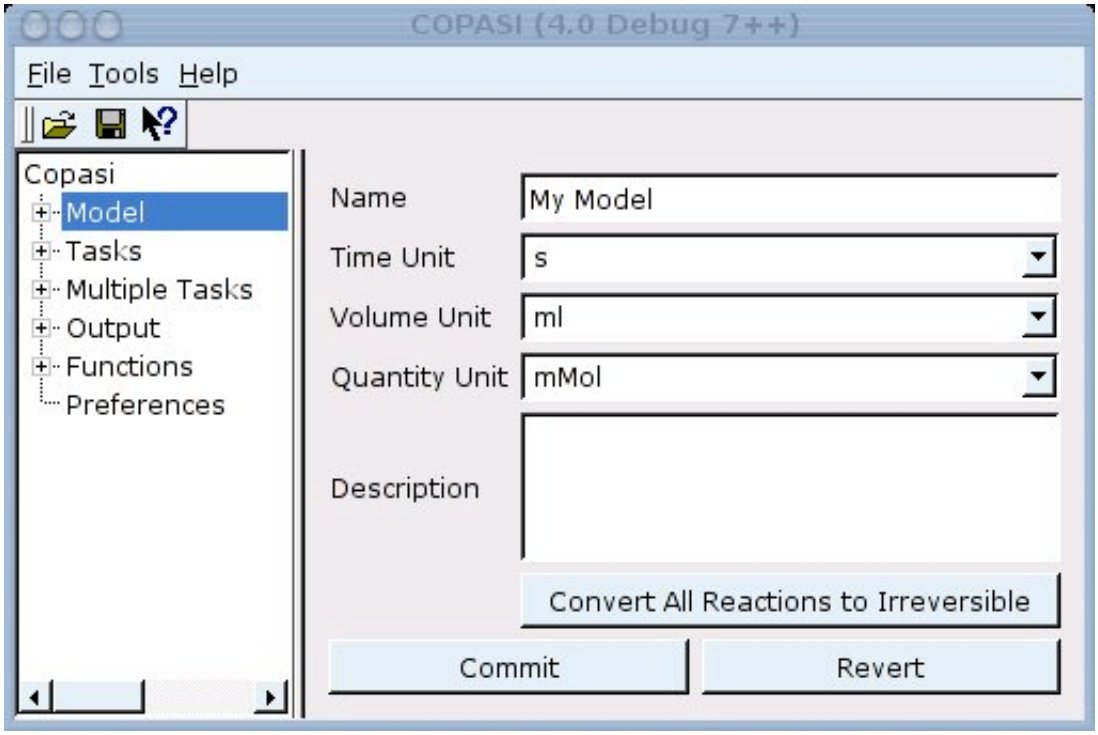
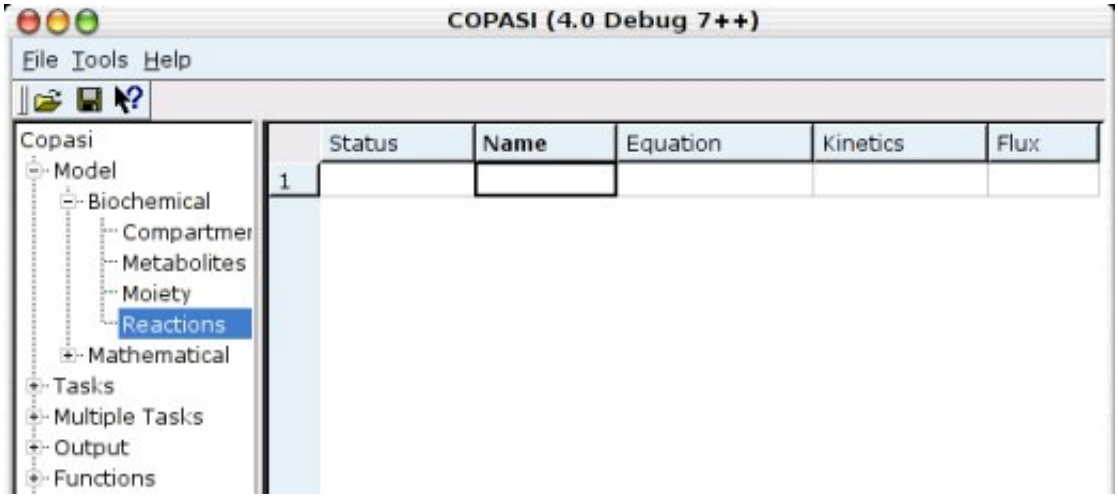
## Step 1: Model Settings

