together (through the addition of separators).

See the *ModelMaker Reference Manual* for a list of ModelMaker's toolbar icons.

4. Basics

This chapter deals with ModelMaker's utility commands.

Starting ModelMaker

There are several ways to start ModelMaker.

From the Start menu

A ModelMaker program item is automatically created during installation.

- Select Start|Programs|ModelMaker 4|ModelMaker 4 from the Windows Taskbar Start Menu

From Windows Explorer

- Access *Windows Explorer* or *My Computer*

The default ModelMaker installation is to C:\Program Files\Cherwell Scientific\ModelMaker 4\mm.exe

- Locate and double click the file *mm.exe*

From a shortcut

You can create a shortcut to ModelMaker on your Windows desktop:

- Select the *mm.exe* file in Windows Explorer
- Select RMB|Create Shortcut
- Drag the new shortcut onto your desktop

To start ModelMaker from the shortcut:

- Double click the desktop icon

Closing ModelMaker

To close ModelMaker:

- Select File|Exit, or:
- Click the Close button (**x**) in the upper right hand corner of the ModelMaker window

You will be prompted to save any changes to models you have been working on.

Opening a model

To open a model in ModelMaker:

- Click the Open icon, or:
- Select File | Open

The Open dialog box opens.

- Use the *Look in* drop-down list to locate your model
- Click *Open*

To open a new model:

- Click the New icon, or:
- Select File | New

Alternatively, you can open a model from the recent models list:

- Select File | 'recent model.mod'

Closing a model

To close a model:

- Select File | Close
- Click the close icon (**x)** in the top right hand corner of the model window

You will be prompted to save any changes.

To close all open models:

- Select Window | Close All

Saving a model

ModelMaker saves models with the extension ‘*mod*’. To save a model:

- Click the Save icon, or:
- Select File | Save

To save a model with a new name:

- Select File | Save As

The Save As dialog box opens:

- Use the *Save in* drop-down list to locate your desired drive and folder
- Enter the model name in the *File name* edit box
- Select *Model files (*.mod)* from the *Save as type* drop-down list
- Click *OK*

ModelMaker creates two other types of file when saving models:

1. Model backup files with the extension ‘*mbk*’. When a model is saved to file, a backup copy is made if a previous version already exists.
2. Model save files with the extension ‘*sav*’. As the model is run, ModelMaker saves the calculated values of the model components to file.

Sending a model as an e-mail

To send a model as an e-mail:

- Select File | Send...

A new e-mail message dialog opens with your model attached as a file.

Password protection

To protect a model with a password:

- Select File|Password Protection...

The Add Password Protection dialog box opens.

- Enter a password in the *Password* and *Verify* edit boxes

You will be prompted for the password next time you open the model.

Printing from ModelMaker

Any of the ModelMaker views can be printed:

- Click the Print icon, or:
- Select File|Print

The Print dialog opens.

- Check that the printer details are correct and click *OK*

Use Print Preview to check what a printed document will look like. To access Print Preview:

- Click the Print Preview icon, or:
- Select File|Print Preview

From Print Preview you can:

1. Print the document by clicking on the *Print* icon
2. Scroll through the document pages with the left and right arrows
3. Close the preview by clicking the *Close* icon

Open the Page Setup dialog box to customize your page and printer settings:

- Select File|Page Setup

- Check the settings and click *OK*

Arranging windows

The names of all open models are listed at the foot of the Window menu. Click a model with the LMB to make it the active model. Use the Window menu options to arrange open model windows.

To display model windows in a cascading style:

- Select Window | Cascade

To display model windows vertically across the width of the ModelMaker window:

- Select Window | Tile Vertically

To display model windows in horizontally down the length of the ModelMaker window:

- Select Window | Tile Horizontally

To arrange the icons of minimized model windows:

- Select Window | Arrange Icons

ModelMaker Help

On-line help

Select Help | Contents or Help | Index to launch the on-line Microsoft Windows Help system. Select Help | Using help for help on using and customizing the help system.

Context sensitive help

Context sensitive help takes the form of a question mark (**?**) located in the top right hand corner of dialog boxes. To use context sensitive help:

- Click **?** with the LMB

The cursor changes to indicate context sensitive help is active inside the dialog box.

- Click the dialog text for which you would like more information

A popup window opens. Close this window by clicking the screen with the LMB.

Alternatively, use What's This:

- Click the What's This icon, or:
- Select Help | What's This?

The cursor changes to indicate context sensitive help is active inside the ModelMaker window.

Tip of the Day

To read ModelMaker's Tip of the Day:

- Select Help | Tip of the Day

About ModelMaker

Information about your version of ModelMaker, including licensing codes, is available under About ModelMaker...

Select Help | About ModelMaker...

ModelMaker on the Web

The ModelKinetix.com Home Page and the ModelMaker support site can be accessed directly from ModelMaker:

- Select Help | ModelMaker on the Web |
    - ModelMaker Home Page
    - ModelMaker Support

ModelMaker User Group

To e-mail the ModelMaker User Group:

- Select Help | E-mail ModelKinetix.com | ModelMaker User Group |
    - Send a message
    - Subscribe

5. Working with Models

When a new model is opened, only the Diagram view is represented in the Model Explorer. Model diagrams are built in the Diagram view from the range of components displayed on the toolbar. ModelMaker has 16 types of component which are discussed in more detail in *Chapters 6 to 10*. Each type of component (excluding parameters) is represented by a unique diagram representation and falls into one of the following categories:

1. Component boxes - compartments, variables, defined values, delays, lookup tables, lookup files, independent events, component events, DLL functions and text boxes

2. Component lines – flows and influences

3. Sub-model references – input and output references

Parameters are added to the model via the Parameter View (see *Chapter 10: Parameters*).

Adding components

Each component is represented by a unique diagram representation. Place the mouse cursor over a toolbar icon to display a ToolTip.

To select a component:

- Click the component icon on the toolbar, or:

- Select Component | *component type*

The cursor changes to a cross-hair to reflect the type of component selected.

Adding component boxes

To add a single component box to the model diagram:

- Select the component box icon from the Diagram toolbar

- Move the cursor to the position in the model diagram where you want the component to appear

- Click the LMB

The component box is added to the model diagram at the cursor position or at the nearest grid point if snap to grid is enabled. The cursor returns to its normal pointer shape.

To indicate that the newly added component box is in its uninitialized or empty state, it appears shaded in blue.

Adding component lines

Component lines require a source component and a target component. For flows, the source and target boxes must both be compartments.

To add a component line to the model diagram:

Select the component line icon from the Diagram toolbar

- Click the source component
- Click the target component

The component line is added between the two selected components.

A newly added flow has an invalid equation and therefore appears shaded in red.

If a component line is selected for addition to the diagram and the left mouse button is clicked at an invalid position in the model diagram, ModelMaker beeps to indicate the invalid mouse selection and the cursor returns to its normal pointer shape.

Adding sub-model references

Sub-model references allow communication between parent models and sub-models. To add a sub-model reference:

- Select the sub-model in the model diagram
- Select the sub-model reference icon from the Diagram toolbar
- Click in the model diagram

The sub-model reference is added to the model diagram. A matching reference is added to the diagram of the selected sub-model.

Adding multiple components

Multiple component boxes, lines or references can be added to the model diagram by holding down the <Ctrl> key as the components are added. The cursor remains as a cross-hair, representing the selected component.

Canceling a component selection

If you select a component to add to the diagram and then change your mind, press <Esc> or click the Select icon on the Diagram toolbar to cancel your selection. The cursor returns to its normal pointer shape.

Defining components

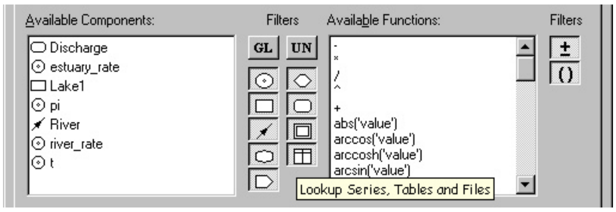
The characteristics of each model component are defined in its component definition dialog box. To access this dialog:

- Double click the component with the LMB, or:
- Select the component and press <Enter>

Alternatively, a number of components can be defined in turn by selecting them together and double-clicking within the selection area. The definition dialog for each of the selected components is accessed in turn. Click the Cancel button in any of the dialogs to stop the process.

Component filter buttons

Most of the component definition dialog boxes (and many other ModelMaker dialogs) contain list boxes which display Available Components. Use the component filter buttons to select the types of component that are displayed. Passing the mouse cursor over each filter will display a ToolTip explaining which components will be filtered. The functions filter buttons work in the same way.



Finding components

Use the Find Component dialog box to find a component's model diagram representation or definition within the model. To open the

Find Component dialog box:

- Click the Find Component icon, or:
- Select Edit|Find Component...

The model's components will be shown in the Components list box.

- Select the component you want to find
- Press *Show* to view the selected component which will be centered within the Diagram view, or:
- Press *Edit* to view the definition dialog box for the selected component

Symbol scope

ModelMaker models can be created as hierarchical structures containing nested sub-models. With the exception of universal components considered below, sub-models are treated as separate models. This means that no two components in the same sub-model can have the same symbol, but components in two different sub-models can have the same symbol.

Influences and flows

In general, if one component references another then they must be connected by an influence or flow. For example, if V1 = V2 * 3 then V2 can be said to influence the value of V1 and an influence must be inserted between V2 and V1. This rule ensures that the diagram represents the structure of the model, with influences and flows showing the way in which different components are interrelated.

However, it is not always possible or practicable to construct models in this manner so ModelMaker defines two exceptions to the rule - global and universal components.

Global components

Global components can be referenced by any other component in the same sub-model or in a lower sub-model. For example, a model component that is used by many components in a sub-model can be defined as global to avoid inserting many influences. Parameters do not have a diagram representation and are therefore considered to be global in scope by default.

Universal components

Universal components can be referenced by any other component in the entire model. For example, a model component that is referenced by many components in different sub-models can be defined as universal to avoid creating many sub-model references.

Since a universal component can be referenced from anywhere within a model, its symbol must be unique.

Whenever you attempt to change the symbol or the universal status of a model component, ModelMaker will alert you to any symbol clashes.

Configuring run symbols

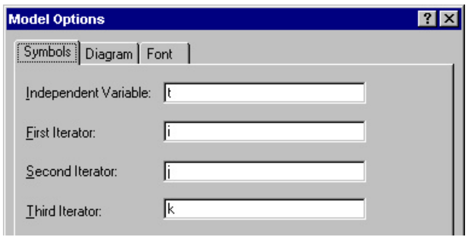
In addition to the symbols defined by the components of the model, ModelMaker requires four further symbols:

- The independent variable. This must be a unique valid symbol. By default, the independent variable is time, represented by the symbol *t*.

- Three array iterator symbols - these must be unique valid symbols. They are used to iterate over the x, y, and z coordinates of array components. By default they are given the symbols *i*, *j* and *k*.

The run symbols for a model are defined using the Symbols tab of the Model Options dialog box, accessed by selecting Options from the Model menu.

The Model Options dialog Symbols tab



Independent Variable: t

First Iterator: i

Second Iterator: j

Third Iterator: k

Component description

Each model component can have a single line of descriptive text associated with it to make the model easier to understand. The description can be displayed with the model component in the Model Diagram view, Parameter view or Definition view.

To display a description:

- Open the component definition dialog box
- Enter your text in the *Description* edit box of the Definition tab
- Select *Show Description*

Component information

A component can also have a longer section of free form information associated with it, in addition to the single line description. This might be used, for example, to give references or provide a more detailed description of the role of the component in the model.

To add information about a component:

- Open the Component Definition dialog box
- Enter your text in the Information tab

The information text is never displayed by ModelMaker but an information indicator can be displayed to show that a component has some information text defined:

- Select *Show Information Icons* on the General tab of the User Preferences dialog box (Edit menu)

Component bitmap image

Model components can be represented as bitmap images in the model diagram.

- Open the Component Definition dialog box
- Enter a name in the *Bitmap File Name* edit box or invoke the *Open* dialog to locate your bitmap file
- Select a *Bitmap sizing* option

Scale component to bitmap will increase the component size to match the bitmap's size (if it is smaller than the bitmap).

Tile bitmap within component will tile the bitmap to fill the component.

Scale bitmap to component will stretch or squash the bitmap to fill the component.

Component shading

ModelMaker uses shading to provide information about the status of model components. Component lines are outlined or completely filled with color, whereas component boxes are shaded with color.

Blue diagonal lines The component is empty, *i.e.* has no equation, event condition, event action, or lookup file name defined. Models containing empty components cannot be run.

Green outline or green diagonal lines The component is global, *i.e.* its symbol can be referenced by other model components in the same sub-model, or a lower sub-model, without a direct influence or flow connection.

Green or green cross-hatching The component is universal, *i.e.* its symbol can be referenced by other model components in the whole model without a direct influence or flow connection.

Red or red cross-hatching The component is in error. Models containing components in error cannot be run.

Text boxes

Text boxes are components that allow the model developer to add informative text to a model; they take no part in model calculations. To add a text box to a model:

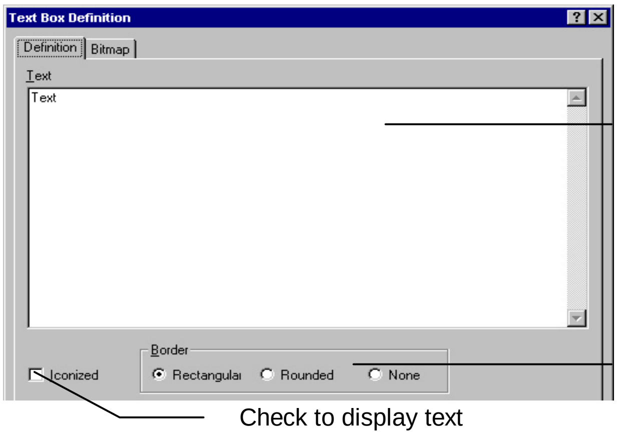
- Select the Text Box icon from the toolbar
- Click in the model diagram with the LMB

Text box definition To access the Text Box Definition dialog box:

- Double click the text box component with the LMB

By default the complete text within a text box is displayed in the model diagram. For some models which contain large amounts of descriptive text, it may be more convenient (and less cluttered) to hide the text until the user wishes to read it. In this case the text box can be displayed as an information icon until opened by the user.

The Text Box Definition dialog box



Text: Text

☐ Iconized

Border: ● Rectangular ○ Rounded ○ None

Enter text

Select border type

Check to display text box as an icon

By default, double-clicking the left mouse button on a text box will access its definition dialog in the normal manner. When model development is complete, this can be changed so that double-clicking the left mouse button will open or close the text box icon by selecting the ‘Double-click opens and closes text box components’ check box in the General tab of the User Preferences dialog box (select Edit | User Preferences).

Selecting components

Components must be selected before they can be moved or resized etc.

To select a Component box:

- Click inside the box with the LMB

To select a Component line:

- Click the arrow with the LMB

Moving components

Components can be moved either singly or in groups. Select the component or components you want to move, hold the left mouse button down within the selection area and drag the components to their new position.

Formatting components

The way in which a model component is drawn can be changed by using the Component Format dialog box. This allows you to change the line thickness, line color, font and font color used to draw the component. For component boxes you can also define how the text within the component is formatted.

Formatting a single component

To format an individual component:

- Select the component to be formatted
- Select Component | Format to open the Component Format dialog box

The Component Format dialog box is divided into two tabs – Diagram and Font. Use the Diagram tab to select line characteristics and text formatting options. Use the Font tab to specify font name, style, size and effects.

Formatting all model components

A model can be formatted in the Model Options dialog box:

- Select Model | Options

The Model Options dialog box is split into three tabs – Symbols (see *Configuring run symbols*), Diagram and Font. Use the Diagram tab to specify line characteristics and set grid options for the model. Use the Font tab to specify font name, style, size and effects.

Sizing components

The size of a component box can be changed by selecting it and dragging the appropriate sizing handle to attain the desired dimensions. ModelMaker automatically reformats the text within the component.

The sizing functions of the align menu can also be used to resize component boxes. Components can be resized to match the widest, narrowest, tallest or shortest component in the model:

- Select the component or components to be resized and the component whose size will be copied

- Select Component | Align and the appropriate alignment function:

    - Widest, Narrowest, Tallest, Shortest

ModelMaker resizes the selected components.

Aligning components

Model diagrams are entirely free-format; ModelMaker draws no functional inferences from the relative positions of model components. However, in order to improve the appearance of a model it is possible to align components. Flows and influences cannot be aligned because their position depends on the positions of their source and target components.

To align a group of components carry out the following steps:

- Select the components to be aligned

- Select Component | Align and the appropriate alignment function:

    - Left, Center Vertically, Right, Top, Center Horizontally, Bottom

ModelMaker aligns the selected components as requested.

The Snap to Grid option in Model | Options can also be used to align model components as they are added, moved and resized.

Using the clipboard

Use the clipboard to move or copy components within or between models. Select the component that you wish to copy or move and click the Copy or Cut icons from the Main toolbar. If components are available in the clipboard they can be pasted into a model using the Paste button. If component symbols clash you are prompted to supply alternative symbols.

Scrolling and zooming the model diagram

Use the scroll bars to move around the model diagram.

To zoom the model diagram out *i.e.* to view a greater area of the model diagram:

- Select View | Zoom Out

The model diagram will be re-drawn at a smaller scale. It is possible to zoom the model diagram out successively six times.

To zoom into the model diagram *i.e.* to view a smaller area of the model diagram:

- Select View | Zoom In

The cursor changes to the zoom in magnifying glass.

- Move the cursor to the position of interest and click the LMB

The model diagram is re-drawn at a larger scale centered on the cursor position. If the model cannot be zoomed in or out, the Zoom In or Zoom Out menu items are grayed out.

Setting user preferences

In the User Preferences dialog box, you can set a variety of model editing, model running and output properties. The properties set are saved with a model, but the default settings that ModelMaker applies to a new model can also be changed. To open the User Preferences dialog box:

- Select Edit | User Preferences

The User Preferences dialog box is divided into two tabs – General and Output.

