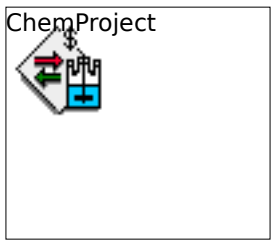
ChemProject

A Synthesis Calculation & Analysis Program



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Introduction to ChemProject

What it is

ChemProject is a program for the evaluation of a chemical synthesis in terms of material amounts and their costs, featuring a highly intuitive graphical interface. A synthesis can consist of a main branch and up to 15 connected branches. Data are analyzed for process efficiency according to a wide selection of criteria. Material prices may conveniently be imported from customizable and freely combinable price lists. A variety of detailed, carefully designed print reports is provided (the demo-version allows previews only).

System requirements

ChemProject was written using the “FoxPro for Macintosh” database program from Microsoft. However, since ChemProject was compiled as a stand alone program, you don't need “FoxPro” to run it. The database language is VERY slow on less powerful Macs. *It is therefore strongly suggested to run ChemProject on 68040 based Macs and PowerMacs*. It also runs on 68030 based Macs, but you will need a lot of patience for calculations and interface responses.

The minimum hardware requirements are:

- Mac LC III or higher (68040 processor or PowerMac recommended).
- System 7.01 or higher.
- 4.5 MB free RAM (native PPC-version: 8 MB RAM; 4 MB when virtual memory or RAM Doubler are on).
- 6 MB free hard disk space.
- 1640x480 pixel screen or larger.

Limitations

Since ChemProject has been written in a fourth generation database language, some direct programming control was not available and some compromises had to be taken in rare cases. E.g. double clicking a ChemProject file will launch the program, but not open the corresponding file. You will have to do this from within the program. Also, project files and price list files need to have DOS-like suffixes (".syn" and ".prc", respectively) to be recognized by the program.

About this manual

This manual combines both a program reference, printed in plain black font, and a tutorial, *printed in italic dark blue font* in a single continuous text. Beginners to ChemProject are guided through all relevant aspects of the program by this combination of information and tutorial. More experienced users can selectively consult the reference areas, occasionally utilizing the tutorial areas as an additional illustration. In all example pictures within this manual the highlight color is pink. This color might vary from user to user according the individual setting in the color control panel.

Part 1

VIEWING THE PROJECT

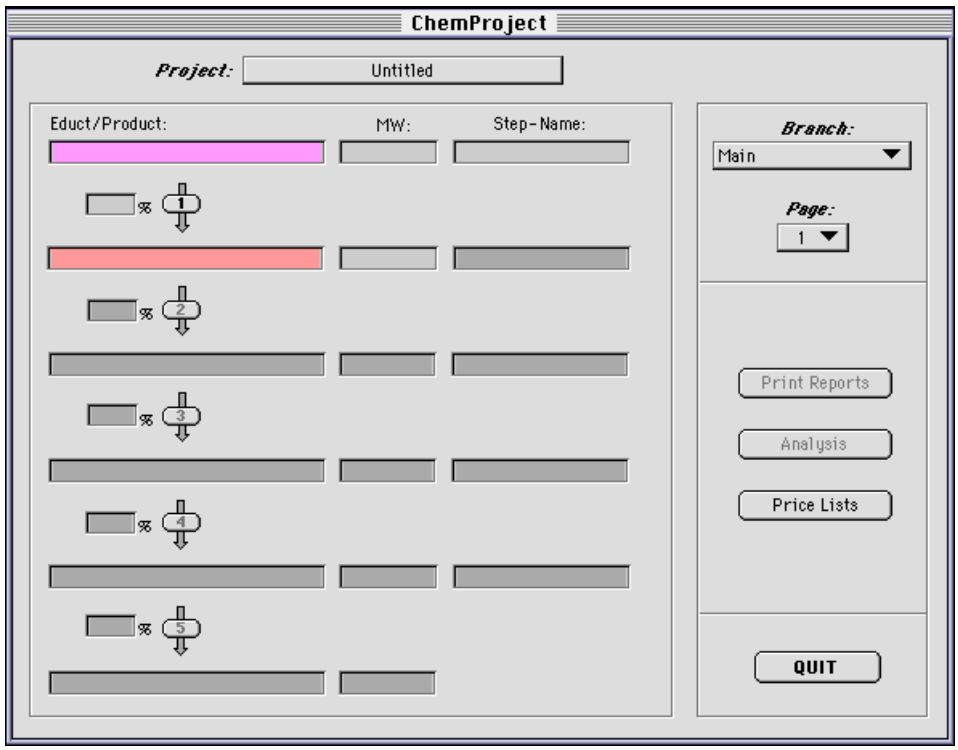
The Startup Screen

Launch ChemProject by double clicking its program icon: its main window appears. There are two options to proceed from here:

- You can open an existing project by clicking the project field (initially containing the word "untitled") once. This will bring up a file dialog, from which the desired file can be selected. You can alternatively use the **Open** command from the **File** menu.
  => *see next page*

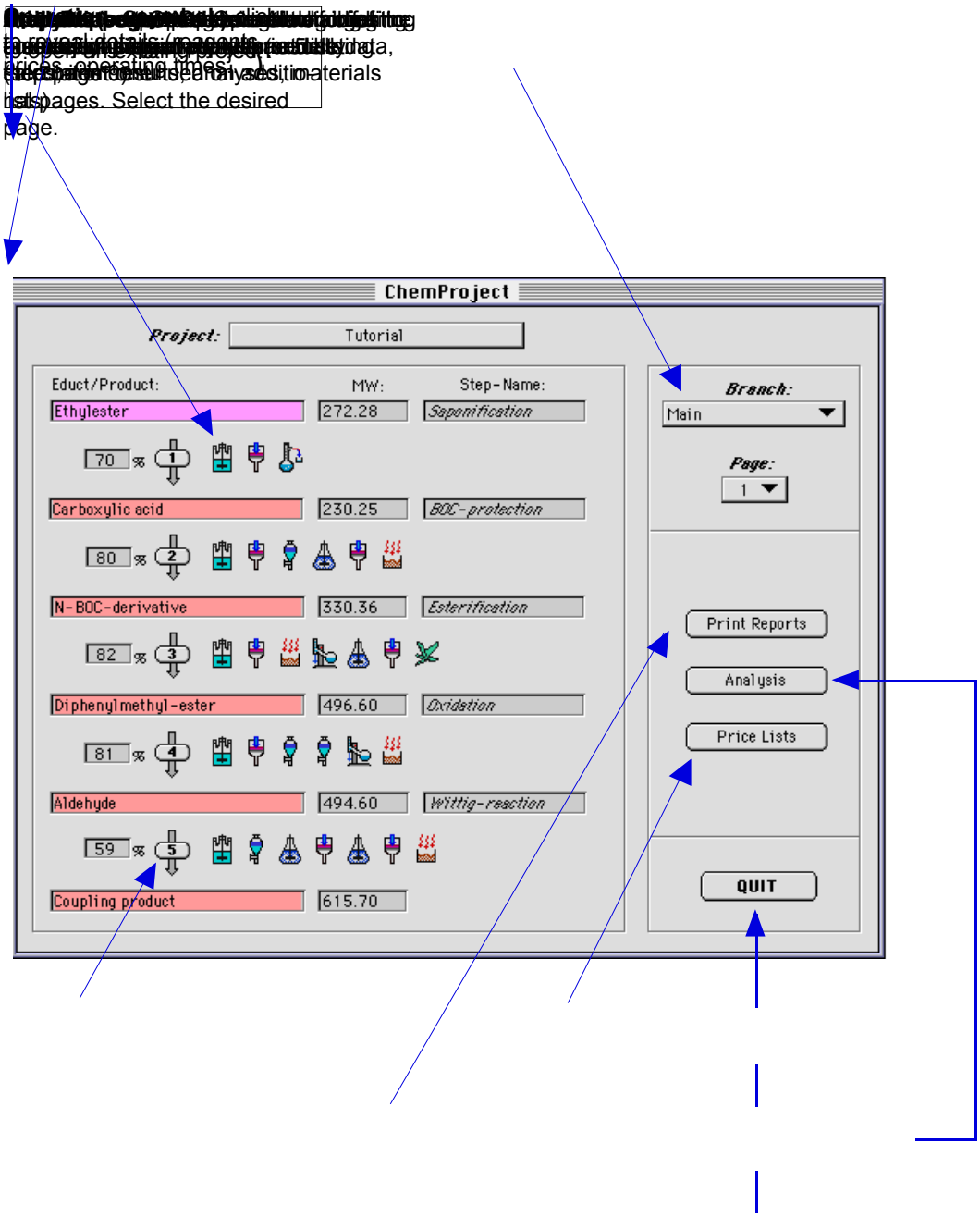
- Or you can start entering a new project by filling in the data fields of the first step.
  => *see page 11*