Once you start Copasi, the first dialog you will see shows a tree on the left, where you can select the individual elements of Copasi. The element that is selected per default is the tree node that corresponds to the current model. On the right side, you can see the settings for this model, which are the name of the model, the units that copasi will use in the model and a description of the model. Here you should give the model a more expressive name and maybe a short description.

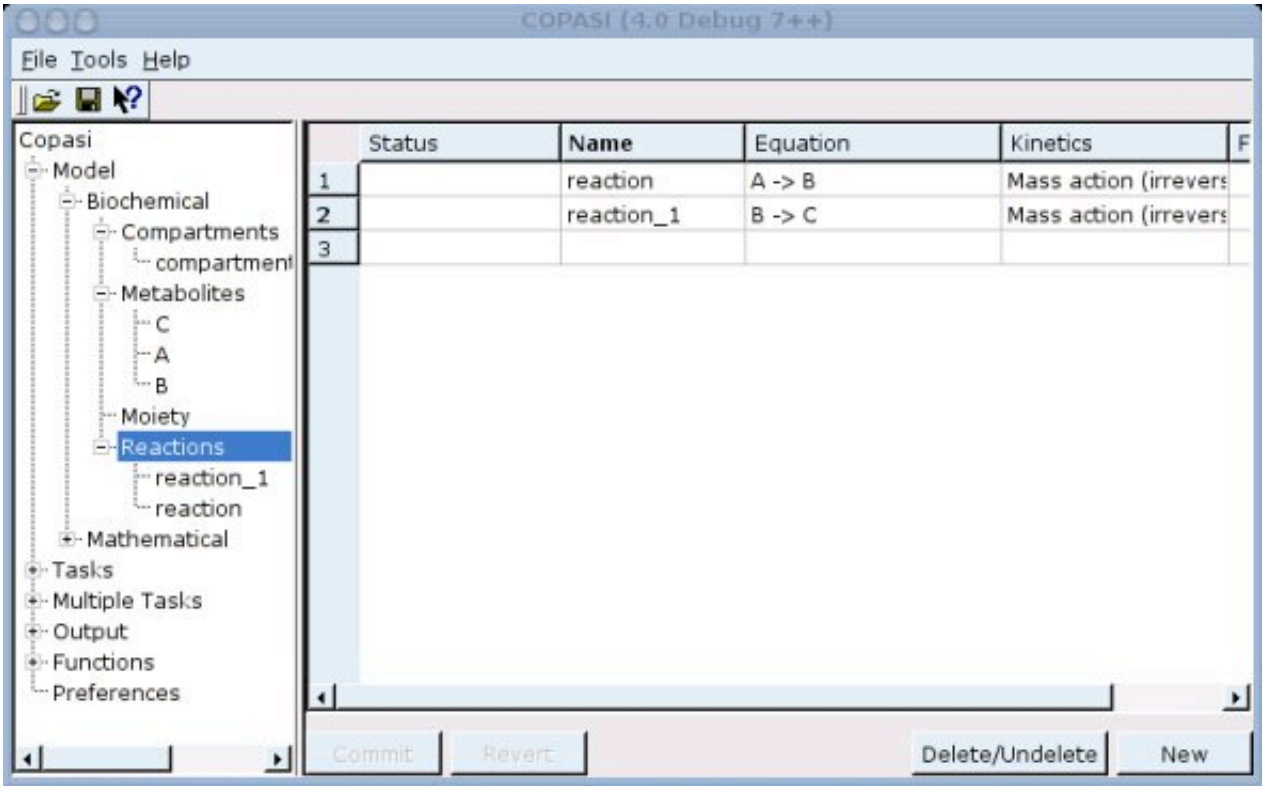



## Step 2: Reaction Input

There are several ways to define the set of reactions for the model. The fastest one is probably to type them into the reaction overview table. You find this reaction overview in the tree on the left under `Model->Biochemical->Reactions.`