Use the General tab to:

1. Select or deselect quiet editing mode

2. Request that equations are updated when flows are added or removed

3. Show information icons

4. Set double click to open and close text box icons

5. Set the Maximum Undo Level – set to 20 by default

6. Warn when all components are initially zero

7. Collect debug information

This will enable the Debug Information dialog box once a model has been run. Select Model | Debug Information to open the debugger.

8. Save selected component values

9. Update graphs during a model run

10. Display a final elapsed time message

Use the Output tab to:

1. Specify the name of a report file and choose to overwrite existing files

2. Enable tracing, specify a trace file name and choose to overwrite existing files

Several of the actions which an event can trigger control the output of trace messages, which can be of assistance when debugging a model. The TraceMessage event action is used to output a message to the trace file, and the message can be labeled by assigning it to one of nine trace levels. The TraceOn and TraceOff event actions are used within a model to switch tracing on or off.

The Enable Tracing check box acts as a master switch for controlling whether ModelMaker processes event actions to do with tracing. The Active Levels check boxes determine which trace messages are written to the trace file. For example, if only the Level 1 check box is selected then only messages output by the TraceMessage action as level 1 messages will be written to file. See *Chapter 8: Components – Independent and Component Events* for more information on using events.

6. Components – Compartments, Flows, Variables and Defined Values

Compartments, flows, variables and defined values share two important characteristics – they can all be defined as:

1. Conditional or unconditional components

2. Arrays of component elements

Compartments

Compartments represent integrators in a model. The value of a compartment represents the quantity held within it, and is calculated using a differential equation which gives the rate of change of the value:

$$\frac{\mathrm{d}\,Compartment}{\mathrm{d}\,t} = f(\,)$$

where *f( )* is a function of the values of components defined in the model, and *t* is the independent variable of the model, usually time.

A compartment must also have an initial value which is used to define its value at the start of the model run. The initial value may be zero, but if all compartments have an initial value of zero a warning dialog will show when the model is run. The initial value equation is of the form:

$$\text{Initial value} = g(\,)$$

where *g( )* is a function of defined values and model parameters.

The value of a compartment may also be set by the actions of an independent or component event.

Flows

Flows represent the movement of something from one compartment to another, *i.e.* some quantity is subtracted from the source compartment and added to the destination compartment. The value of this flow is expressed as an equation of the form:

$$\text{Flow} = f(\,)$$

where *f( )* is a function of the values of components defined in the model– often a proportion of the value of the flow's source compartment.

By default, when a flow is added to the model diagram, the equations of its source and target compartments are updated to reflect its presence. The process is reversed if the flow is removed. In some models this may be inappropriate, in which case the updating of the compartment equations can be switched on or off by selecting the appropriate check box on the General tab of the User Preferences dialog box (Edit menu).

Influences Influences show where the value of one component affects the value of another. Influences do not have a symbol or a definition dialog box.

Variables

Variables have values which are calculated as the model is run. The value of a variable is expressed as an equation of the form:

$$\text{Variable} = f(\,)$$

where *f( )* is a function of components defined in the model.

Defined values

Defined values are constant values calculated at the start of a model run. The value of a defined value is expressed as an equation of the form:

$$\text{Defined value} = g(\,)$$

where *g( )* is a function of defined values and model parameters.

The value of a defined value may also be set by the actions of an independent or component event.

Defining unconditional and conditional components

Unconditional components

The value of an unconditional component is defined using a single equation which is always used when evaluating the component. This is the default state for new components.

Conditional components

The value of a conditional component is defined using a list of conditions which have associated equations. When the component is to be evaluated ModelMaker works down the list of conditions until it finds one which is true. It then uses the associated equation to work out the value of the component. If no true condition is found, an error is generated.

The Unconditional and Conditional Definition dialog boxes for compartments, flows, variables and defined values are very similar.

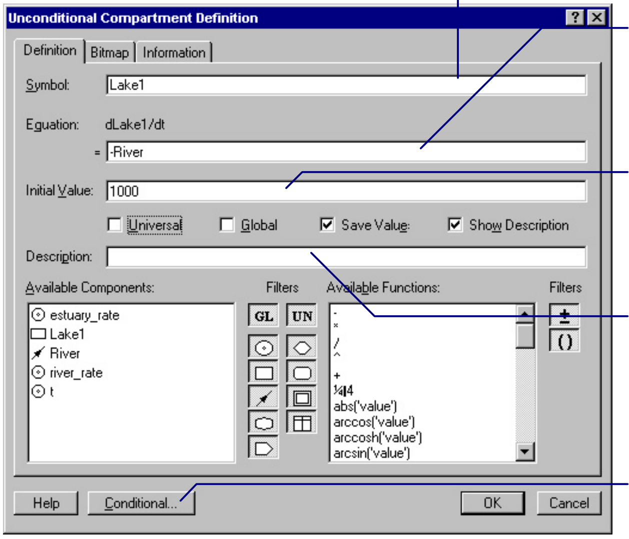
Defining unconditional components

Open the unconditional definition dialog box:

- Double click the component to be defined with the LMB
- Specify the component characteristics
- Click *OK*

The Unconditional Component Definition dialog Definition tab

Enter a unique symbol or an array element range expression



Unconditional Compartment Definition

Definition | Bitmap | Information

Symbol: Lake1

Equation: dLake1/dt

= -River

Initial Value: 1000

□ Universal □ Global ☑ Save Value ☑ Show Description

Description:

Available Components:

- estuary_rate
- Lake1
- River
- river_rate
- t

Enter a mathematical expression defining the component value

Enter a mathematical expression defining the initial value (compartments only)

Enter a description for the component (optional)

Make the component conditional

Defining conditional components

Open the Conditional Component dialog box:

- Click the *Conditional* button in the Unconditional Component Definition dialog box

The Conditional Definition dialog box is invoked with the currently entered equation as the default equation.

The Conditional Component Definition dialog Definition tab

Enter a unique symbol or an array element range expression

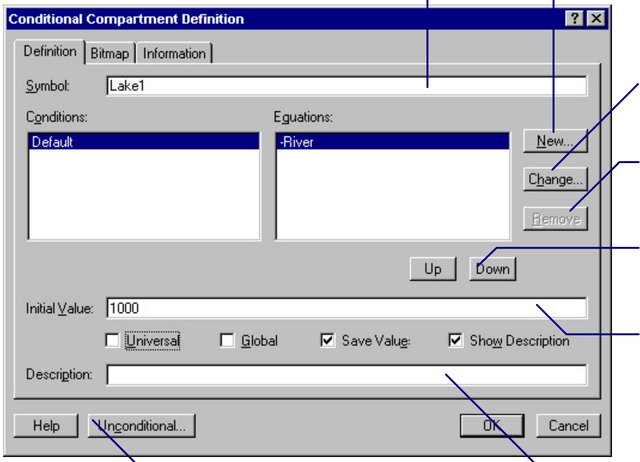
Create a new conditional expression

Edit the currently selected expression

Delete the currently selected expression

Change the evaluation order

Enter a mathematical expression defining the initial value (compartments only)



Symbol: Lake1

Conditions: Default

Equations: River

Initial Value: 1000

□ Universal □ Global ☑ Save Value ☑ Show Description

Make the component unconditional

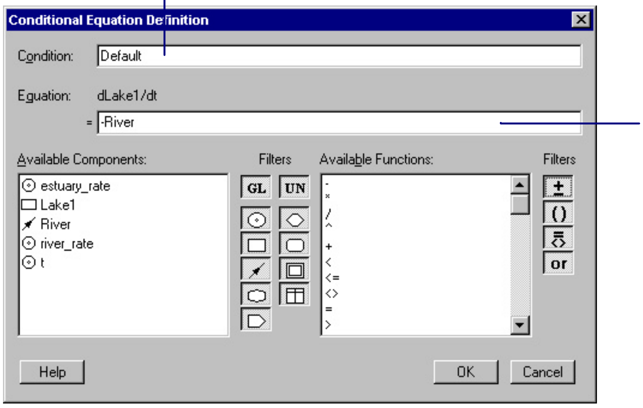
Enter a description for the component (optional)

- Use the New, Change, Remove, Up and Down buttons to manage the conditional equations

Selecting New or Change opens the Conditional Equation Definition dialog box.

- Enter values in the *Condition* and *Equation* edit boxes
- Click *OK*

The Conditional Equation Definition dialog box



Conditional Equation Definition

Condition: Default

Equation: dLake1/dt

= -River

Available Components:

- estuary_rate
- Lake1
- River
- river_rate
- t

Enter a conditional expression or leave blank for default

Enter a mathematical expression defining the component value

Default equations

If the Condition field of the Conditional Equation Definition dialog box is left blank or contains the word 'Default', ModelMaker will always evaluate the condition as being true. Thus any conditional equations which appear below a default equation in the equation list of a component will never be evaluated.

If, when evaluating a conditional component, ModelMaker reaches the end of an equation list without finding a condition which is true, it is unable to evaluate the component and terminates the model run with an appropriate error message. Thus, using a default equation at the end of an equation list prevents accidental conditional evaluation errors.

Defining arrays of component elements

Component array symbols

A single compartment, flow, variable or defined value component can represent an array or part of an array of component elements in up to three dimensions. A component is defined as an array of elements by adding an array range expression after the component symbol in the Symbol field of the appropriate definition dialog box. For example, a compartment with the symbol C1[0..1, 0..1] represents a 2 × 2 array of compartment elements.

Component element definition

The component elements defined by an array component are evaluated using the same equation (or set of conditional equations). ModelMaker defines three iterator symbols (*i*, *j*, and *k* by default) to allow the definition of component elements to reflect their position within an array. These iterator symbols are defined in the Symbols tab of the Model Options dialog box:

- Select Model | Options

Thus a one-dimensional array (vector) of elements can be defined in terms of *i*, a two-dimensional array of elements in terms of *i* and *j* and a three-dimensional array of element in terms of *i*, *j* and *k*. For example, if a defined value were defined as:

D1[0..1, 0..1] = i + (j+1) * 10

then its elements would take the following values:

D1[0,0] = 0 + (0 + 1) * 10 = 10

D1[0,1] = 0 + (1 + 1) * 10 = 20

D1[1,0] = 1 + (0 + 1) * 10 = 11

D1[1,1] = 1 + (1 + 1) * 10 = 21

Array elements may also refer to other elements in the same array (and in other arrays) using iterator expressions. For example, given two 2 × 2 arrays, one may be defined like this:

V1[0..1, 0..1] = C1[i, j]

In this case the values of the elements of *C1* will be copied to the elements of *V1*.

Component array sections

When not all the elements within an array of component elements can be defined by the same equation (or set of conditional equations) they can be defined in more than one section. This commonly arises when modeling the edge effects of an area or volume. In this case two model components are given the same symbol but different array element ranges. For example, a 2 × 2 defined value could be defined in two sections as follows:

D3[0..1, 0] = i * 10

D3[0..1, 1] = i * 100 + j

Its elements would then take the following values:

D3[0,0] = 0 * 10 = 0

D3[0,1] = 0 * 100 + 1 = 1

D3[1,0] = 1 * 10 = 10

D3[1,1] = 1 * 100 + 1 = 101

When taken together the sections of an array must define a complete, contiguous array of elements with no elements missing. For example, a defined value array with sections D3[0..1] and D3[3..4] is illegal because there is no definition for element D3[2].

7. Components – Lookup Tables and Lookup Files

Lookup files and lookup tables provide a mechanism for linking models with external numerical data. With lookup files, the data are held in a text file which is attached to a model component. Lookup tables hold their data in a lookup view which allows direct entry of data into the model.

Lookup series

A lookup table or file can have many lookup series associated with it, where each series symbol represents a column of data within the Table view or attached file. Lookup series work in the same way for tables and files. There are four types of series.

Control series

A control series is assigned to a column of data which contains values of an existing model component. Thus a control series does not have a value or symbol of its own but uses the value of the model component to determine which data points are to be used to calculate the value of a controlled series.

Controlled series

A controlled series is assigned to a column of data which contains the data from which the value of the series is to be evaluated. A controlled series has its own unique symbol which is used by other model components to refer to its value. A controlled series must also be assigned a control series which determines which data points are to be used to calculate its value.

Once the required data points have been identified the values of the series are calculated by interpolation. Interpolation can be constant, linear, polynomial or rational. See the *ModelMaker Reference Manual* for more information about interpolation.

Data series

A data series is assigned to a column of data from which single values can be picked. A data series has its own unique symbol but can only be evaluated using the lookup function. Data series are used to extract a data value from a specific index in a column of data.

Data series are not assigned a control series and cannot be interpolated.

Unused series

An unused series is assigned as a place holder to a column of data that is not used by the model.

Configuring lookup files

Lookup files are configured in the Lookup File Definition dialog box. To open the Lookup File Definition dialog box:

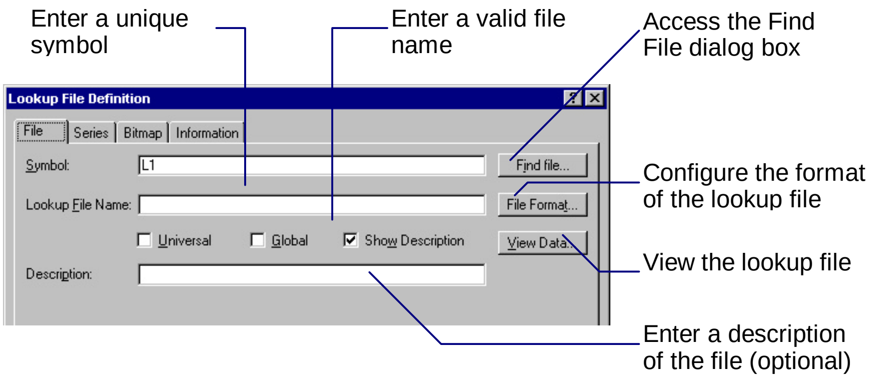
- Double click the lookup file (from either the model diagram or Definition view)

The Lookup File Definition dialog box is divided into four tabs – File, Series, Bitmap and Information. See *Chapter 5: Working with Models* for more details on using the Bitmap and Information tabs.

Configuring the File tab

- In the File tab, enter text in the *Symbol* and *Lookup File Name* edit boxes

The Lookup File Definition dialog File tab



Lookup File Definition

Symbol: L1

Lookup File Name:

□ Universal □ Global ☑ Show Description

Description:

Enter a unique symbol

Enter a valid file name

Access the Find File dialog box

Configure the format of the lookup file

View the lookup file

Enter a description of the file (optional)

Configuring the Series tab

- Select the Series tab
- Select the lookup series to be configured and configure its type, symbol and characteristics

  For a Control series:

  - Select a component from the *Available Components* drop-down list

  For a Controlled series:

  - Enter a unique symbol (global or universal) in the *Series Symbol* edit box

  - Select a controlling series

  - If required, define the series as repeated

  - Select an interpolation method

  For a Data series:

  - Enter a unique symbol (global or universal) in the *Series Symbol* edit box

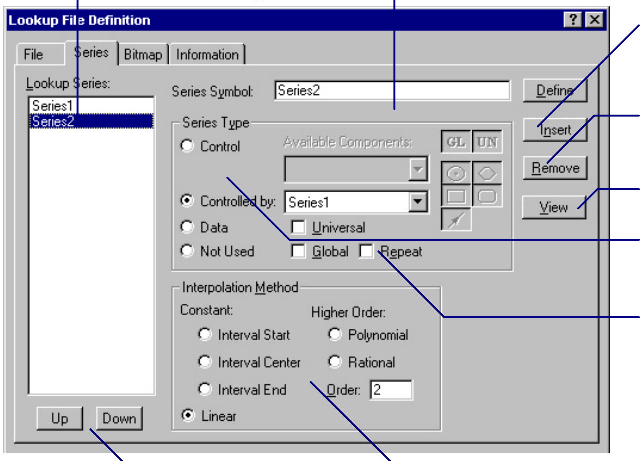
  - If required, define the series as repeated

  For an Unused series:

  - No other selections are required

- Click *OK*

The Lookup File Definition dialog Series tab



Lookup Series:
Series1
Series2

Series Symbol: Series2

Series Type
○ Control
Available Components:
● Controlled by: Series1
○ Data
☐ Universal
○ Not Used
☐ Global
☐ Repeat

Interpolation Method
Constant:
○ Interval Start
○ Interval Center
○ Interval End
● Linear
Higher Order:
○ Polynomial
○ Rational
Order: 2

Select the lookup series to configure

Enter a symbol for the series

Add a new lookup series

Remove the selected lookup series

View series

Select the lookup series type

Check to repeat data beyond available data. Repeat series can extend infinitely above and below the available data

Use Up and Down to change the series order

Select the interpolation method to use

Configuring lookup tables

Lookup tables are configured in the Lookup Table Definition dialog box. To open the Lookup Table Definition dialog box:

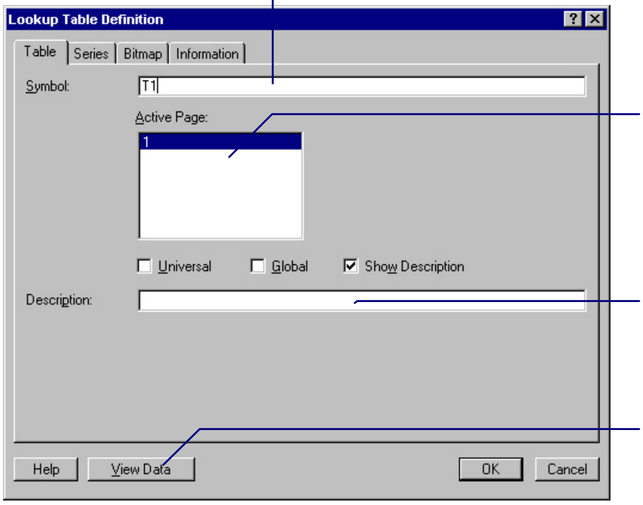
- Double click the Lookup Table (from either the model diagram or the Definition view)

The Lookup Table Definition dialog box is divided into four tabs – Table, Series, Bitmap and Information. See *Chapter 5: Working with Models* for more details on using the Bitmap and Information tabs.