- *To start with, let's open an existing project. Click inside the project field (the one containing the word "untitled"). From the appearing file dialog, select the "tutorial" project located inside the ChemProject folder.*



The Main Window (View)

The main window provides an overview over a branch of the current synthesis. Each step of the branch is divided into operations (e.g. reaction, filtration, crystallization...), which are represented in a pictographic form. This cartoon-like sequence of operations allows a fast and selective access to operational data detail and an instant assessment of the complexity of a step.

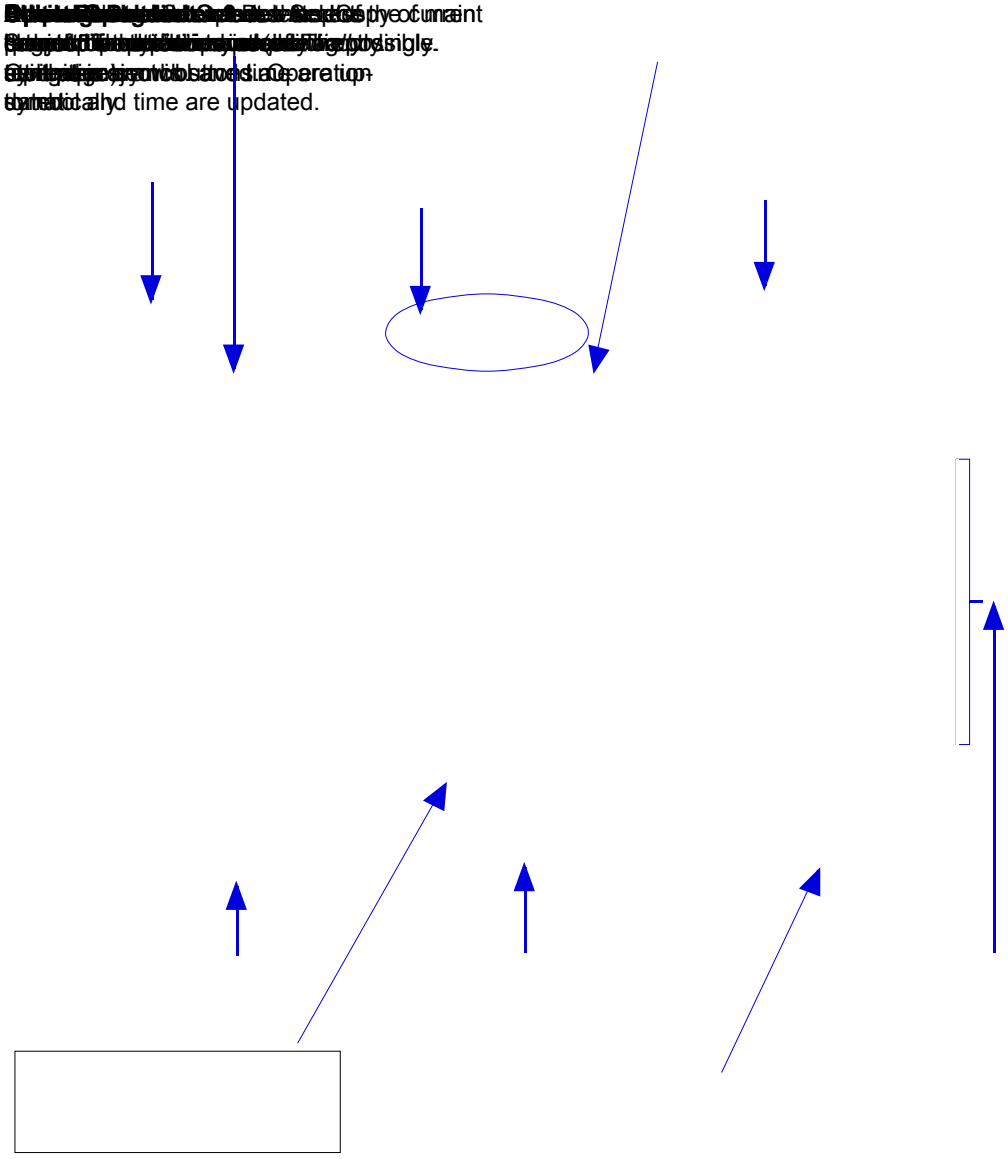


- *Move to page two of the current branch ("Main") using the "Page" pop up menu.*
- *Move through the three branches of the "tutorial" project using the "Branch" pop up menu.*
- *Then go back to the "Main" branch and click the first operation symbol of the first step:*

The Source Data Window (View)

This window contains the original data of an operation. You may have entered these from your lab journal, a publication or any other source. Each step is independent from another in its scale: one step may have been entered in e.g. 120 g scale, while the following one is entered in 32 ton scale. Chemproject will automatically adjust the scales of all steps during project calculation. Of course, all *operations* of a single step must be of the same scale.

You can conveniently navigate through the whole project from this window without the need to switch back to the main window.