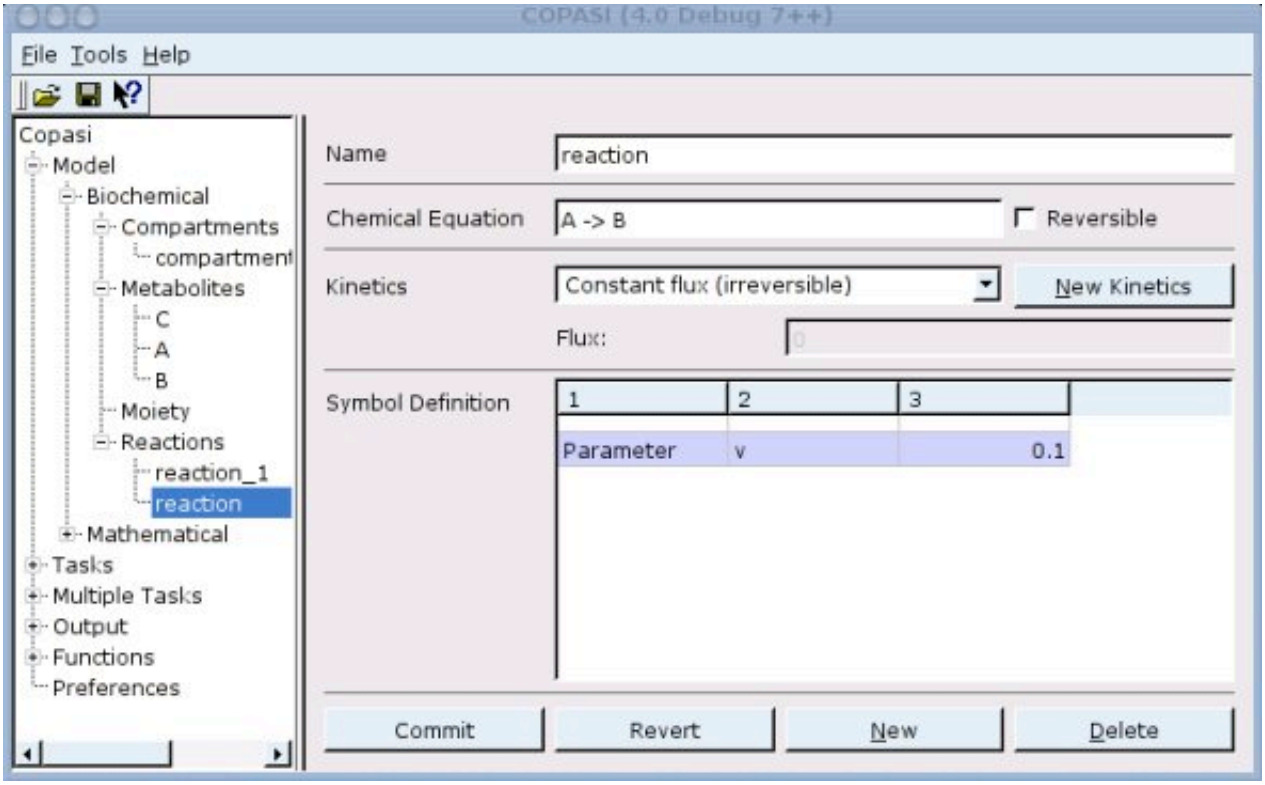



To create a new reaction just click on the empty cell in the *Equation* column and start typing. When you are finished with typing the reaction equation, hit the return key. Now you are in the next row and can type the next reaction. Once you have created all reaction, you click the **"commit"** button at the bottom of the screen, this will create all the reactions as well as the necessary metabolites and compartments. All reactions are created with an irreversible mass-action kinetic with a kinetic constant of 0.1, all metabolites have an initial concentration of 0.1 standard concentration units (the ones specified in the *Model Settings* dialog.) and the single compartment has a volume of 1 standard volume units.