Configuring the Table tab

- In the Table tab, enter text in the *Symbol* edit box

Enter a unique symbol



Select the data page to be active at the start of the model run

Enter a description of the table (optional)

Activate the Lookup Table view

The Lookup Table Definition dialog Table tab

Configuring the Series tab

- Select the Series tab

The Lookup Table Definition dialog Series tab works in the same way as the Lookup File Definition dialog Series tab. To configure the Series tab, refer to the section *Configuring the Series tab* described under *Configuring Lookup Files.*

Entering lookup table data

Once the form of the lookup table has been defined, the data values can be entered in the Lookup Table view. To access the Lookup Table view:

- Click *View Data* at the bottom of the definition dialog

This activates the Lookup Table view where data values can be defined. The Lookup Table view is discussed in more detail below.

- Enter your data into the table

Select File | Import File to import a text file into the active lookup table. The Import File dialog box opens. Select *Format* to configure the file format options.

Using the Lookup Table view

Creating the Lookup Table view

To create the Lookup Table view:

- Select the lookup table in the model diagram and select RMB | Lookup Table Data

If the Lookup Table view already exists, it becomes the active view. The view is created with an empty sheet (*Page 1*) under the sub-view T1 (or the Lookup Table Symbol name if it has been defined). Further sheets can be added to T1 as Page 2, Page 3 etc. Further Lookup Tables can be added to the Lookup Table view as T2, T3 etc.

Selecting the active page

- Select the lookup table sub-view *e.g.* T1, T2 etc
- Select the option that corresponds to your desired active page

Adding pages

To add a new page to the Lookup Table view:

- Select View | Add Page

Copying pages

To copy the currently active data page:

- Select View | Copy Page

Changing pages

To change the name of the currently active data page:

- Select View | Change Page

Deleting pages

To remove the currently active page of data from the table:

- Select View | Delete Page

Inserting columns and rows

Use the Lookup Table view toolbar icons to insert or delete rows and columns. Use the options under the View menu to insert or delete cells.

Configuring the lookup table

The Lookup Table Definition dialog box can be accessed directly from the Lookup Table view:

- Click the Series icon

Alternatively, selected lookup series may be configured individually. From the Lookup Table view:

- Double click in the column header of the series to be configured

The Lookup Table Series Definition dialog box opens for the selected series.

Changing a lookup data source

ModelMaker allows the data source of a lookup table or lookup file to be changed during a model run. For lookup tables this involves changing the active page of the lookup view and for lookup files it means changing the configured lookup file.

Changing the active lookup table page

The Lookup view associated with a lookup table can have more than one page of data, each with the same lookup series configuration and a unique identifying number.

At the start of a model run, ModelMaker calculates the values of its configured lookup series from the data contained on the active page. It is possible to change the active page during the model run by using the following event actions:

- SetPage(*lookup_table*, *page_number*)

  This attempts to set the active page of the lookup table with the symbol *lookup_table* to the page with the identifier *page_number*. If the lookup table does not have a page with the given identifier, an error message is displayed and the model run is terminated.

For example, the action

SetPage(MetData, 1)

sets the active page of the lookup table *MetData* to the page with the identifier 1.

- GetPage(Message, Title, *lookup_table*)

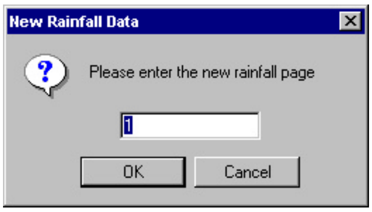
  This displays a dialog box with the given message and title prompting the user to enter the identifier of the page which is to be made the active page of the lookup table with the symbol lookup_table. The currently active page identifier is used as the default value. If the lookup table does not have a page with the entered identifier, an error message is displayed and the user is prompted to enter another value.

  If the user clicks Cancel the model run is terminated.

  For example, the action

  GetPage("Please enter the new rainfall page", "New Rainfall Data", MetData)

  displays the following dialog box and sets the active page of the lookup table *Rainfall* to the page with the entered identifier.


New Rainfall Data

Please enter the new rainfall page

1

The event action QueryLookupPage can also be used to return the identifier of the currently active page for a lookup table.

Changing the configured lookup file

It is often appropriate to arrange datasets into several different files, *e.g.* a separate file for each year of observed sunshine hours or for the sunshine hours observed at several different meteorological stations.

At the start of a model run ModelMaker loads the configured file and calculates the values of its configured lookup series from the loaded data. It is possible to change the loaded file during the model run by using the following event actions:

- SetFileName(*lookup_file*, *file_name*)

This attempts to set the active page of the lookup file with the symbol *lookup_file* to the page with the identifier *page_number*. If the new file does not exist or cannot be loaded, an error message is displayed and the model run is terminated.

For example, the action

SetFileName(Sunshine, “sun2.dat”)

loads the file sun2.dat from the current directory into the lookup file *Sunshine*.

- (Message, Title, *lookup_file*)

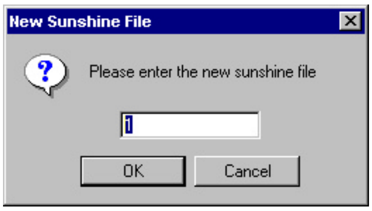
This displays a dialog box with the given message and title and prompting the user to enter the name of a file to load into the lookup file which has the symbol *lookup_file*. The name of the currently loaded file is used as the default file name. If the new file does not exist or cannot be loaded, an error message is displayed and the user is prompted to enter another file name.

If the user clicks Cancel the model run will be terminated.

For example, the action

GetFileName(“Please enter the new sunshine file”, “New Sunshine File”, Sunshine)

displays the following dialog box and loads the file with the entered name into lookup file *Sunshine.*



New Sunshine File

Please enter the new sunshine file

1

8. Components – Independent and Component Events

ModelMaker provides two types of event component to accommodate discontinuous models – independent and component events.

Events exploit the fact that ModelMaker uses initial value integration methods. ModelMaker starts every integration step as though it was the first, treating current component values as initial values and discounting what has gone before. Consequently, an event can adjust model component values at the end of an integration step without affecting the accuracy of the integration.

Event triggers

Independent and component events differ only in the way in which they are triggered.

Independent events

Independent events are triggered at user-defined values of the independent variable as the model is run. They can be periodic (*e.g.* trigger every 5 days starting on day 10) or non-periodic (*e.g.* trigger on the first Tuesday of the month) or a combination of the two (*e.g.* trigger on weekends and every first Tuesday).

Component events

Component events are triggered when a user-defined condition becomes true. This condition can be defined in terms of any other component value (*e.g.* when the lake is full, open the sluice gates).

Event active status

The active status of an event can be:

1. Configured to be active or inactive at the start of a model run

2. Configured to be re-activated or de-activated after having been triggered

3. Activated or de-activated by the actions of other events

Event actions

When an event is triggered a list of user-defined actions is performed. There is no difference in the way in which independent and component events behave once they have been triggered. In addition to simply changing the component values, events can:

1. Re-initialize selected components or the whole of the model

2. Display messages

3. Ask the model user for a Yes / No answer or a new value for a compartment or defined value

4. Change the data source for lookup tables and files

5. Control other events

6. Evaluate DLL functions

7. End the model run

Events can also include loops and conditional statements in their list of actions.

Event calculation order

The calculation order of events can be defined by the model designer. For all other components, except DLL functions, ModelMaker calculates their values in the order which is implicit in their definition, *i.e.* if component A uses the value of component B, component B will be evaluated first. Since events have such freedom to change the state of the model, ModelMaker has no way of defining exactly how events should be ordered and must leave the job to the user. This only becomes important for models with many interacting events.

Use the Component Order dialog box to determine the order in which events and DLL functions will be evaluated. To open the Component Order dialog box:

- Select Component | Evaluation Order

Use the Up and Down buttons to change the evaluation order.

Defining events

Events are configured in the Event Definition dialog box. To open the Event Definition dialog box:

- Double click the event in the model diagram

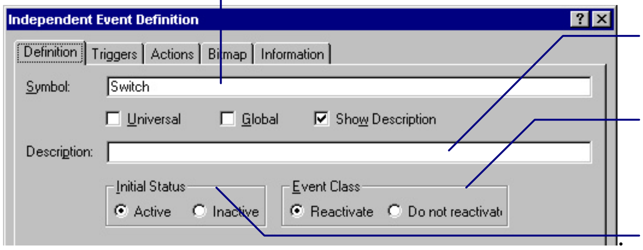
The Event Definition dialog box is divided into five tabs – Definition, Trigger, Actions, Bitmap, Information.

Configuring event definition

Independent and Component Events use the same configuration process in the Definition tab to define the symbol and type.

- In the Definition tab, enter text in the *Symbol* edit box
- Select *Initial Status* and *Event Class* options

The Event Definition dialog Definition tab



Independent Event Definition

Definition | Triggers | Actions | Bitmap | Information

Symbol: Switch

☐ Universal ☐ Global ☑ Show Description

Description:

Initial Status: ● Active ○ Inactive

Event Class: ● Reactivate ○ Do not reactivat

Enter a unique symbol

Enter a description of the event (optional)

Define whether the event is re-activated once triggered

Define whether the event is initially active

Configuring component event triggers

The component event trigger condition and tolerance are configured in the Trigger tab of the Component Event Definition dialog box.

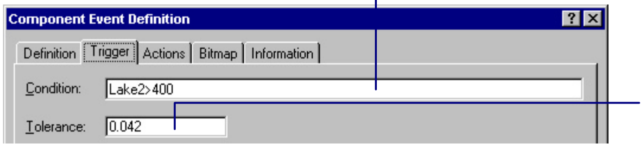
- Select the Trigger tab
- Enter a Boolean expression in the *Condition* edit box

This may contain references to any model value in order to decide whether the event should be triggered.

- Enter a value in the *Tolerance* edit box

When a component event whose condition is true is encountered, the step length of the model integration method is adjusted in order to trigger the event within the defined tolerance value.

The Component Event Definition Trigger tab



Condition: Lake2>400

Tolerance: 0.042

Enter the conditional trigger expression

Enter the trigger tolerance value

Configuring independent event triggers

Independent events are triggered at user-defined values of the independent variable in the Triggers tab of the Independent Event Definition dialog box.

To define a periodic trigger:

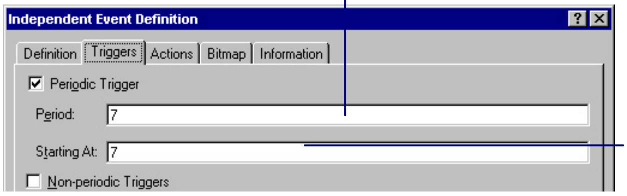
- Select *Periodic Trigger*
- Enter values in the *Period* and *Starting At* edit boxes

To define a non-periodic trigger:

- Select *Non-periodic Triggers*
- Use the New, Change and Remove buttons to add, edit and delete non-periodic triggers

ModelMaker must be able to evaluate periodic and non-periodic triggers at the start of the model run. As a result they must be defined in terms of model parameters, defined values and numeric expressions.

The Independent Event Definition dialog Triggers tab



☑ Periodic Trigger

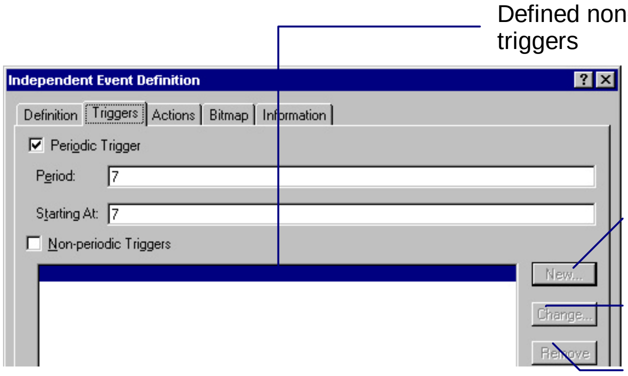
Period: 7

Starting At: 7

☐ Non-periodic Triggers

Enter the trigger period expression

Enter the trigger start value expression



☑ Periodic Trigger

Period: 7

Starting At: 7

□ Non-periodic Triggers

Defined non-periodic triggers

Create a new non-periodic trigger

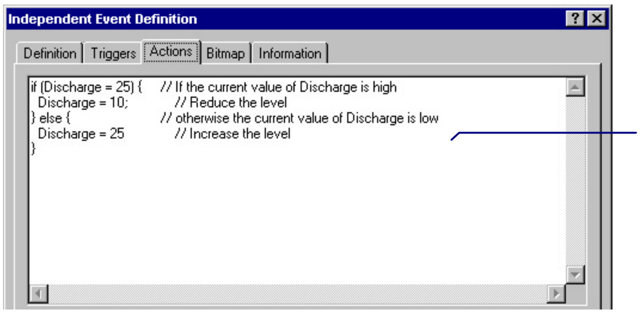
Edit the selected non-periodic trigger

Delete the selected non-periodic trigger

Configuring event actions

The Actions tab of the Independent and Component Event Definition dialog boxes is used to define the actions which an event will perform when it is triggered.

The Event Definition dialog Actions tab



```
if (Discharge = 25) {    // If the current value of Discharge is high
  Discharge = 10;          // Reduce the level
} else {                 // otherwise the current value of Discharge is low
  Discharge = 25           // Increase the level
}
```

Defined event actions

Event actions consist of a list of action statements, each separated by a semi-colon. The actions of an event may:

1. Assign new values to certain model components

2. Call actions

3. Use conditional statements to execute different groups of actions based on the condition of the model

Comments

To make the actions of an event easier to understand comments can be added. Any text on a line to the right of a double slash '/ / 'is ignored by ModelMaker. For example:

```
                         // Change the state of the model
Year = 0                 // Reset the year counter
```

Assigning model component values

Event actions can assign new values to compartments and defined values. The iterator symbols (*i*, *j* and *k* by default) are also available and can be assigned integer values. For example:

```
C1 = 10;

D1 = C1 * 2.5536;

D2= D1 * cos(t/2);

i    = j + 1;
```

To allow the assignment of new values to arrays of compartments and defined values ModelMaker makes use of the iterator symbols to define a shorthand syntax as follows:

component[*range_specification*] = *iterated_expression*

where *range_specification* defines a valid range of the elements of the component and *iterated_expression* is a mathematical expression in which the iterator symbols appropriate to the dimension of the component iterate over the defined range. Thus if the component is a one-dimensional array, the first iterator symbol (*i* by default) will iterate over the range and if it is a two-dimensional array the first and second iterator symbols will be available (*i* and *j* by default).

For example, given a 2 × 2 array of compartments C1[0..1, 0..1], the expression

```
C1[0..1, 0..1] = (i + 1) + (j * 10);
```

assigns values to the elements of *C1* as follows:

```
C1[0,0] = (0 + 1) + (0 * 10) = 1

C1[0,1] = (0 + 1) + (1 * 10) = 11

C1[1,0] = (1 + 1) + (0 * 10) = 2

C1[1,1] = (1 + 1) + (1 * 10) = 12
```

The following expression the value 10 to array elements C2[a,0] and C2[a+1,0],where a is another component value:

```
        C2[a .. a + 1, 0] = 10;
```

The next expression copies the reflection of the array *D2* about its main diagonal into *D1*:

```
        D1[0..10, 0..10] = D2[ j, i ];
```

Calling actions

ModelMaker provides a wide range of actions for communicating with the model user and adjusting the state of the model. A complete list of event actions can be found in the ModelMaker Reference Manual.