## Step 3: Refining the Model

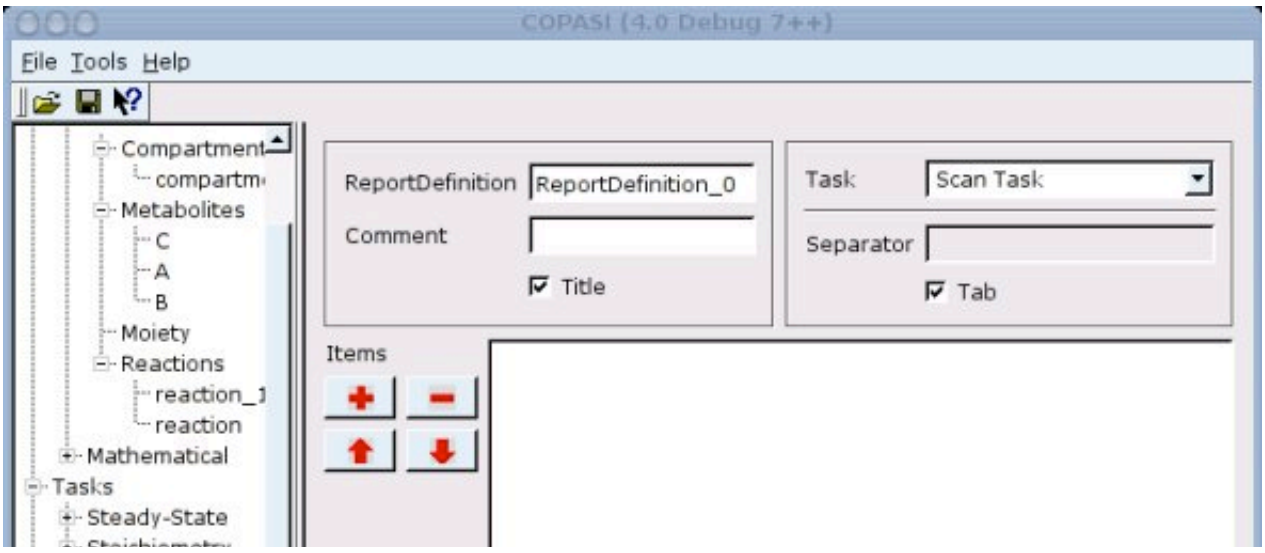
Your reaction probably don't all have a mass-action kinetic, so before you can run the actual simulation, you have to specify the correct kinetics for all the reactions. In order to do this, you navigate in the tree on the left to the reaction that you want to change. Or you can double click on the reaction in the reaction overview table. In the *Reaction Settings* dialog you can change all attributes of the reaction, especially the kinetics and the associated kinetic parameters.



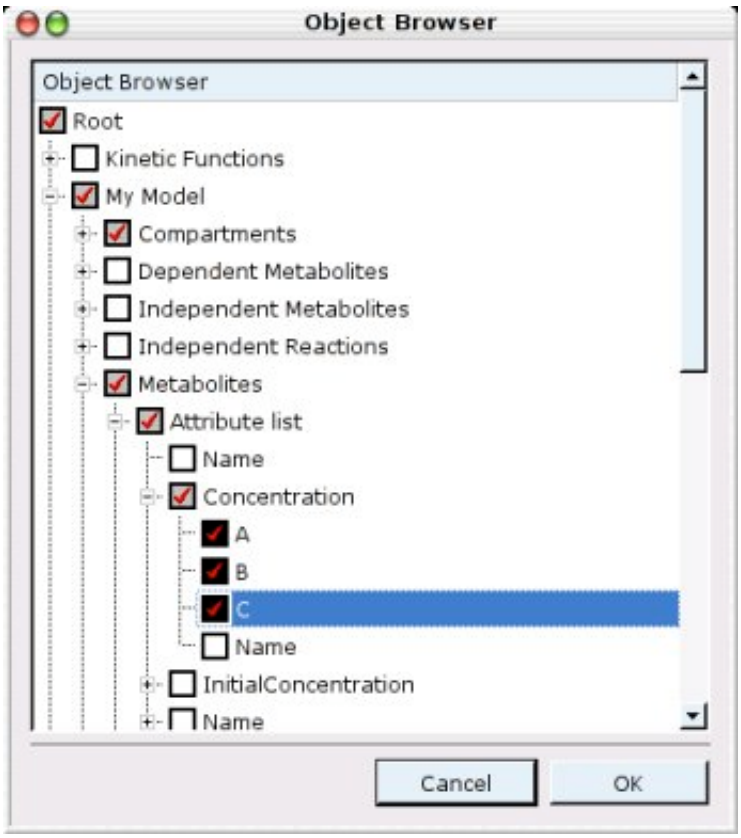

If necessary, you can do the same for the metabolites and the compartment. Just use the tree on the left to navigate to the model element you want to change and make the necessary changes in the dialog on the right.

## Step 4: Creating a Report Definition

Now that we have a model, we could actually go ahead and do a simulation. But in order for copasi to know what to do with the calculated data from the simulation, we have to define some which kind of output we want. This can either be a plot (which we will do a later) or a report. If we don't define an output , copasi will not store the results. In order to create a report definition, you navigate in the tree to `Output->Reports` and click the **`"new"`** button on the bottom and then on the **`"commit"`** button. If you now double click on the new entry in the table you will find yourself in the dialog for the report definition.