Event actions can be divided into two types:

1. Those which return a value (e.g. GetChoice(...), QueryPage(...))

2. Those which do not return a value (e.g. Message(...), SetPage(...))

Actions which return a value can be used to assign values to model components, e.g.

```
   D1 = GetChoice(“Do you want to model water flow?”, “Model
          Configuration”);
   D2 = QueryPage(T1);           // Get the chosen lookup table data
                                    page
```

Actions which do not return a value must be used on their own, *e.g.*

```
   InitializeAll;
   GetValue(“Which Year ?”, “Question”, D1, D1 > 90 and D1 <= 99);
```

Control statements

ModelMaker provides a set of control statements for conditionally controlling which actions are executed when the event is triggered.

if and if-else statements

The if and if-else statements allow the conditional execution of actions. The syntax of the if statement is as follows:

```
   if (expression is true)
      execute action or group of actions;
```

Thus if the bracketed expression is true, the action or group of actions which follows it is evaluated. If the expression is false, the specified action or group of actions is ignored and execution passes on to the next statement. For example:

```
if (D1 > 10)                // If D1 is too big
    D1 = 10;                // Set D1 to its upper limit
```

Actions can be grouped together using braces (curly brackets) ‘{’and ‘}’. All of the actions within the braces are executed when the if statement expression is true.

```
if (year = 0) {// If the first time
    D1 = 0;                 // Initialize components.
    D2 = 10;                // Note: semi-colon must still be used
                               to
}                           // separate the actions within the
                               braces.
```

The if statement can be extended by using the if-else form as follows:

```
if (expression is true)
    execute first action or group of actions;
else
    execute second action or group of actions;
```

Thus if the expression in brackets is true, the first action or group of actions is executed. If the expression is false, the second action or group of action is executed instead. For example:

```
if (D1 < 10)                // If not too big
    D1 = D1 + 1;            // increment D1
else                        // if too big
    D1 = 0;                 // start again
```

Again, braces can be used to group actions to be executed. For example:

```
if (weight > 10) {          // if things have got too heavy
    store  = store + weight; // store the product
    weight = 0;             // and start again
} else {                    // if still spare capacity
```

```
        weight = weight + 10;       // take the load
    }
```

while loop

The while loop allows actions to be repeated while a specified expression is true. The syntax of the while statement is as follows:

```
    while (expression is true)
        execute action of group of actions;
```

Thus for as long as the expression in the brackets is true, the action or group of actions following it is repeatedly evaluated. When the expression is false, execution passes to the next action. For example:

```
    while (D1 < 10)                 // while D1 is small enough
        D1 = D1 + D2;               // add the value of D2
```

Braces can be used to group actions to be executed. For example:

```
    while (D2 < 100) {              // while there is still room left
        D2 = D3 * D4;               // add the product of D3 and D4
        D3 = D3 + D4;               // increment D3
    }
```

do-while loop

The do while loop is similar to the while statement, allowing actions to be repeated while a specified expression is true. The difference lies in that the expression is evaluated at the end of the loop rather than at the beginning. The syntax of the do-while statement is as follows:

```
    do
        action or group of actions;
    while (expression is true);
```

Thus the action or group of actions following the do statement is executed once, and then repeatedly for as long as the expression in the brackets is true. When the expression is false, execution passes on to the next action. This means that the actions or group of actions will always be executed at least once. For example:

```
    do
        D1 = D1 + D2;               // always increment D1 at least once
    while (D1 < 10);                // repeat until D1 is too big
```

Braces can again be used:

```
do {
    D2 = D3 / D4;
    D3 = D3 = D4;
} while (D2 < 100);
```

for loop

The for loop allows actions or groups of action to be executed a specified number of times. The syntax of the for statement is as follows:

```
for (initial assignment; condition ; increment assignment)
    action or group of actions;
```

The for loop uses three expressions to control the execution of actions:

1. Initial assignment - this is evaluated before the loop is started

2. Condition - this must be true for the loop to be executed

3. Increment assignment - this is executed at the end of the loop before the condition is re-evaluated to decide whether to repeat the loop again

For example:

```
for (i = 0; i < 10; i = i + 1)       // increment i from 0 to 9
    Message("D1[%i] = %f", "info", i, D1[i]);
                                     // display the value of each array
                                        element
```

Braces can be used to group actions:

```
for (D1 = 0; D1 < 10; D1 = D1 + D2) {
                                     // starting from 0 increment D1
    GetValue("How much to add?", "Question", D2, D2 < 10);
                                     // Get an increment from the user
    total = total + D2;              // keep track of the total
}
```

break statement

The break statement is used with while, do-while and for loops to break out of the loop and transfer execution to the next action following the loop. For example:

```
for (i = 0; i < 10; i = i + 1) {     // increment i from 0 to 9
```

```
        D1[i] = D1[i] + 1;          // add to the elements of D1
        if (D1[i] > 5) {            // if an element is too big
            break;                  // break from the for loop
        }
    }
```

continue statement

The continue statement is used with while, do-while and for loops to return execution to the top of the loop without executing the actions which follow the continue statement.
For example:

```
    for (i = 0; i < 10; i = i + 1) {    // increment i from 0 to 9
        if (i = 5) {
            continue;                   // do not add to element D1[5]
        }
        D1[i] = D1[i] + 1;              // add to the elements of D1
    }
```

goto statement

The goto statement allows the unconditional transfer of execution to a particular action. The goto statement has the following syntax

```
    goto label;
```

where label is a text identifier within the list of actions. A label is identified by appending a colon to it. For example:

```
    if (D1 > 10) {                  // if D1 is too big
        goto no_add;                // skip the increment
    }
    D1 = D1 + 10;                   // increment D1
    no_add:  // transferred to here when D1 > 10
```

The goto statement can be used anywhere in the action list, although it is recommended that its use be kept to a minimum in order to maintain clarity.

9. Components – Sub-models, Delays and DLL functions

Sub-models

Sub-model components are used to create hierarchical structure within a model. As a model grows in size and complexity the ease with which it can be understood and manipulated is greatly increased by dividing it into groups of components. Each group, termed a sub-model, typically represents a logical section of the model. Each sub-model may contain further sub-models - ModelMaker does not place a limit on how deeply sub-models can be nested.

Sub-model hierarchies define the scope of the symbols of the components within them. Thus two components may have the same symbol as long as they are in separate sub-models and neither of them is universal.

When a model needs to pass values in and out of the sub-models it contains, there are two options:

1. Use sub-model references

This is generally the recommended method because it preserves the structure of the model.

2. Use a universal component to hold the value to be passed

Making a component universal means that it can be referenced from anywhere in the model and removes the need for direct connection.

The Sub-model view

Sub-models are added to the Diagram view as branches of the main model diagram. By default these branches are called Sub1, Sub2 etc. To activate a sub-model view:

- Double click a sub-model component in the model diagram

Note, selecting View | Parent model will take you up one level into the parent model of the current sub-model. Selecting View | Top-level model will access the model diagram of the top-level model.

Adding sub-model references

There are two types of sub-model reference: input and output. These are used to pass values into and out of a sub-model respectively.

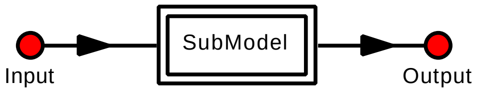
To add a sub-model reference to a parent model:

- Select the sub-model component in the model diagram

The input and output reference icons will be enabled on the toolbar.

- Select a reference icon and click in the model diagram

Sub-model references in the parent model

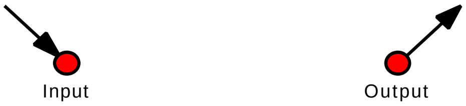


Each sub-model reference is given a unique symbol to distinguish it from other references. To change the symbol of a parent model reference:

- Double click the reference to be renamed
- Enter a new name in the Model Reference Definition dialog box

When a sub-model reference is added to a sub-model component a link is made between the sub-model and its parent. An input reference is shown in the parent model as an inward connection with a corresponding inward connection inside the sub-model. Similarly an output connection is shown as an outward connection inside the sub-model, with a corresponding outward connection in the parent model.

Corresponding references inside the sub-model



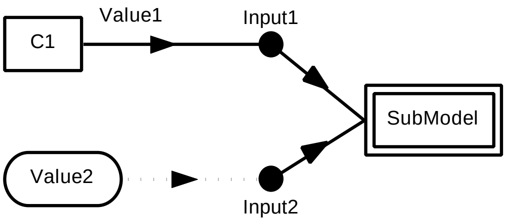
To change the symbol or arrow position of a corresponding sub-model reference:

- Double click the reference to be customized
- Select its new properties in the Model Reference Definition dialog box

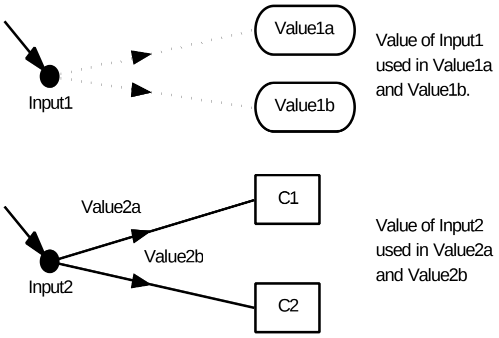
Input references

Connecting a model component to an input reference in the parent model passes the value of the component into the sub-model, making it available to the components inside the sub-model. The connection can be made using a flow (from a compartment) or an influence.

If a flow is connected to the input reference, the value of the flow is passed into the sub-model. If an influence is connected, the value of the source component of the influence is passed. Only one component may be connected to the parent end of an input reference.



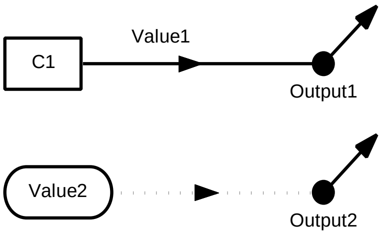
Inside the sub-model the input reference takes the value of the connected component in the parent model. This value can be used in the normal way by using the symbol of the input reference.


Value1a
Input1
Value1b
Value of Input1 used in Value1a and Value1b.
Value2a
C1
Value2b
Input2
C2
Value of Input2 used in Value2a and Value2b

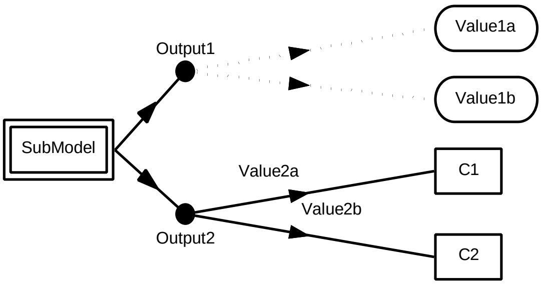
Output references

Connecting a model component to an output reference inside its sub-model passes the value of the component out of the sub-model making it available to the components in the parent model. The connection can be made using a flow (from a compartment) or an influence.

If a flow is connected to the output reference, the value of the flow is passed out of the sub-model. If an influence is connected, the value of the source component of the influence is passed. Only one component may be connected to the sub-model end of an output reference.



In the parent model the output reference takes the value of the connected component in sub-model. This value can be used in the normal way by using the symbol of the output reference.



Value of Output1 used in Value1a and Value1b.

Value of Output2 used in Value2a and Value2b

Delays

In many systems not everything happens at once, and the consequences of certain occurrences may not be felt by the model until some period of time has passed. To accommodate this, ModelMaker provides a delay component which takes the value of another model component and delays it for a defined, but not necessarily constant, period before feeding it back into the model.

A delay component is specified in terms of:

1. The component whose value is to be delayed.

2. A value or mathematical expression defining the duration of the delay.

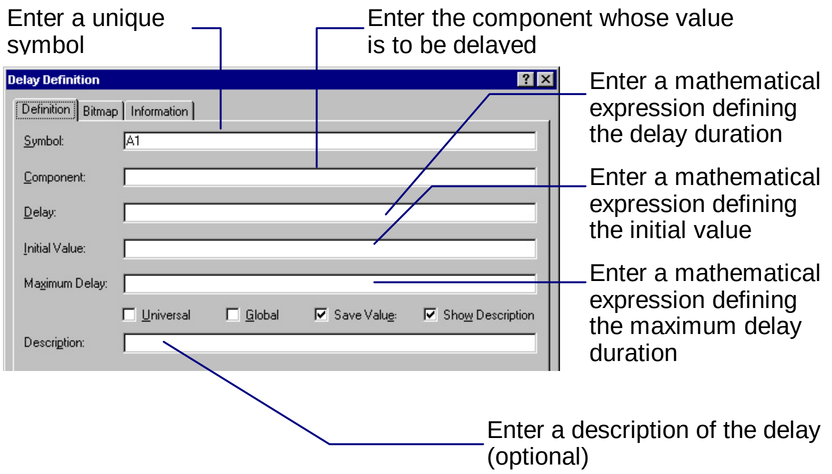
3. An initial value. At the start of the model run ModelMaker does not know what the delayed value of the component should be, so a value or defining mathematical expression must be supplied.

4. The maximum delay. ModelMaker has to maintain a buffer of past values in order to calculate delayed values and needs to know how big to make this buffer. If the delay is variable, you should set this field to the largest value of delay you expect. If, during the model run, the delay duration exceeds this value, the run is halted with an appropriate error message

ModelMaker must be able to evaluate the delay duration, initial value and maximum delay at the start of the model run, requiring that they all be defined in terms of model parameters, defined values and numeric expressions.

A delay is defined using the Delay Definition dialog box which can be accessed by double clicking the delay component.

The Delay Definition dialog box



Delay Definition

Definition | Bitmap | Information

Symbol: A1

Component:

Delay:

Initial Value:

Maximum Delay:

☐ Universal ☐ Global ☑ Save Value ☑ Show Description

Description:

Enter a unique symbol

Enter the component whose value is to be delayed

Enter a mathematical expression defining the delay duration

Enter a mathematical expression defining the initial value

Enter a mathematical expression defining the maximum delay duration

Enter a description of the delay (optional)

DLL functions

DLL functions allow ModelMaker models to be connected to external functions defined in Windows DLL (Dynamic Link Library) modules. Such functions may contain special calculations or dialog interfaces written for a particular purpose outside the normal scope of a ModelMaker model. Refer to the ModelMaker Reference Manual for more information on writing DLL functions.

ModelMaker communicates with functions held in DLLs by passing and receiving two sets of values. The values passed or input to the functions are defined by a user-defined list of mathematical expressions. The values output by the functions are each assigned a symbol and can then be used by other model components in the normal way.

DLL function evaluation

A DLL function can be one of two types – normal or integration.

Normal DLL functions behave in a similar way to variables and are designed to carry out straightforward calculations. In addition to the configured input value they receive the current value of the independent variable.

Integration DLL functions behave in a similar way to compartments and are designed to carry out integration-type calculations over the same calculation steps as those ModelMaker uses to evaluate the rest of the model. In addition to the configured input values they receive the values of the independent variable at the start and at the end of the last successful integration step undertaken by ModelMaker.

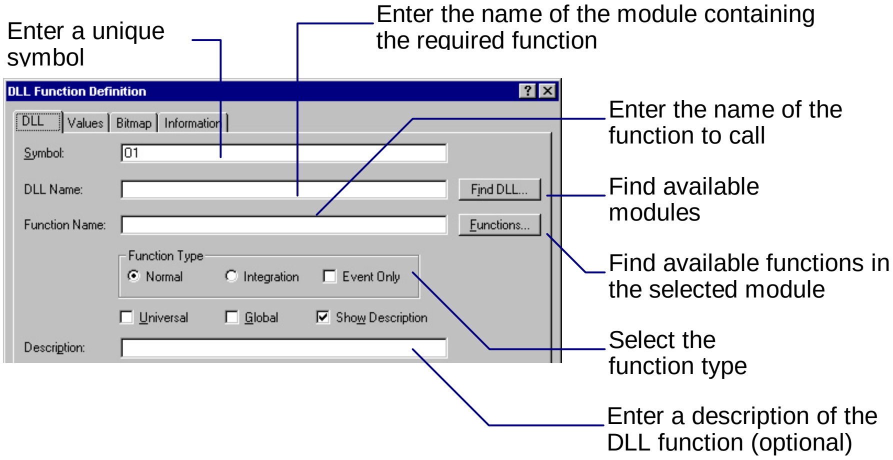
In addition to being normal or integration, a DLL function can be defined to be 'event only'. By default a DLL function is evaluated (*i.e.* the external function is called) for every calculation step made by ModelMaker. For some external functions this is not appropriate. In such cases, event only DLL functions (which can be evaluated only by an event using the EvaluateFunction action) can be used.

For example, a DLL function which uses a dialog box to ask the user for model initialization information might only be called at the start of a model run. In this case the DLL function would be made event only and would be evaluated by an event triggered at the start of the model run.

DLL function definition

The DLL tab of the DLL Function Definition dialog box is used to configure the component symbol, DLL module and function. Open the DLL Function Definition dialog box by double clicking the DLL component.

The DLL Function Definition dialog DLL tab



Enter a unique symbol

Enter the name of the module containing the required function

Enter the name of the function to call

Find available modules

Find available functions in the selected module

Select the function type

Enter a description of the DLL function (optional)

DLL Function Definition

DLL | Values | Bitmap | Information

Symbol: 01

DLL Name:

Function Name:

Function Type: ● Normal ○ Integration □ Event Only

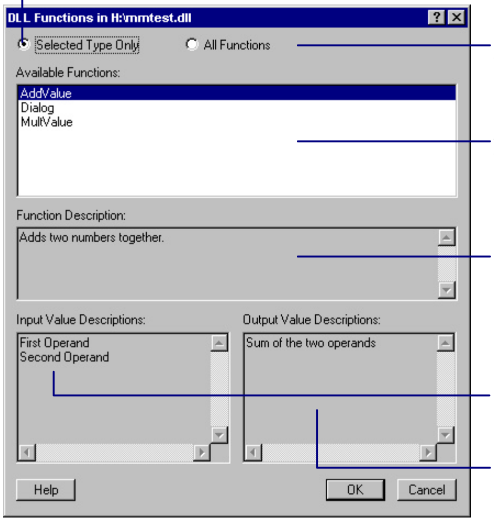
□ Universal □ Global ☑ Show Description

Description:

Each DLL module may contain many functions which can be used by a DLL function component. The ModelMaker function interface allows the developer of the DLL to provide the names of the functions available in a DLL and information about their use and input and output values. If this information is available for the specified DLL, the Functions button will be activated. Click the Functions button to activate the DLL Functions dialog box.

The DLL Functions dialog box

Only display those functions which match the DLL function type



● Selected Type Only ○ All Functions

Available Functions:

AddValue
Dialog
MultValue

Function Description:

Adds two numbers together.

Input Value Descriptions:

First Operand
Second Operand

Output Value Descriptions:

Sum of the two operands

Display all functions in the module

Available functions

Description of the selected function

Description of the input values

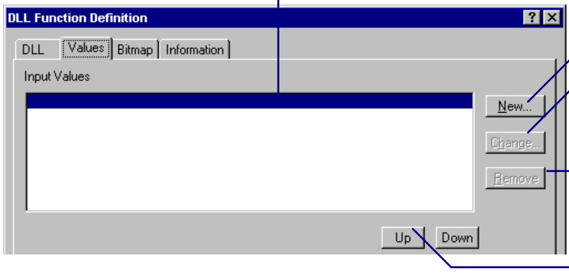
Description of the output values

DLL function value definition

The values input to a DLL function are specified by a list of mathematical expressions defined in terms of the other components in the model. The input values are defined using the Values tab of the DLL Function Definition dialog box.

The DLL Function Definition dialog Values tab – Input Values

Defined input value expressions



Create a new input value

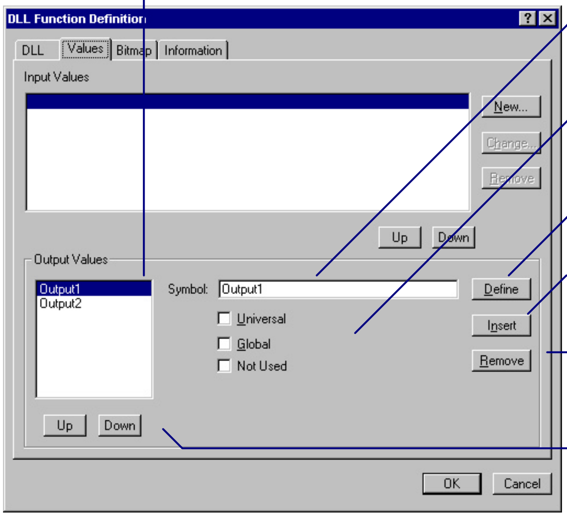
Change the currently selected input value

Delete the currently selected input value

Use Up and Down to change the input value order

Each of the output values from a DLL function is given a unique symbol so that it can be used by other components in the model. The output values are defined using the Values tab of the DLL Function Definition dialog box.