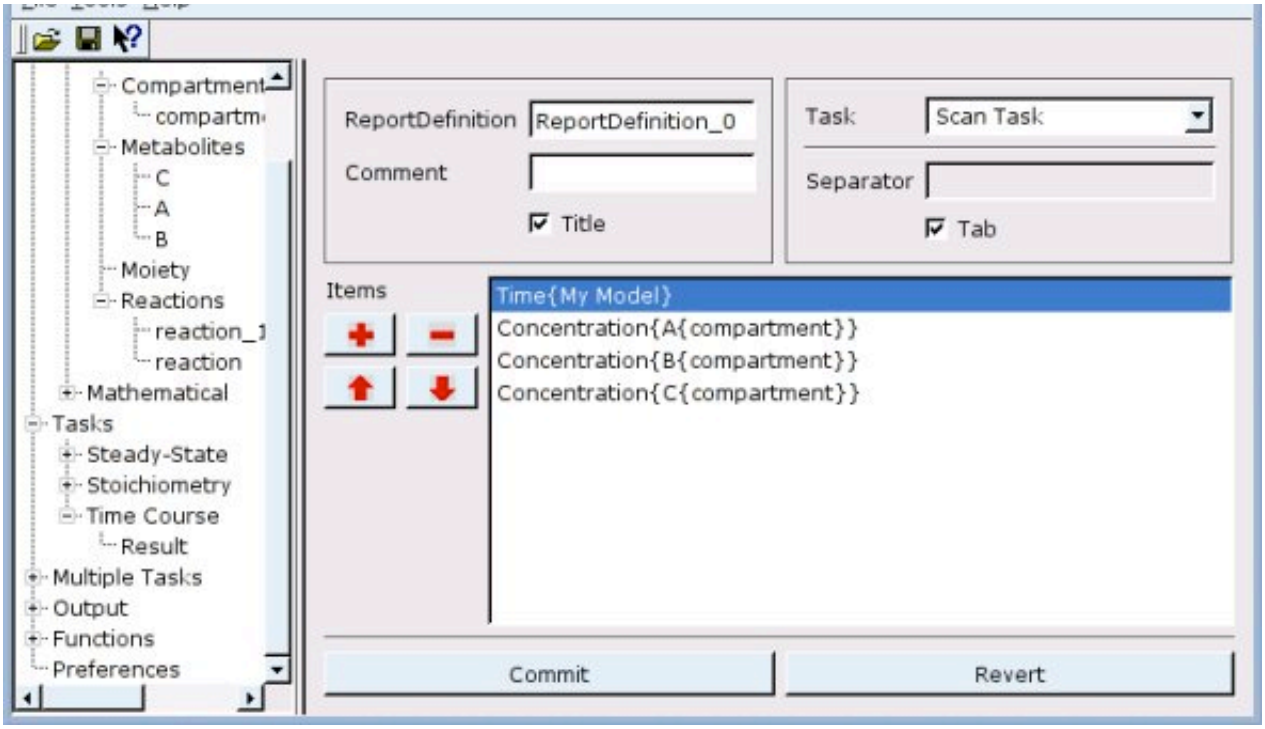



At first the list widget is empty, that means that nothing will be put into the report. In order to add items for the output, you click on the **"+"** button which is located to the right of the empty list. This will open the *Object Browser* dialog where you can select any available object. For now, we will limit ourselves to the *time* object and the concentrations of the metabolites. If you look at the tree, you will see one node that has the name of your model as specified in Step 1. Opening this node will show you all the objects available in the model. Now open the *Metabolites* node and in the metabolites subtree you open the *Attribute list* node and in there you will find the *Concentration* node. Open the *Concentration* node and click the check boxes with the names of the metabolites.




Likewise click the check box for the *time* attribute which you will find directly under the node for the model (same level as the *Metabolites* node). Once you have selected all the attributes for the output, you finish the selection by clicking the **"OK"** button.

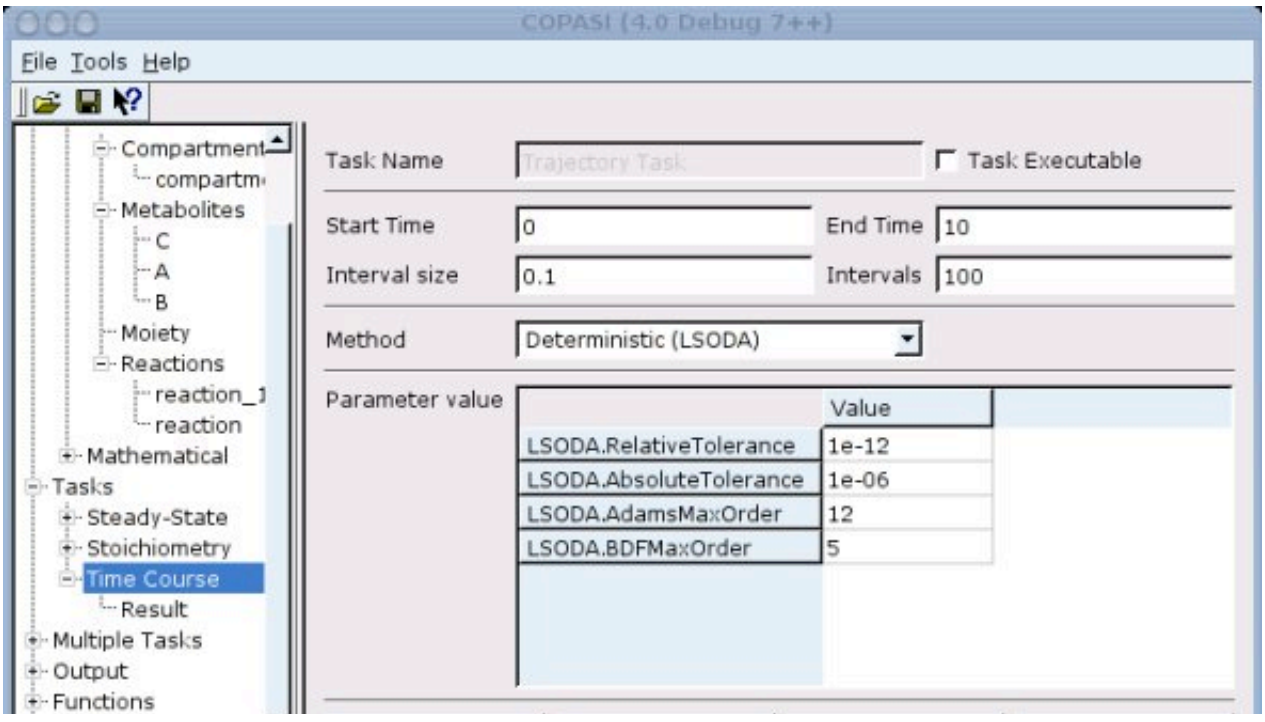
The attributes that you see in the list widget now, will be written to file in same the order as the appear in the list. If you want the time to appear in the first column of your output instead of the last, you have to change the order of the selected elements. You can change the order of the elements by selecting an item in the list and moving it up or down via the arrow buttons on the left. You can also delete an element by selecting it and then pushing the **"–"** button.




## Step 5: Calculating a Time Course

In the tree on the left under Tasks you can find the entry called *Time Course*. Selecting this entry in the tree will bring you to the time course settings dialog.

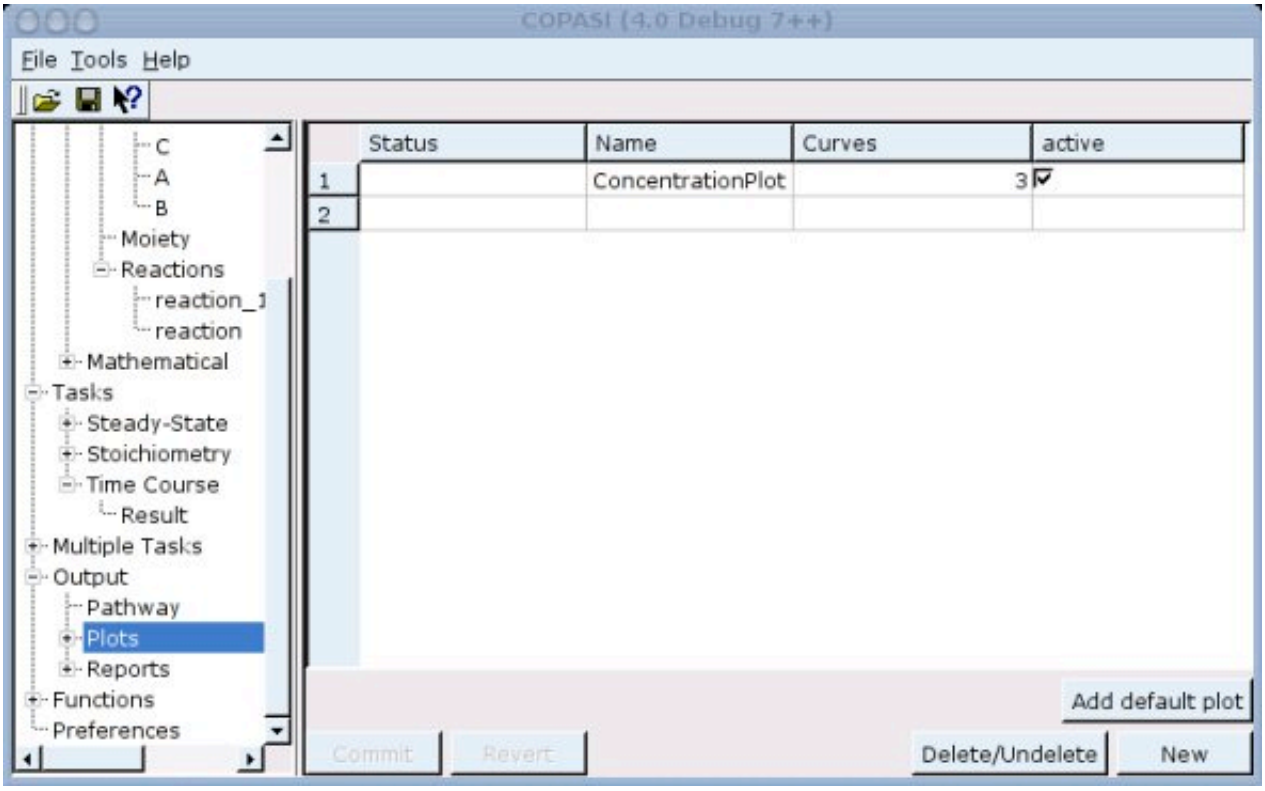
Here you can set all parameters for calculating a time course like starting time, end time, how many data points are to be stored and last but not least the method for calculating the trajectory. So far you can choose between deterministic simulation or stochastic simulation. Depending on the simulation method, you have some more parameters that can be changed in the table toward the bottom of the dialog, but the default values should suffice most of the time.