The DLL Function Definition dialog Values tab – Output Values



Output1
Output2

Symbol: Output1

☐ Universal
☐ Global
☐ Not Used

Defined output value expressions

Enter a unique symbol for the output value

Define the output value type

Accept the output value definition

Create a new output value

Delete the currently selected output value

Use Up and Down to change the output value order

DLL evaluation order

Use the Component Order dialog box to determine the order in which events and DLL functions will be evaluated. To open the Component Order dialog box:

- Select Component|Evaluation Order

Use the Up and Down buttons to change the evaluation order.

10. Parameters

Parameters store constant values within a model. They do not have a diagram representation and are considered to be global. Instead of a having a representation in the Diagram view, parameters are added, viewed and manipulated in the Parameter view.

Using the Parameter view

Creating the Parameter view

To create the Parameter view:

- Click the Parameters icon, or:
- Select View | Parameters

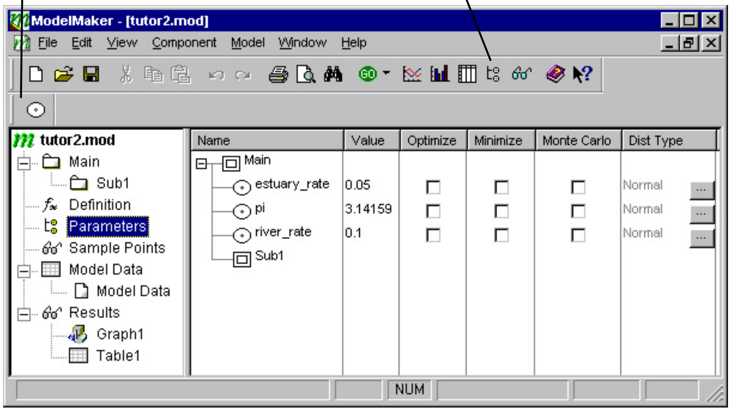
If the Parameter view already exists, it becomes the active view.

The Parameter view is divided into six fields – Name, Value, Optimize, Minimize, Monte Carlo and Dist Type.

The Parameter view

Use the Parameter icon to add parameters to the view

Use the Parameters icon to create or activate the view



Name	Value	Optimize	Minimize	Monte Carlo	Dist Type
Main					
estuary_rate	0.05	□	□	□	Normal
pi	3.14159	□	□	□	Normal
river_rate	0.1	□	□	□	Normal
Sub1					

The Name field provides a tree view of a model's structure with each branch representing a sub-model or parameter array range. Expand and collapse branches by double clicking the plus and minus icons. Parameters are presented in alphabetical order within each sub-model.

Use the Optimize, Minimize, Monte Carlo and Dist Type check boxes to select parameters to investigate during analysis. See *Chapter 14: Optimization; Chapter 15: Minimization; Chapter 16: Monte Carlo Analysis.*

Adding parameters

Specify which sub-model you want to add a new parameter to by clicking the appropriate sub-model entry with the LMB. To add a parameter:

- Click the Parameter icon, or:
- Select Component|Parameter

Defining parameters

Parameters are defined in the Parameter Definition dialog box. To open this dialog:

- Double click with the LMB on the parameter to be defined

The Parameter Definition dialog box is divided into four tabs – Definition, Constraints, Estimation and Information. See *Chapter 5: Working with Models* for more details about the Information tab.

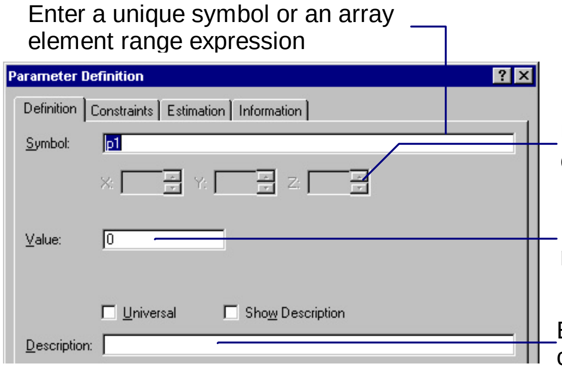
Configuring the Definition tab

Use the Definition tab to characterize the parameter. The value of the parameter is shown in the Value field of the Parameter view.

- Enter a name in the *Symbol* edit box
- Enter a value in the *Value* edit box

The Parameter Definition dialog Definition tab

Enter a unique symbol or an array element range expression



Symbol: p1

Value: 0

□ Universal □ Show Description

Description:

Use to define each element of the parameter array

Enter a value for the parameter element

Enter a description for the component (optional)

Configuring the Constraints tab

Use the Constraints tab to define parameter constraints during optimization and minimization calculations. Constraints can be defined as unconstrained, a range (multiplicative or absolute) or fixed.

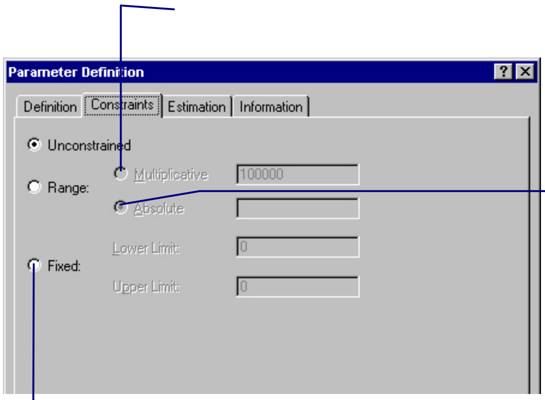
Unconstrained is the ModelMaker default selection and means that parameters can take any value during optimization and minimization.

A constraint range provides a way to control the range of parameter values used during analysis. Select Range to set a constraint range in relation to the parameter value. For example, a range of 10 sets the multiplicative range to 0.1*value<value<10*value and the absolute range to value±10.

Select *Fixed* to set the constraint range to lie between fixed upper and lower limits.

The Parameter Definition dialog Constraints tab

Check for a multiplicative range and enter a value in the edit box



● Unconstrained

○ Range: ○ Multiplicative 100000

○ Absolute

○ Fixed: Lower Limit: 0

Upper Limit: 0

Check for an absolute range and enter a value in the edit box

Check for fixed constraints and enter limits in the edit boxes

Configuring the Estimation tab

Use the Estimation tab to set limits on parameter estimation before optimization. Parameter estimation can be defined as default, none, a range (multiplicative, fractional or absolute) or fixed.

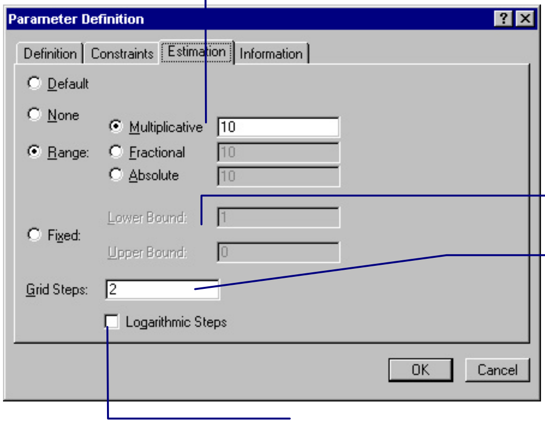
Default sets parameter estimation as the default search range defined in the Optimization Settings dialog Estimation tab.

None sets the parameter value to remain fixed.

Range constrains the parameter estimation to a value within a range that is relative to the parameter value. Multiplicative allows a wide estimation range to be set, *e.g.* 10 sets the estimation range as 0.1*value<value<10*value. Fractional allows a narrow estimation range to be set, *e.g.* 0.1 sets the estimation range as value*(1±0.1). Absolute sets an absolute estimation range, *e.g.* 10 set the range as value±10.

Fixed sets the estimation range as an absolute range.

The Parameter Definition dialog Estimation tab



Parameter Definition

Definition | Constraints | Estimation | Information

○ Default

○ None

● Range: ● Multiplicative 10 / ○ Fractional 10 / ○ Absolute 10

○ Fixed: Lower Bound: 1 / Upper Bound: 0

Grid Steps: 2

□ Logarithmic Steps

OK | Cancel

Check a range type and enter a value in the corresponding edit box

Check Fixed and enter upper and lower limits

Sets the size of the grid steps when using Grid search during Range and Fixed estimation

Sets the grid step sizes to be taken in logarithmic sizes

Deleting parameters

To delete parameters from the Parameter view:

- Select the parameter to be deleted
- Select Edit | Delete or press the <Delete> key

The selected parameter will be removed from the Parameter view. To undelete the parameter:

- Select Edit | Undo Component Delete

Arrays of parameters

To define a parameter as an array:

- Double click the parameter to be defined

The Parameter Definition dialog box opens.

- Select the Definition tab
- Enter an array range expression in the *Symbol* edit box

Click outside the symbol field to enable the X, Y and Z spin boxes. You can now assign individual values to the array elements:

- In the available X, Y or Z spin box click the up / down arrow to scroll to the appropriate array element number
- Enter a number in the *Value* edit box
- Repeat until you have defined the whole array

For example, a parameter with the symbol p[0..1, 0..1] represents a 2x2 array of parameter elements, each of which can have a different value.

Unlike compartments, flows, variables and defined values, parameter arrays may only be defined as a single section. This is because each parameter element must be individually defined.

Note, you can also use the shortcut menu to add and define parameters *i.e.* select RMB | New Parameter or RMB | Edit Parameter. Parameters can be updated with optimized or minimized values – see *Chapter 14: Optimization* or *Chapter 15: Minimization*.

11. Running a Model

Once a model has been defined by inserting and configuring all the necessary model components, it can be run. This is the process of solving all the model component equations using the selected integration method, over the desired range of the model's independent variable.

To run a model:

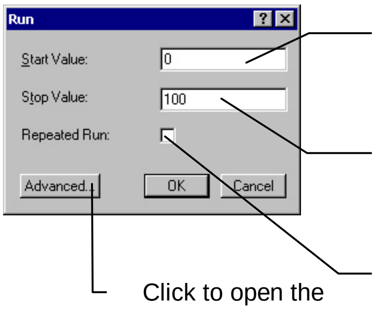
- Click the Integrate icon, or:
- Select Model|Integrate

The Run dialog box opens.

- Click *OK*

The model is run using the default run options.

The Run dialog



Run

Start Value: 0

Stop Value: 100

Repeated Run: □

Enter the starting value of the independent variable for the run

Enter the stop value of the independent variable for the run

Check to initiate repeated run options

Click to open the Run Options dialog

Configuring run options

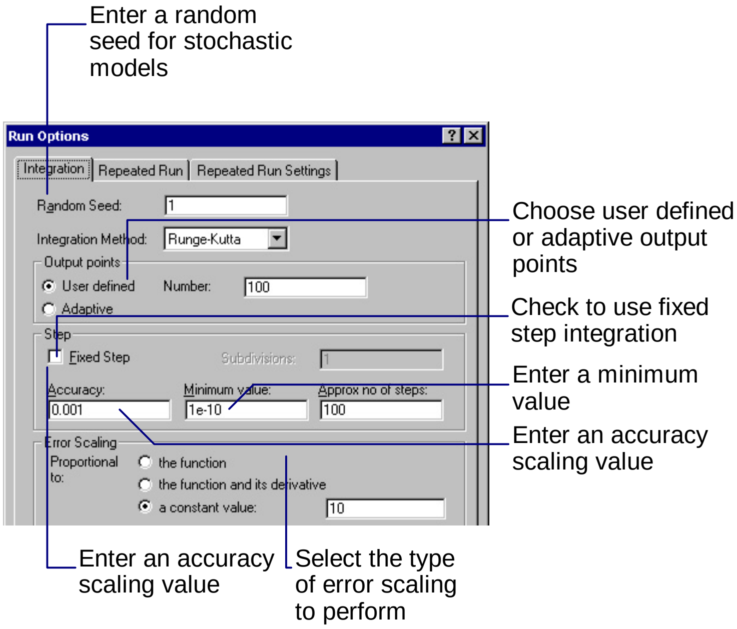
More advanced run options can be configured from the Run Options dialog box. To open the Run Options dialog:

- Click the Advanced button in the Run dialog, or:
- Select Model|Configure>Integration

The Run Options dialog is divided into three tabs – Integration, Repeated Run and Repeated Run Settings.

Configuring the integration method

The integration method that is used to solve the model is selected and configured in the Integration tab. See the *ModelMaker Reference Manual* for more information about the available integration methods.



Run Options

Integration | Repeated Run | Repeated Run Settings

Random Seed: 1

Integration Method: Runge-Kutta

Output points

● User defined Number: 100

○ Adaptive

Step

□ Fixed Step Subdivisions: 1

Accuracy: 0.001 Minimum value: 1e-10 Approx no of steps: 100

Error Scaling

Proportional to:

○ the function

○ the function and its derivative

● a constant value: 10

The Run Options dialog Integration tab

Enter a random seed for stochastic models

Choose user defined or adaptive output points

Check to use fixed step integration

Enter a minimum value

Enter an accuracy scaling value

Enter an accuracy scaling value

Select the type of error scaling to perform

Random seed

Stochastic models require a random seed value for the pseudo-random number generator. The default value is 1.

Integration method

Choose from five integration methods – Euler, Mid-Point, Runge-Kutta, Bulirsch-Stoer and Gear. Runge-Kutta is the default method. Gear's method has different run options which are discussed below.

Output points

This is the number of output points for plotting or displaying in a table, and is used to control the amount of data generated. You can choose user defined or adaptive output points. With user defined, the number of output steps must also be entered (the default value is 100). With adaptive output points, ModelMaker will calculate the number of output points depending on the nature of the function, *i.e.* more output points will be calculated for curved regions of the function than for straight functions. Note that adaptive output points are not compatible with repeated runs.

Step

The step panel configures the integration step calculation. Using the default step options, the initial step length is equivalent to the full range of the integration divided by the approx no. of steps. Accuracy is used to scale the integration method's error calculation. The smaller the accuracy value the more accurate the model calculation is but the longer the model takes to run. Minimum value is also used in the error calculation, and prevents numerical overflow when the values of model components are very small.

With user defined output points, fixed step integration can be selected – select *Fixed Step* and enter a value in the *Subdivisions* edit box. Thus with this option, the total number of calculations will be equal to the number of output points multiplied by the number of subdivisions.

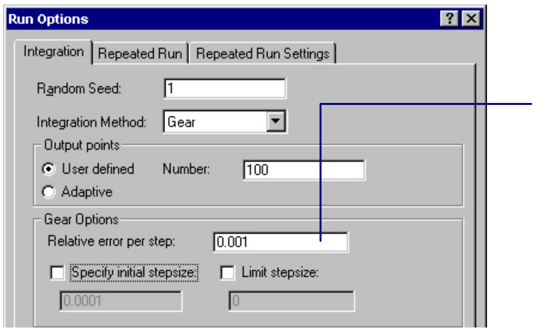
Error scaling

Choose how the method error is scaled. The default method sets error scaling to be proportional to a constant value of 10.

Configuring Gear's method

If Gear is selected as the integration method, the Integration tab options change. Gear's method is an appropriate solver for stiff simulations where processes happen on very different time scales. It automatically adjusts the size of integration steps to match the timescale on which the simulation is evolving. Note that Gear's method may be a memory intensive calculation.

If the *Specify initial stepsize* and *Limit stepsize* check boxes are left clear, ModelMaker will select values.



Random Seed: 1

Integration Method: Gear

Output points

● User defined Number: 100

○ Adaptive

Gear Options

Relative error per step: 0.001

□ Specify initial stepsize: 0.0001

□ Limit stepsize: 0

Enter a relative error per step. *E.g.* An error of 0.001 ensures an error on each component in one integration step of less than 0.1%.

Configuring a repeated run

Repeated run operation provides the ability to run a model many times whilst preserving the final state of the model from one run to the next. This is particularly useful for periodic models and for stochastic models where many runs are required to assess the effect of random factors.

Repeated runs are configured in the Repeated Run and Repeated Run Settings tabs of the Run Options dialog.

To set up a repeated run:

- Select the Repeated Run tab
- Enter a value in the *Number of Runs* edit box
- Select components in the *Components to Include* list box

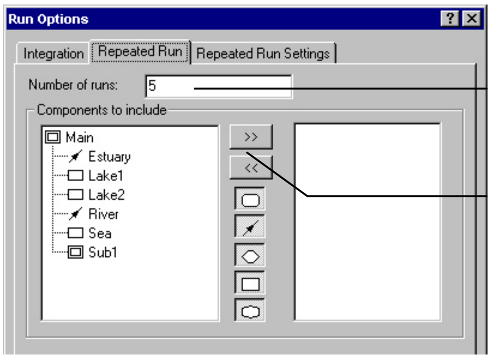
The calculated data are saved for the selected components. These retained series are available for inclusion in graphs and tables.

- Click '>>' to move the selected components into the opposite list box
- Select the Repeated Run Settings tab
- Select the *Repeated Run* option button
- Select components in the *Preserved Component* list box

The values of these components are preserved from one run to the next.

- Click '>>' to move the selected components into the opposite list box
- Click *OK* in the Run Options dialog
- Select *Repeated Run* in the Run dialog
- Click *OK* in the Run dialog

The Run Options dialog Repeated Run tab



Number of runs: 5

Enter the number of repetitions

Use >> and << to select the components whose values are to be saved

Pressing <Esc> will cancel the repeated run calculation.

Configuring sensitivity analysis

During sensitivity analysis the value of a selected parameter is systematically adjusted to obtain an indication of how sensitive the calculated values of other model components are to this change.

To set up sensitivity analysis:

- Select the Repeated Run tab
- Select components in the *Components to Include* list box

The calculated data are saved for the selected components. These retained series are available for inclusion in graphs and tables.

- Click '>>' to move the selected components into the opposite list box
- Enter a value in the *Number of Runs* edit box

This is the number of runs required to reach the Stop Value.

- Select the Repeated Run Settings tab
- Select the *Sensitivity Analysis* option button
- Select or clear the *Logarithmic Steps* check box
- Select a parameter

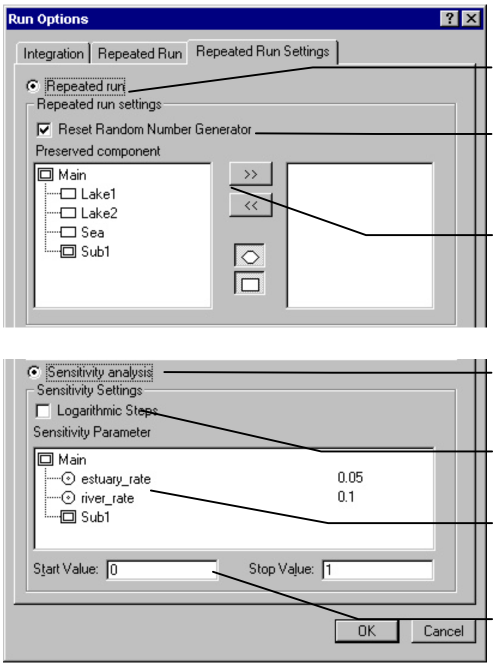
This parameter will be adjusted during the analysis.

- Enter values in the *Start Value* and *Stop Value* edit boxes

These are the initial and final values of the parameter.

- Click *OK* in the Run Options dialog
- Select *Repeated Run* in the Run dialog
- Click *OK* in the Run dialog

The Run Options dialog Repeated Run Settings tab



● Repeated run

Repeated run settings

☑ Reset Random Number Generator

● Sensitivity analysis

Sensitivity Settings

□ Logarithmic Steps

estuary_rate	0.05
river_rate	0.1

Start Value: 0 Stop Value: 1

Check to perform a repeated run

Check to use the same random number series for each run

Use >> and << to select components whose values are to be preserved

Check to perform sensitivity analysis

Check for logarithmic steps

Select the parameter to be varied

Enter parameter stop and start values

Retained series

During a repeated run or sensitivity analysis, ModelMaker creates a retained series of data for each selected model component for each run of the model. Each retained series is labeled with the number of the run or parameter value for which it was created. For example, a repeated run for component *C1* produces retained series *C1:Run1, C1:Run2* etc; sensitivity analysis of component *C1* (based on the adjustment of parameter *P1* at values 0.1, 0.2 etc.) produces retained series *C1:P1=0.1, C1:P1=0.2.*

In most circumstances only one series of data is created for the independent variable as the component retained series are calculated for the same values of the independent variable. If, however, the run is halted, the final value in the series may be calculated at a unique value of the independent variable. In this case ModelMaker creates a retained series of data for the independent variable.

The retained series created by a repeated run or sensitivity analysis are available for inclusion in tables and graphs by opening the Graph Selection or Table Selection dialog boxes. See *Chapter 12: Graphs* and *Chapter 13: Tables* for more information on graphs and tables.

If, at the start of the run, retained series exist from a previous sensitivity analysis or repeated run, ModelMaker replaces the old series with the new series.

12. Graphs

Graphs provide an easy way to view both calculated and Model Data values. Graphs, like tables (see *Chapter 13*), can be archived and restored at a later date so that the effects of changes to the model can be examined. Graphs are stored under the Results view as Graph1, Graph2 etc. Histograms are stored under the Results view as Histo1, Histo2 etc. and are discussed in *Chapter 16: Monte Carlo Analysis.*

The values of Compartments, Variables, Flows, Defined values and Delays can be shown on graphs. Note that component values are only available for plotting if *Save Value* is selected in each component definition dialog box. However, all component values are saved if *Save selected component values* is cleared in the User Preferences dialog box (Edit menu).

Creating graphs

To create a graph:

- Click the Graph icon, or:
- Select View | Graph

The Graph Selection dialog box opens. Use this dialog to specify which component values are to be presented on the vertical and horizontal axes.

- Select components in the *Components* list box

These components will be plotted on the vertical axis

- Click '>>' to move the selected components into the *Vertical Axis* list box

Double clicking components also moves them from one list box to the other.

- Select a component in the *Horizontal Axis* list box

This component will be plotted on the horizontal axis. By default, the independent variable (normally time) is used for the horizontal axis but any other suitable component can be chosen.

Now the graph is ready to plot:

- Click *OK*

Repeat the steps described above to add further graphs to the Results view.

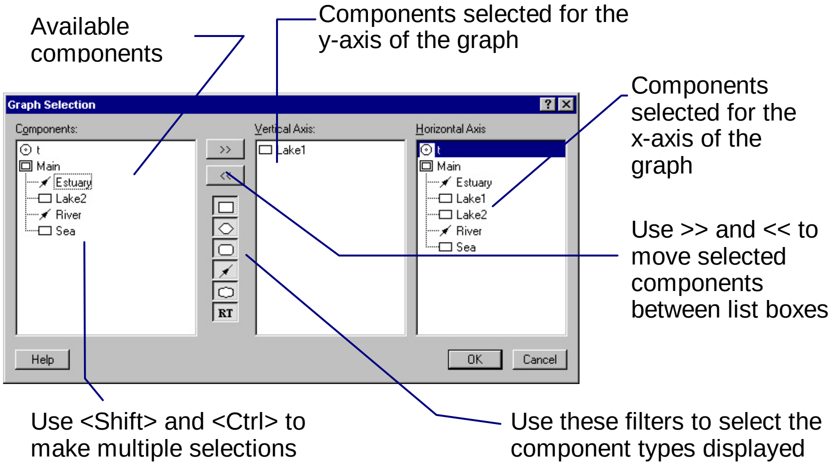
Changing the graph selection

Your component selection can be changed at any time by re-opening the Graph Selection dialog box:

- Click the Selection icon on the Graph toolbar, or:
- Select View | Selection

Use ‘>>’ and ‘<<’ to change your component selection.

The Graph Selection dialog box



Available components

Components selected for the y-axis of the graph

Components selected for the x-axis of the graph

Use >> and << to move selected components between list boxes

Use <Shift> and <Ctrl> to make multiple selections

Use these filters to select the component types displayed

Customizing graphs

The graph series, title, axes and legend can be customized in order to present the graph in the most effective way.

Customizing the graph series

When a model component is selected for the vertical axis of a graph, a graph series is created to display the values associated with the component. A graph series can be associated with the following sets of values:

1. Model values *i.e.* values calculated from the model.

2. Data points *i.e.* data configured in the Model Data view. See *Chapter 14: Optimization*.

3. Error bars *i.e.* error calculated for the data points. Error bars are based on the default optimization error which is configured in the Weighting tab of the Optimization Settings dialog box. Error values can also be configured in the Model Data view. See *Chapter 14: Optimization*.

The series options for a graph are defined in the Graph Series dialog box:

- Click the Series icon, or:

- Select View | Series

The Graph Series Options dialog box opens.

- Select a graph series in the *Series* list box and define its marker and line attributes etc.

- Click *Define*

The options for the series are saved.

- Use *Up* and *Down* to change the graph series selection

- Click *OK* to save the series options and dismiss the dialog

Adding model data points

If model data have been configured for the components plotted on a graph, these data can be added to the graph as data points.

In the Graph Series Options dialog box:

- Select *Data Points* for each series with model data

If more than one page of data has been configured in the Model Data view, you can choose to display all model data or selected sheets only.

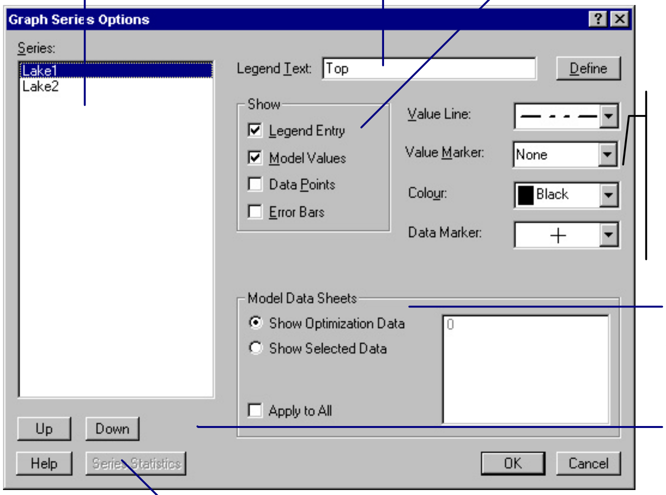
- Select *Show Optimization Data* or *Show Selected Data*

With *Show Selected Data*, you must also select the page number of one or more sheets.

- Select *Apply to All* to apply this setting to all series

See *Chapter 14: Optimization* for more information about configuring the Model Data view.

The Graph Series Options dialog box



Graph Series Options

Series:
Lake1
Lake2

Legend Text: Top

Show
☑ Legend Entry
☑ Model Values
☐ Data Points
☐ Error Bars

Value Line: — - - —
Value Marker: None
Colour: ■ Black
Data Marker: +

Model Data Sheets
● Show Optimization Data
○ Show Selected Data
0
☐ Apply to All

Select the graph series to define

Enter legend text

Select series values to show

Select the line type, line color and marker type for model values and data points

Show data configured in the Model Data view (if available)

Use Up and Down to change the graph series selection

Select to open the Series Statistics dialog (Histograms only)

Customizing graph axes

When a graph is created it is given a default axis configuration depending on the value of the series. You can change the following characteristics of a graph axis:

1. Maximum and minimum values.

2. Major and minor tick intervals.

3. Crossing point.

4. Grid lines.

5. Axis title text, position, color and font.

6. Axis label numeric format, color and font.

To customize a graph axis:

- Click the X-Axis or Y-Axis icon, or:
- Select View | X-Axis or View | Y-Axis

The appropriate Graph Axis Configuration dialog box opens.

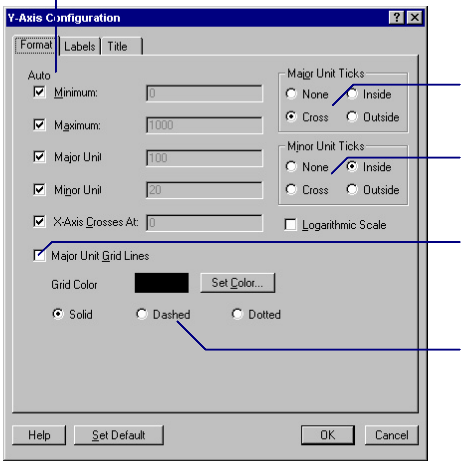
- Define the new axis characteristics
- Click *OK*

The Graph Axis Configuration dialog boxes are divided into three tabs – Format, Labels and Title.

Use the Format tab to define the axis limits, tick marks, crossing point and grid lines.

The Graph Axis Configuration dialog Format tab

Clear these flags to enter a fixed value for the axis characteristic



Y-Axis Configuration

Format | Labels | Title

Auto

☑ Minimum: 0

☑ Maximum: 1000

☑ Major Unit 100

☑ Minor Unit 20

☑ X-Axis Crosses At: 0

Major Unit Ticks: ○ None ○ Inside ● Cross ○ Outside

Minor Unit Ticks: ○ None ● Inside ○ Cross ○ Outside

□ Logarithmic Scale

□ Major Unit Grid Lines

Grid Color ■ Set Color...

● Solid ○ Dashed ○ Dotted

Select the major unit tick mark type

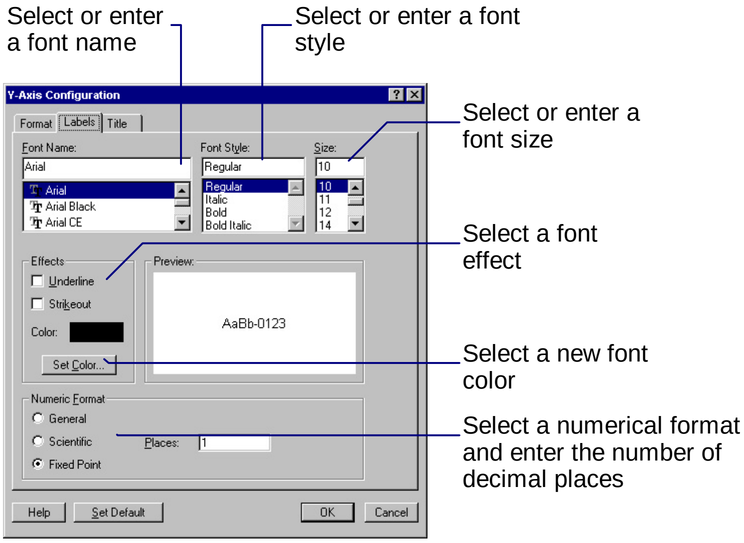
Select the minor unit tick mark type

Select the minor unit tick mark type

Customize grid

Use the Labels tab to define the font and numeric format for the axis labels.

The Graph Axis Configuration dialog Labels tab



Select or enter a font name

Select or enter a font style

Select or enter a font size

Select a font effect

Select a new font color

Select a numerical format and enter the number of decimal places

Y-Axis Configuration

Font Name: Arial

Font Style: Regular

Size: 10

□ Underline

□ Strikeout

Color: ■

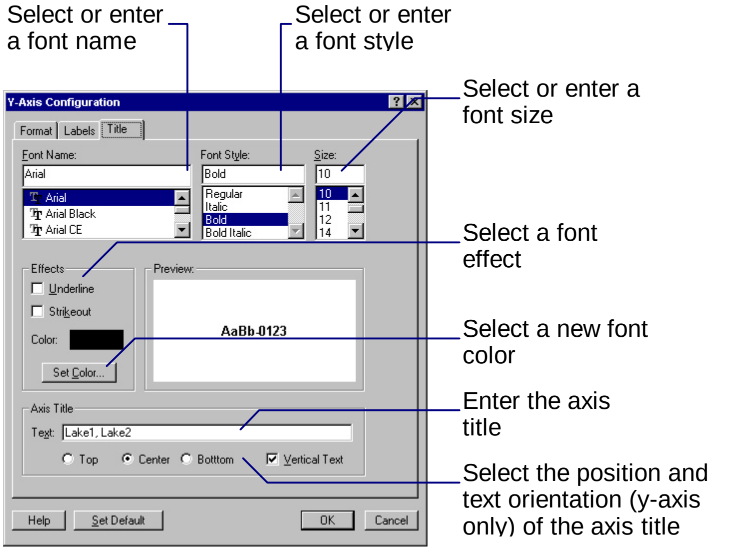
Preview: AaBb-0123

Numeric Format: ○ General ○ Scientific ● Fixed Point

Places: 1

Use the Title tab to define the font, text, position and orientation of the axis title.

The Graph Axis Configuration dialog Title tab



Select or enter a font name

Select or enter a font style

Select or enter a font size

Select a font effect

Select a new font color

Enter the axis title

Select the position and text orientation (y-axis only) of the axis title

Y-Axis Configuration

Font Name: Arial

Font Style: Bold

Size: 10

□ Underline

□ Strikeout

Color: ■

Preview: AaBb-0123

Axis Title

Text: Lake1, Lake2

○ Top ● Center ○ Botttom ☑ Vertical Text

Axis scaling during a model run

As a model is run, the values of model components displayed on a graph may exceed the bounds of the current graph scale. You can configure the axis to expand its scale during the model run by selecting the *Minimum* and *Maximum* fields in the Format tab of the Graph Axis Configuration dialog box. If these options are selected, the axis will adjust during the model run (if necessary), and at the end of the run in order to display the best presentation of the data.

Customizing the title, legend, background and frame

The following graph attributes can be changed:

1. Title text, position, color and font.

2. Legend position, color and font.

3. Graph background color and frame properties.

To customize the title and legend:

- Click the Attributes icon, or:

- Select View | Attributes

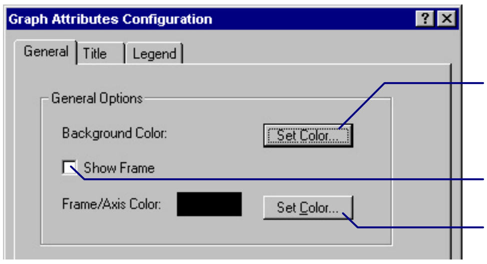
The Graph Attributes dialog box opens.

- Define the new title, legend, frame and background characteristics

- Click *OK*

The Graph Attributes dialog box is divided into three tabs – General, Title and Legend.

The Graph Attributes dialog General tab



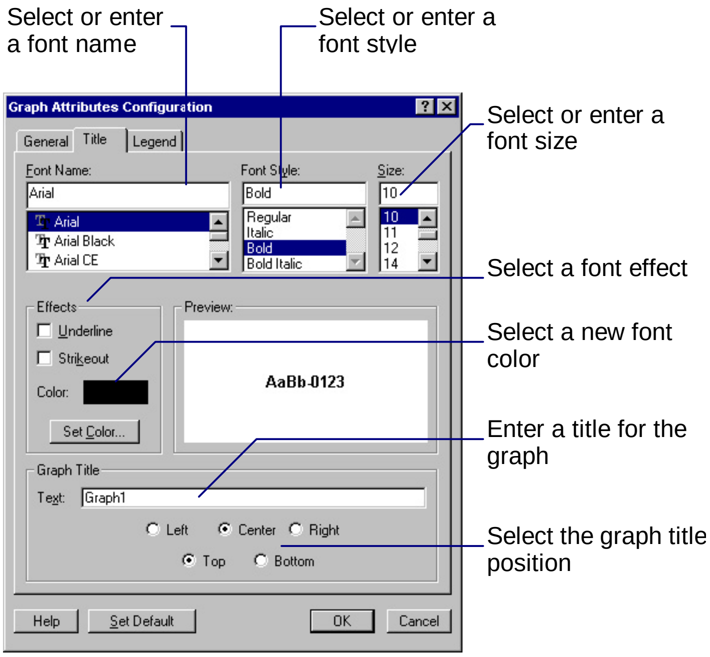
Select a graph background color

Check to add a frame

Select frame color

Use the General tab to change the background color and frame properties of the graph.