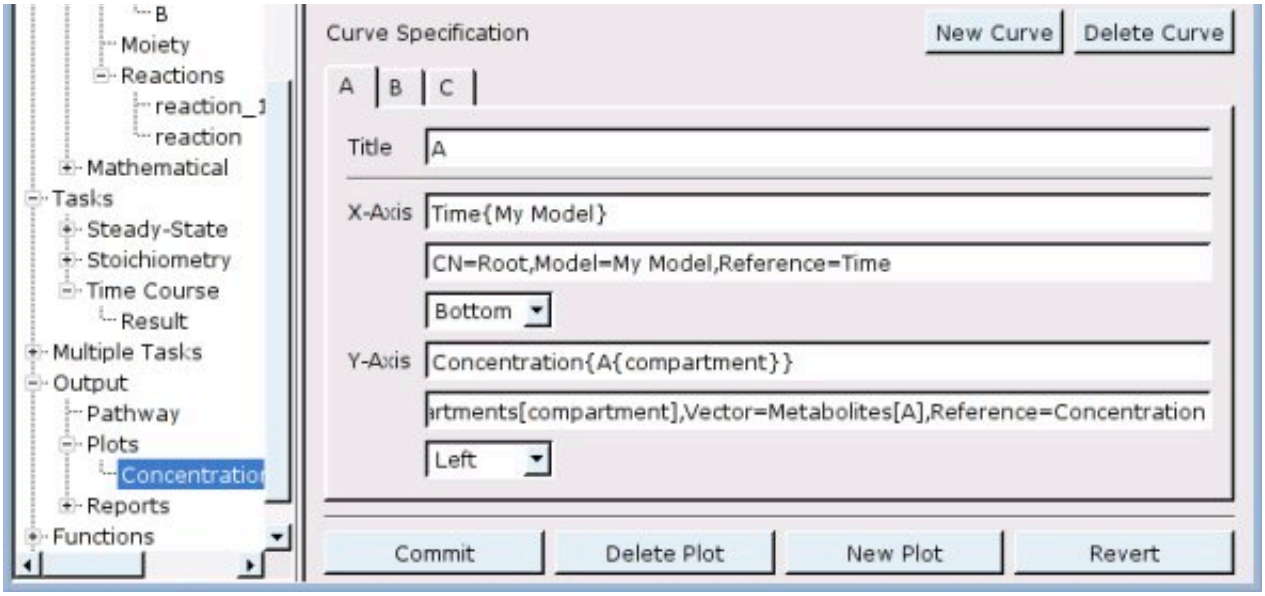

Before we can calculate the actual trajectory, we have to specify a report definition to use for the output and a filename for this report definition. To do this, you have to click on the **"ReportDefinition"** button at the bottom. In the dialog that pops up, you choose the report definition that you created in the last step and specify a file name in the *Target* field. You can either type the filename, or browse the file system by clicking the **"browse"** button. When you are finished, click the **"confirm"** button. You are now ready to calculate the time course by clicking the **"Run"** button at the bottom of the *Time Course* dialog. To verify that copasi really did calculate something, look at the file you just specified, it should now contain the data of the time course simulation.

## Step 6: Plotting

In the object tree on the left in the *Output* node, you can find the entry called *Plots*. Selecting this will bring you to the plot definition overview which will probably be empty.




If you click on the **"Add default plot"** button at the bottom, a default plot that contains the concentrations of all metabolites against the time will be created. To edit this plot definition, double click on the entry.




In this dialog you can add more curves, delete curves or change the way individual curves are plotted. Once you are finished with the plot definition, you go back to the *Time Course* dialog and push the **"Run"** button again. Now you a new plot window like the one below, with the concentrations of all metabolites on the y axis plotted against the time on the x axis, should pop up.