The Graph Attributes dialog Title tab



Select or enter a font name

Select or enter a font style

Select or enter a font size

Select a font effect

Select a new font color

Enter a title for the graph

Select the graph title position

Graph Attributes Configuration

Font Name: Arial

Font Style: Bold

Size: 10

Color: ■

Preview: AaBb 0123

Graph Title

Text: Graph1

○ Left ● Center ○ Right

● Top ○ Bottom

Use the Title tab to define the graph title characteristics.

The Graph Attributes dialog Legend tab is similar to the Title tab but is used to configure the legend characteristics.

Note that the graph dialog boxes can also be accessed from the RMB, or by double clicking with the LMB on appropriate areas of the graph. For example, double click the graph title to open the Graph Attributes Configuration dialog box.

Graph cross-hairs

To allow values to be read quickly and easily, cross-hairs can be displayed on the graph:

- Press and hold down the LMB in the graph until the cross-hairs appear

The *x* and *y* values at the current mouse position are shown on the message bar. The accuracy of the values shown depends on the size of the graph window. Thus, the greatest accuracy is achieved with a maximized graph window.

Archiving graphs

You may want to store several sets of results in order to investigate changes to your model. You can do this by archiving results:

- Select the Results view in the Model Explorer
- Select RMB | Archive...

All views in the current Results view are archived to a new view called Archive1. The current Definition view is also copied to the archived view. Additional results sets will be archived as Archive2, Archive3 etc. The archived results will not be updated as you make changes to your model.

Saving a graph as a text file

To save the values from the active graph as a tab-separated text file:

- Select View | Save View as Text...

The Save View As Text dialog box opens with the default file specification of the model name and the extension '.txt'.

- Enter a file name in the *File name:* edit box
- Click *OK*

The graph is saved in a tab-separated format with the selected file name.

Copying a graph

To copy the active graph to the Windows clipboard:

- Select Edit | Copy or click the Copy icon

The graph is copied to the Windows clipboard as tab-separated text, a Windows metafile or a bitmap image and can be used by other Windows applications.

Renaming graph sub-views

To rename a graph sub-view:

- Select the graph in the Model Explorer
- Select RMB|Rename View...

The View Name dialog box opens.

- Enter a name in the *View Name* edit box and click *OK*

13. Tables

Tables provide access to the values calculated by ModelMaker during a model run. Tables, like graphs (see *Chapter 12*), can be archived and restored at a later date so that the effects of changes to the model can be examined. The values of Compartments, Variables, Flows, Defined values, Delays and the independent variable can be shown on tables. Tables are stored under the Results view as Table1, Table2 etc.

Creating tables

To create a table:

- Click the Table icon, or:
- Select View | Table

The Table Selection dialog box opens. Use this dialog to specify which components are to be presented in your table.

- Select components in the *Components* list box

These components will be tabulated.

- Click '>>' to move the selected components into the *Selected* list box

Double clicking components also moves them from one list box to the other.

- Click *OK*

Repeat the steps described above to add further tables to the Results view.

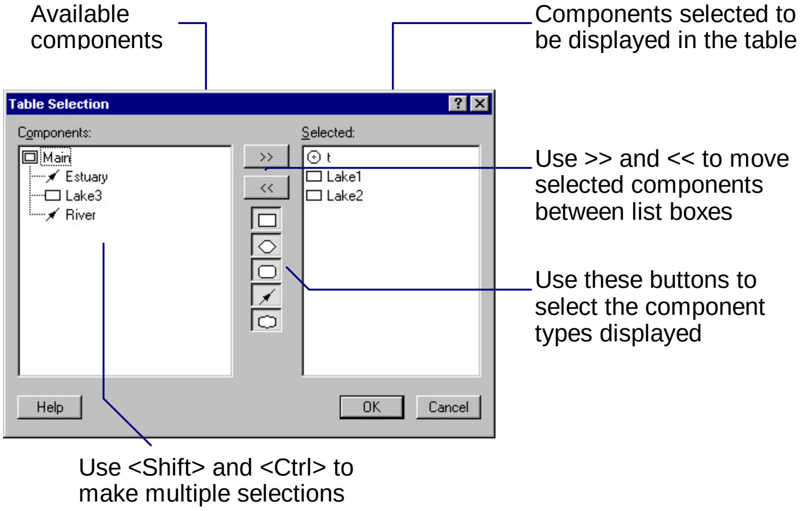
Changing the table selection

Your component selection can be changed at any time by re-opening the Table Selection dialog box:

- Click the Selection icon on the Table toolbar, or:
- Select View | Selection

Use '>>' and '<<' to change your component selection.

The Table Selection dialog box



Available components

Components selected to be displayed in the table

Use >> and << to move selected components between list boxes

Use these buttons to select the component types displayed

Use <Shift> and <Ctrl> to make multiple selections

Customizing tables

The table series, title and numerical format can all be customized in order to present tabulated values in the most effective way.

Customizing the table series

When a model component is selected for a table, a tables series is created to display the values associated with the component. The display of each of these sets of values is controlled using the Table Series dialog box. To define the options for a table series:

- Click the Series icon, or:
- Select View | Series

The Table Series dialog box opens.

- Select a table series in the *Series* list box and define its title and numerical format etc.
- Click *Define*

The options for the series are saved. Use the Up and Down buttons to change the table series selection. Click OK to save the series options and dismiss the dialog.

The Table Series dialog box

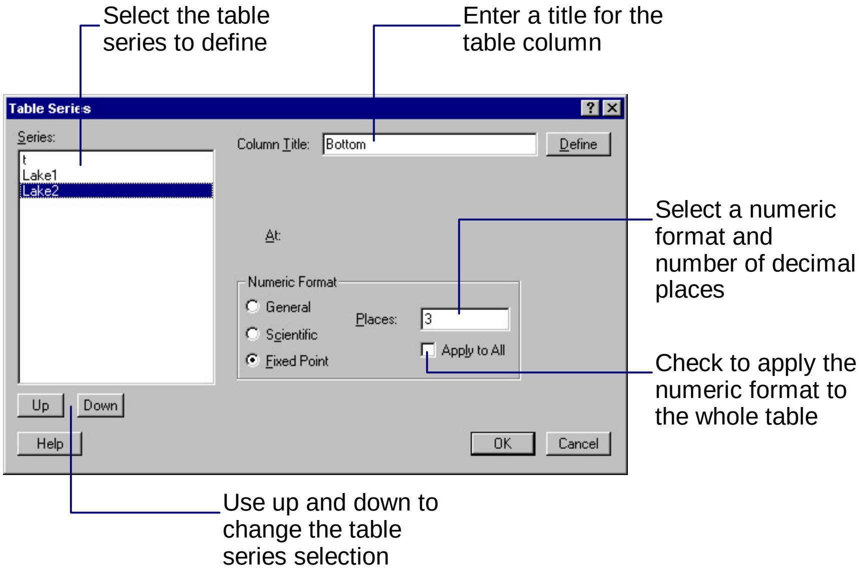


Table Series

Series:
t
Lake1
Lake2

Column Title: Bottom

At:

Numeric Format
○ General
○ Scientific
● Fixed Point

Places: 3

□ Apply to All

Select the table series to define

Enter a title for the table column

Select a numeric format and number of decimal places

Check to apply the numeric format to the whole table

Use up and down to change the table series selection

Note the table selection and series dialog boxes can also be accessed from the RMB, or by double clicking with the LMB on appropriate areas of the table. For example, click the table header to open the Table Series dialog box.

Archiving tables

You may want to store several sets of results in order to investigate changes to your model. You can do this by archiving sets of results:

- Select the Results view in the Model Explorer
- Select RMB | Archive...

All views in the current Results view are archived to a new view called Archive1. The current Definition view is also copied to the archived view. Additional results sets will be archived as Archive2, Archive3 etc. The archived results will not be updated as you make changes to your model.

Saving a table as a text file

To save the values from the active table as a tab-separated text file:

- Select View | Save View as Text

The Save View As Text dialog box opens with the default file specification of the model name and the extension '.txt'

- Enter a file name in the *File name:* edit box
- Click *OK*

The table is saved in a tab-separated format with the selected file name.

Copying a table

To copy a selection of the active table to the Windows clipboard:

- Select the cells of the table which are to be copied
- Select Edit | Copy or click the Copy icon

The data are copied to the Windows clipboard as tab-separated text values which can be used by other Windows applications.

Renaming table sub-views

To rename a table sub-view:

- Select the table in the Model Explorer
- Select RMB | Rename View...

The View Name dialog box opens.

- Enter a new name in the *View Name* edit box

14. Optimization

Calculated values produced by running a model can be compared with experimental data using the optimization feature. During optimization, selected model parameters are systematically adjusted to find the best agreement between the model and the experimental data.

In ModelMaker, simple analytical methods such as linear regression are not generally applicable. Therefore, iterative numerical methods of optimization are used (Marquardt and Simplex). These are very powerful methods of optimization but can be very time consuming. They may not always find the 'perfect' parameter values and may, in certain circumstances, simply not work.

In ModelMaker, input experimental data are called model data and are configured in the Model Data view.

Using the Model Data view

Creating the Model Data view

To create the Model Data view:

- Select View | Model Data

If the Model Data view already exists, it becomes the active view. The view is created with an empty page called Page 1; further pages of data are added as Page 2, Page 3 etc.

Enter your data into the table or select File | Import File to import a text file into the active table. The Import File dialog box will open. Press Format to select the file format options.

Adding pages

To add a new page to the Model Data view:

- Select View | Add Page

Copying pages

To copy the currently active data page:

- Select View | Copy Page

Changing pages

To change the name of the currently active data page:

- Select View | Change Page

Deleting pages

To remove the currently active page of data from the model data table:

- Select View | Delete Page

Inserting columns and rows

Use the Model Data toolbar icons to insert or delete rows and columns. Use the options under the View menu to insert or delete cells.

Configuring the data series

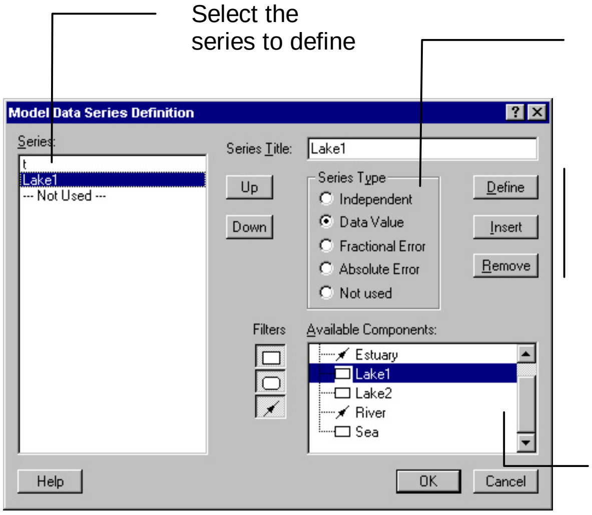
Model data series are configured in the Model Data Series Definition dialog box. To open the Model Data Series Definition dialog box:

- Click the Series icon, or:

- Select View | Series

Select the series to define

Select the series type



The Model Data Series Definition dialog box

Model Data Series Definition

Series:
t
Lake1
--- Not Used ---

Series Title: Lake1

Series Type
○ Independent
● Data Value
○ Fractional Error
○ Absolute Error
○ Not used

Available Components:
Estuary
Lake1
Lake2
River
Sea

Use Define to complete the series definition, Insert to add a new series and Remove to delete a series

Select the series model component

In the Model Data view, one column must represent the independent variable; this is assumed to be the first column. The other columns can be one of four types:

1. Data values associated with a particular model component.

2. Fractional error values associated with a particular data value column.

3. Absolute error values associated with a particular data value column.

4. Not used.

The fractional and absolute errors are used to weight the contribution of the data values during optimization. To use these configured errors, select *Use values from table* in the Weighting tab of the Optimization Settings dialog box (*see below*).

If error values do not exist, default values are configured.

To configure a data series:

- Select the series to be defined
- Select a series type
- Select a component in the *Available Components* list box

The series will represent this component.

- Click *Define*

Configuring optimization

Configuring the Parameter view

- Activate the Parameter view

Select which parameters will be optimized:

- Select the appropriate boxes in the *Optimize* field

Configuring the Model Data view

- Activate the main Model Data view

Assign the Model Data pages to be used in the optimization:

- Select the appropriate boxes in the *Include in optimize* field

Running optimization

- Click the Integrate icon arrow and select *Optimize* from the drop-down menu

The Optimization Run dialog box opens.

- Click *OK*

Your model is optimized with the default settings.

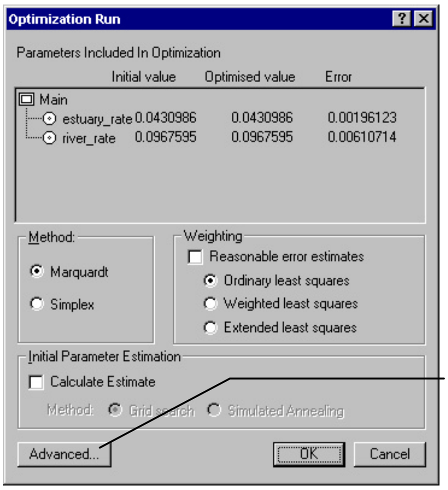
During optimization, ModelMaker compiles the model and collates the selected model data pages. The optimization status is displayed on the message bar, showing the percentage of the independent variable range covered, the time elapsed, the number of convergent steps and the best value calculated. Optimization runs until either the convergence criteria are met or an error is encountered.

Pressing <Esc> will cancel the optimization process.

Optimization settings

Use the Optimization Run dialog to confirm the optimization method and start optimization. The panel at the top of the dialog lists the parameters to be adjusted, their initial values, their optimized values and any error values (Marquardt only).

The Optimization Run dialog box



Optimization Run

Parameters Included In Optimization

	Initial value	Optimised value	Error
Main			
estuary_rate	0.0430986	0.0430986	0.00196123
river_rate	0.0967595	0.0967595	0.00610714

Method:
● Marquardt
○ Simplex

Weighting
□ Reasonable error estimates
● Ordinary least squares
○ Weighted least squares
○ Extended least squares

Initial Parameter Estimation
□ Calculate Estimate
Method: ● Grid search ○ Simulated Annealing

Click to open the Optimization Settings dialog box

Optimization method

Choose between Marquardt and Simplex methods of optimization. Marquardt is the default and recommended optimization method. Simplex is only recommended for experienced users.

Error weighting

Select Reasonable error estimates to use the error estimates indicated on the Weighting tab of the Optimization Settings dialog box. Clear this check box to choose a least squares method to calculate the scaling of the differences between the model values and the experimental data – ordinary least squares, weighted least squares or extended least squares (Marquardt only). Extended least squares is an option for situations where the errors in the data values are not known.

Parameter estimation

Select *Calculate Estimate* to enable initial parameter estimation using either Grid search or Simulated annealing. The Grid search and Simulated annealing options are configured in the Estimation tab of the Optimization Settings dialog box.

Advanced optimization settings

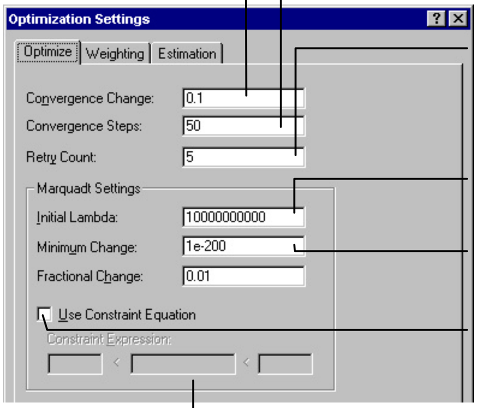
Click the Advanced button of the Optimization Run dialog box to open the Optimization Settings dialog box where more complex optimization options can be set. The Optimization Settings dialog box is divided into three tabs – Optimize, Weighting and Estimation. This dialog can also be opened from the Model menu:

- Select Model | Configure>Optimization

The Optimize tab

Use the Optimize tab to configure the general settings for optimization *i.e.* convergence criteria, parameter settings for Marquardt optimization, and a constraint equation that limits the values of parameters. (The constraint expression can include more than one parameter).

The Optimization Settings dialog Optimize tab



Convergence Change: 0.1

Convergence Steps: 50

Retry Count: 5

Marquadt Settings

Initial Lambda: 10000000000

Minimum Change: 1e-200

Fractional Change: 0.01

□ Use Constraint Equation

Constraint Expression: [ ] < [ ] < [ ]

Enter the size of the convergent step

Enter the number of convergent steps before optimization terminates

Enter the number of times the optimization will retry the last convergent steps

Enter the initial lambda value

Enter the minimum change in lambda

Check to apply an additional constraint expression

Enter a lower value, a condition and an upper value

The Weighting tab

Use the Weighting tab to configure weightings and error magnitude for error calculations. The data weighting options only apply to the reasonable error estimates and weighted least squares weighting schemes. Data weighting may be:

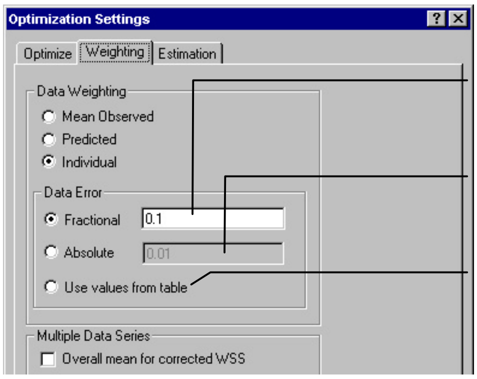
1. Mean Observed *i.e.* if you have a number of data points for one X value, the weighting can be taken as the mean of these values.

2. Predicted *i.e.* uses the predicted model values for the error weighting.

3. Individual *i.e.* use if you have individual data points with their own errors. Choose the magnitude from the Data Error panel.

Select *Overall mean for corrected WSS* if you have several data sets and would like to use the mean of all the data sets for the corrected weighted sum of squares instead of the sum of the individual means.

The Optimization Settings dialog Weighting tab



Data Weighting
○ Mean Observed
○ Predicted
● Individual

Data Error
● Fractional 0.1
○ Absolute 0.01
○ Use values from table

Multiple Data Series
□ Overall mean for corrected WSS

Set the error as a fraction of the size of the data value

Set the error as an absolute value

Use the errors configured in the Model Data view

The Estimation tab

Use the Estimation tab to configure the initial parameter estimation method and settings if *Calculate Estimate* is selected in the Optimization Run dialog. Note that parameter estimation is only available with Marquardt optimization.

The aim of optimization is to find the parameter set that corresponds to the global minimum deviation between the experimental and calculated data. For many problems however, multiple local minima may exist. These can cause problems for the Marquardt and Simplex algorithms (if you do not have a good initial parameter value) because they cannot distinguish a local minimum from a global minimum.

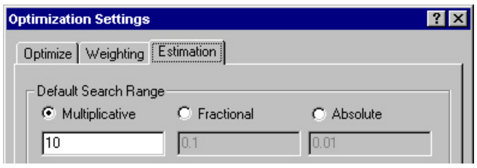
Simulated annealing and grid search are methods of parameter estimation and can be used when the initial parameter value is poor.

The Estimation tab is split into three panels – default search range, simulated annealing and grid search.

Default search range

Default search range sets the parameter estimation range (for simulated annealing and grid search) in relation to its value. For example, 10 sets the multiplicative range to 0.1*value<value<10*value, 0.1 sets the fractional range to value*(1±0.1), and 0.01 sets the absolute range to value±0.01.

The Optimization Settings dialog Estimation tab Search Range panel



Optimization Settings

Optimize | Weighting | Estimation

Default Search Range

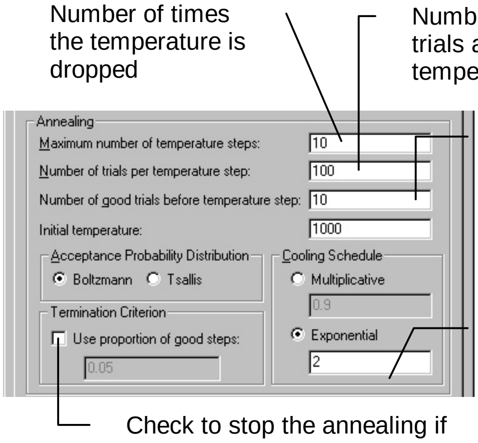
● Multiplicative ○ Fractional ○ Absolute

10 | 0.1 | 0.01

Simulated annealing

Simulated annealing is a standard way of optimizing models where several local minima exist in order to find the global minimum. See the *ModelMaker Reference Manual* for further information.

The Optimization Settings dialog Estimation tab Annealing panel



Annealing

Maximum number of temperature steps: 10

Number of trials per temperature step: 100

Number of good trials before temperature step: 10

Initial temperature: 1000

Acceptance Probability Distribution: ● Boltzmann ○ Tsallis

Termination Criterion: ☐ Use proportion of good steps: 0.05

Cooling Schedule: ○ Multiplicative 0.9 ● Exponential 2

Number of times the temperature is dropped

Number of trials at each temperature

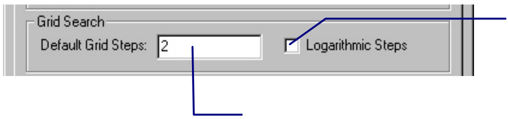
Number of trials accepted before the temperature is dropped. Trials are accepted or rejected by comparison to a Boltzmann or Tsallis distribution

Select whether the temperature is dropped by multiplicative or exponential cooling

Check to stop the annealing if the proportion of good trials falls below a specified level

Grid search

The Optimization Settings dialog Estimation tab Grid Search panel



Default Grid Steps: 2

□ Logarithmic Steps

Sets the grid step sizes to be taken in logarithmic sizes

Sets the size of the grid steps when using Grid search during parameter estimation

Optimization results

The Parameter Results view

The parameter results from the optimization are displayed under the Results view as a sub-view called Parameter Results. Parameter Results provides a tree view of a model's structure, with each branch representing a sub-model. Branches can be expanded and collapsed by double clicking the plus and minus icons. The optimized parameter values are presented in fields called Optimize result and Optimize error.

Update the model parameters

To update your model parameters with the optimization results:

- Activate the Parameter Results view
- Select the parameter to be updated
- Select RMB | Update parameter

The Optimization Statistics view

The optimization statistics are displayed under the Results view as a sub-view called Optimization Statistics. Select the Optimization Statistics view in the Model Explorer to display a summary of the optimization statistics. The statistics presented in the summary are:

1. Degrees of freedom (DF).
2. Weighted sum of squares (WSS) *i.e.* the variation attributed to each component.
3. Mean square (MS) *i.e.* the variation per degree of freedom where MS = WSS / DF.
4. Total uncorrected sum of squares.

5. r^2 value *i.e.* r^2 = Model WSS / Total WSS.

6. *F*-value *i.e.* the variance ratio, where *F* = Model MS / Residual MS.

7. *P*-value *i.e.* probability that the model explained the variation by chance (Marquardt only).

8. *Q*-value *i.e.* probability that the differences between the model and data have occurred by chance (Marquardt only).

The optimized values of the parameters σ and ζ are also reported during extended least squares calculation. These values are calculated for each configured data series. See the *ModelMaker Reference Manual* for more information on extended least squares and other statistical background.

Archiving results

Optimization results can be archived together with graphs and tables:

- Select the Results view in the Model Explorer
- Select RMB | Archive...

15. Minimization

During minimization, the parameter values used in the model are adjusted to find the smallest value of a particular component at a selected point in the model run. ModelMaker uses the *downhill simplex* method of minimization.

The Sample Points view is used to create sample points for both minimization runs and Monte Carlo analysis. A sample point is a result of the simulation, *i.e.* the value of a component at a particular moment in time. The model will be run up to this time point and no further in order to obtain the value of the component with the minimum computational effort.

Using the Sample Points view

Creating the Sample Points view

To create the Sample Points view:

- Click the Sample Points icon, or:
- Select View | Sample Points

If the Sample Points view already exists, it becomes the active view. The Sample Points view is divided into five fields – Name, Component, Time Point, Monte Carlo and Minimize.

Adding sample points

To add a sample point:

- Click the Sample Point icon

A sample point called SP1 will be added to the view; further sample points can be added as SP2, SP3 etc.

Defining sample points

Sample points are defined in the Sample Point Definition dialog box:

- Double click with the LMB on the sample point to be defined

The Sample Point Definition dialog box opens.

- Enter values in the *Time Point* and *Name* edit boxes
- Select a component in the *Component* list box

- Click *OK*

In the Sample Points view:

- Select the *Monte Carlo* check box and / or the *Minimize* option button

Configuring minimization

Configuring the Parameter view

- Activate the Parameter view

Select the parameters to be adjusted:

- Select the appropriate boxes in the *Minimize* field

There is no limit to the number of parameters which ModelMaker can adjust during minimization, but the more that are selected the longer the process takes.

Configuring the Sample Points view

- Activate the Sample Points view
- Configure a sample point for minimization
- Select the *Minimize* option button for the configured sample point

Only one Minimize option button can be selected.

Running minimization

Once parameters and sample points have been configured correctly, minimization is enabled.

- Click the Integrate icon arrow and select *Minimize* from the drop-down menu

The Start Minimization dialog box opens.

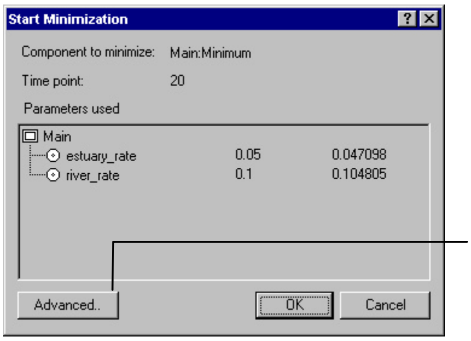
- Click *OK*

The minimization is run with the default settings.

During minimization, ModelMaker compiles the model and displays the minimization status on the message bar, showing the percentage of the independent variable range covered, the time elapsed, the number of convergent steps and the best value calculated for the minimization component. Minimization runs until either the convergence criteria are met or an error is encountered.

Pressing <Esc> will cancel the minimization process.

The Start Minimization dialog box



Start Minimization

Component to minimize: Main:Minimum

Time point: 20

Parameters used

Main		
estuary_rate	0.05	0.047098
river_rate	0.1	0.104805

Click to open the Minimization Configuration dialog box

The Parameter Results view

The parameter results from the minimization are displayed under the Results view as a sub-view called Parameter Results. Parameter Results provides a tree view of a model's structure, with each branch representing a sub-model. Branches can be expanded and collapsed by double clicking the plus and minus icons. The new parameters are displayed in a field called Minimize result.

Update the model parameters

To update your model parameters with the minimization results:

- Activate the Parameter Results view
- Select the parameter to be updated
- Select RMB | Update parameter

Archiving results

Minimization results can be archived together with graphs and tables:

- Select the Results view in the Model Explorer
- Select RMB | Archive...

Advanced minimization configuration

Clicking the Advanced button of the Start Minimization dialog box opens the Minimization Configuration dialog box. This dialog can also be accessed from the Model menu:

- Select Model|Configure>Minimization

Constraint range

The constraint range provides a way to control the range of parameter values used during the optimization process. The constraint range selected is used as the default range for all the parameters selected for the minimization process. Alternatively, parameters can be assigned their own constraint range which overrides the default (See *Chapter 10: Parameters*).

Convergence change

This is the fractional change in the value of the model component being minimized which is considered to be convergent.

Fractional change

This is the fractional change in the parameters which is used to calculate the vertices for the simplex method. For example, if a parameter has a value of 10.0 and the fractional change is 1.0E-3, the model is run with the parameter set to 10.0 + 10.0 × 1.0E-3 = 10.01 in order to calculate the vertex of the simplex.

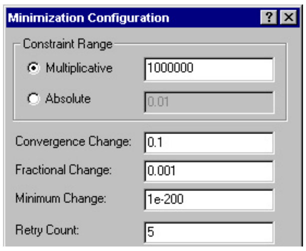
Minimum change

This is the minimum absolute change in the value of a parameter which is allowed when calculating the vertices for the simplex method. For example, if a parameter has a value of 0.1, the fractional change is 1.0E-3 and the minimum change is 1.0E-2 then the model is run with the parameter set to 0.1 + 1.0E-2 = 0.11 because the fractional change in the parameter is less than the minimum change.

Retry Count

Retry count is the number of times minimization retries a calculation if a parameter violates its constraint range. The parameter is set to the nearest extent of its constraint range and the simplex step is repeated.

The Minimization Configuration dialog box



Minimization Configuration

Constraint Range

● Multiplicative 1000000

○ Absolute 0.01

Convergence Change: 0.1

Fractional Change: 0.001

Minimum Change: 1e-200

Retry Count: 5

16. Monte Carlo Analysis

Monte Carlo analysis enables model parameters to be specified as random distributions. A model is run for a specified number of times, and during each run the value of the parameter is taken from a specified probability distribution. In this way, the effect of varying parameters on a component value can be investigated.

Monte Carlo output is plotted as a histogram, giving a distribution of a particular model value that is produced by the variation of the model parameters.

To perform Monte Carlo analysis on a simulation, one or more sample points must be specified. A sample point is a result of the simulation, *i.e.* the value of a component at a particular moment in time. Sample points for Monte Carlo analysis and minimization runs are created in the Sample Points view. See *Chapter 15: Minimization* for more information about using the Sample Points view.

Configuring Monte Carlo analysis

Configuring the Parameter view

- Activate the Parameter view

Choose the parameters to be varied:

- Select the appropriate check boxes in the Monte Carlo field

...

This enables the ... button in the Dist Type field

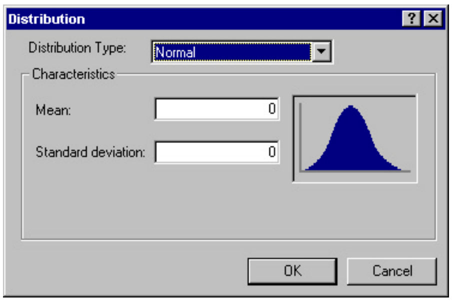
- Click the ... button

The Distribution dialog box opens. Use this dialog to choose a random number distribution:

- Select a *Distribution Type*, enter the required *Characteristics* and click *OK*

Normal, Triangular, Uniform, Exponential, Weibull, Beta, Gamma, Logistic, Pareto, Extreme Value, Binomial, Poisson, Geometric and Log Normal distribution types are available. Each requires different characteristics which must be defined to suit your parameter distribution.

The Distribution dialog box



Distribution

Distribution Type: Normal

Characteristics

Mean: 0

Standard deviation: 0

Configuring the Sample Points view

- Activate the Sample Points view
- Configure a sample point for Monte Carlo analysis
- Select the Monte Carlo check box for the configured sample point

You may configure and select any number of sample points. Use the RMB (click the Monte Carlo header) to select all sample points, clear the selection and toggle the selection.

Running Monte Carlo

Once parameters and sample points are correctly configured, Monte Carlo analysis is enabled.

- Click the Integrate icon arrow and select Monte Carlo

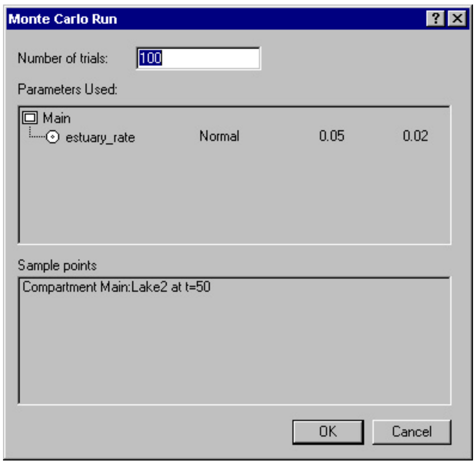
The Monte Carlo Run dialog box opens. This dialog summarizes the parameters and sample points that have been selected for Monte Carlo analysis. Use this dialog to specify the number of trial runs.

- Enter a value in the *Number of trials* edit box
- Click *OK*

During Monte Carlo analysis, ModelMaker compiles the model and displays the analysis status on the message bar, showing the time elapsed and the current run number.

Pressing <Esc> will cancel the analysis.

The Monte Carlo Run dialog box



Number of trials: 100

Parameters Used:

Main			
estuary_rate	Normal	0.05	0.02

Sample points

Compartment Main:Lake2 at t=50

Creating histograms

The results of the Monte Carlo analysis can be viewed in the form of a histogram. To create a histogram:

- Click the Histogram icon, or:
- Select View | Histogram

The Histogram Selection dialog box opens.

- Select sample points to plot in the *Sample Points* list box
- Click '>>' to move the selected components into the *Selected* list box
- Enter a value in the *Number of bins* edit box
- Click *OK*

Histograms are stored under the Results view as Histo1, Histo2 etc.

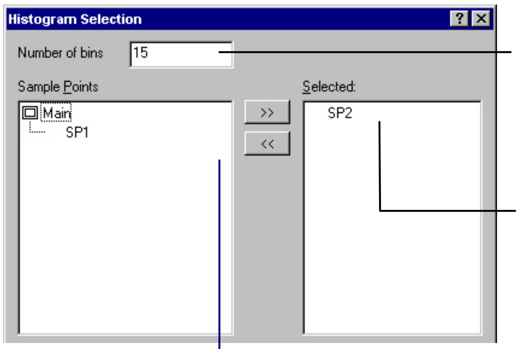
Repeat the steps described above to add additional histograms to the Results view.

Changing the histogram selection

Your sample point selection can be changed at any time by re-opening the Histogram Selection dialog box:

- Click the Selection icon on the Graph toolbar

The Histogram Selection dialog box



Number of columns into which the data are divided

Sample points selected to plot on the histogram

Available sample points

Customizing histograms

Like graphs, the histogram series, title, axes and legend can be customized in order to present the graph in the most effective way. See *Chapter 12: Graphs* for more information about histogram customization.

Archiving histograms

As histograms are stored under the Results view, they can be archived. See *Chapter 12: Graphs* for more information about archiving results.

Saving a histogram as a text file

Histogram data, like other graphs and tables, can be saved as a tab-separated text file. See *Chapter 12: Graphs* for more information about saving data as a text file.

Monte Carlo statistics

The Monte Carlo statistics for each series can be viewed from the Graph Series Options dialog box:

- Click the Series icon

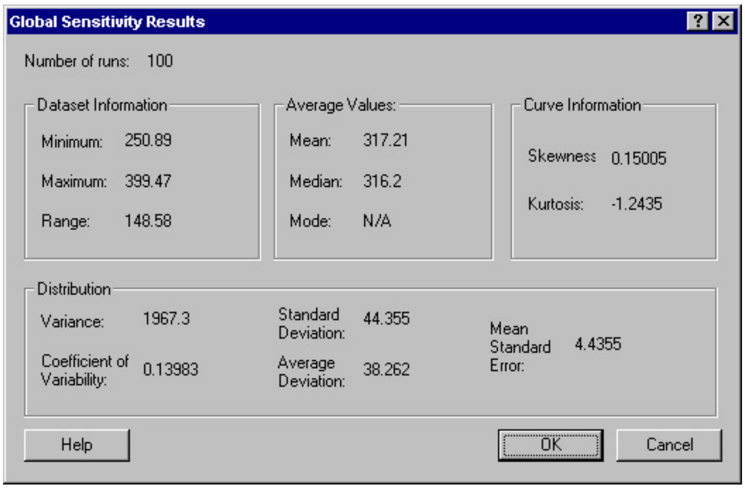
The Graph Series Options dialog box opens.

- Use *Up* and *Down* to select a series

- Click the *Series Statistics* button

The Global Sensitivity Results dialog box opens. This dialog summarizes the statistics for the series, giving dataset information, average values, curve information and distribution data.

The Global Sensitivity Results dialog box



Global Sensitivity Results

Number of runs: 100

Dataset Information

Minimum: 250.89

Maximum: 399.47

Range: 148.58

Average Values:

Mean: 317.21

Median: 316.2

Mode: N/A

Curve Information

Skewness 0.15005

Kurtosis: -1.2435

Distribution

Variance: 1967.3

Coefficient of Variability: 0.13983

Standard Deviation: 44.355

Average Deviation: 38.262

Mean Standard Error: 4.4355

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