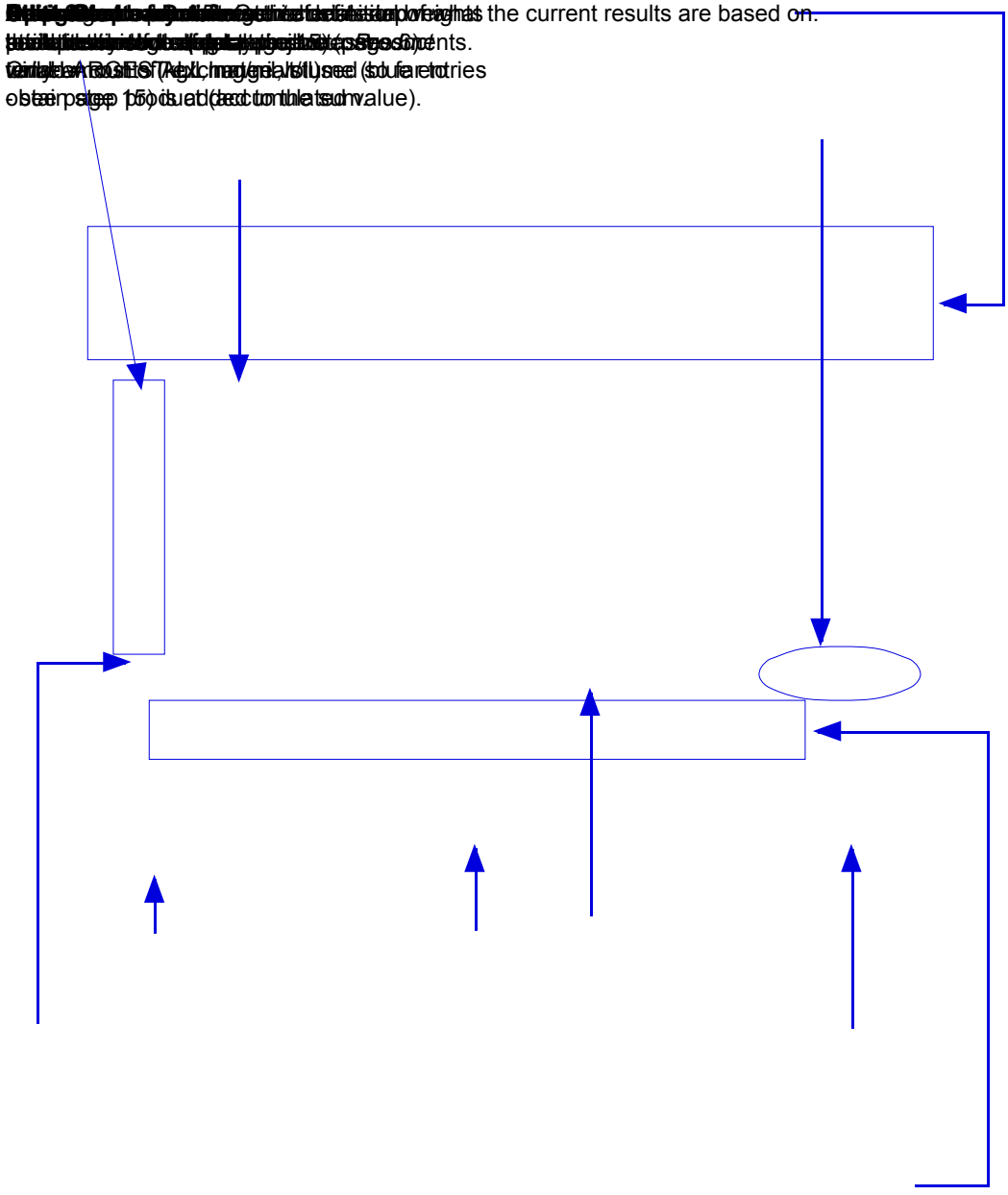


- *Click the "Show Results" button to view the material amounts required by the current operation to obtain a specified amount of synthesis final product.*

The Results Window

This window presents the results of a project calculation. By default, materials and costs are calculated for 1.000 kg of synthesis final product. However, you can enter any other amount into the “values calculated for” area. This will instantly recalculate the project for the new amount. When the pop up menu is changed from “synthesis final product” to “this step’s EDUCT”, the materials and prices are recalculated for the specified amount of the current step’s starting material. This highly useful when the scale of a reaction you currently perform in your lab is changed (use the "Print Step" button to print the new step amounts).

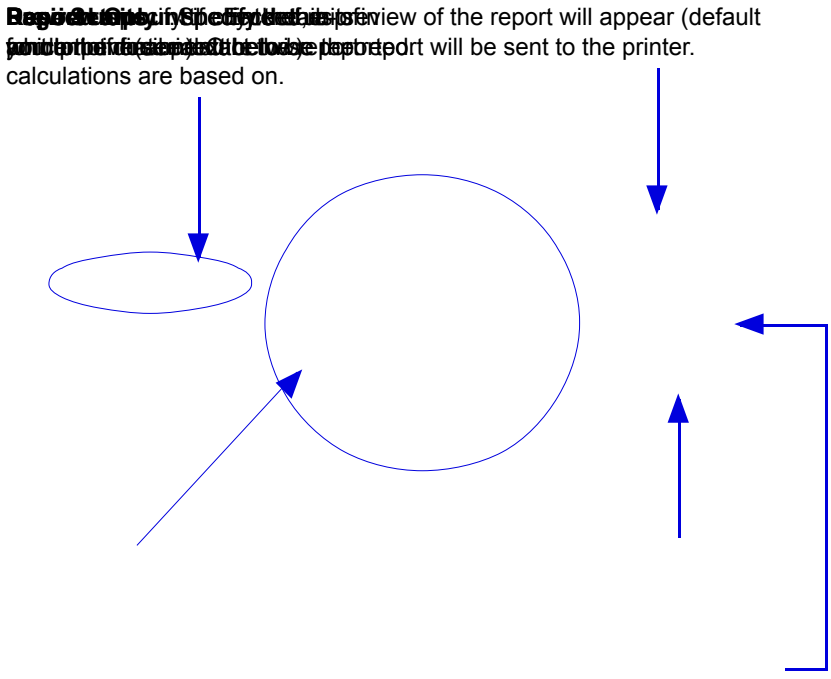
Please note that the step summary summarizes ALL operations of the current step, not only the currently displayed one. Obviously, the reagent cost and product value coincide for the first step of a branch.



- *Click the **DONE** button to go back to the main screen. From there click the **Print Reports** button.*

The Reports Window

Select the type of print report, the amount of final product it is based on, and the destination (printer or preview) from this dialog.



Original Source Data	Original data entered from a lab journal or publication.
Calculation Full	Fully detailed project calculation results.
Calculation Compact	Project calculation results in compact form (less detail).
Materials by Project	Summary of all project materials
Materials by Branch	Summary of all branch materials
Materials by Step	Summary of all step materials
Project Analysis	Results of project analyses (see page 9). Only the 10 most significant items of each category are reported.

All reports except “Original Source Data” and “Project Analysis” are based on the indicated amount of synthesis final product.

- *Preview the different report types. Please note that you will be brought back to the main window after a completed report. Click the “Print Reports” button for accessing the next report).*
- *When done, remain in the MAIN window and press the “Analysis” button.*

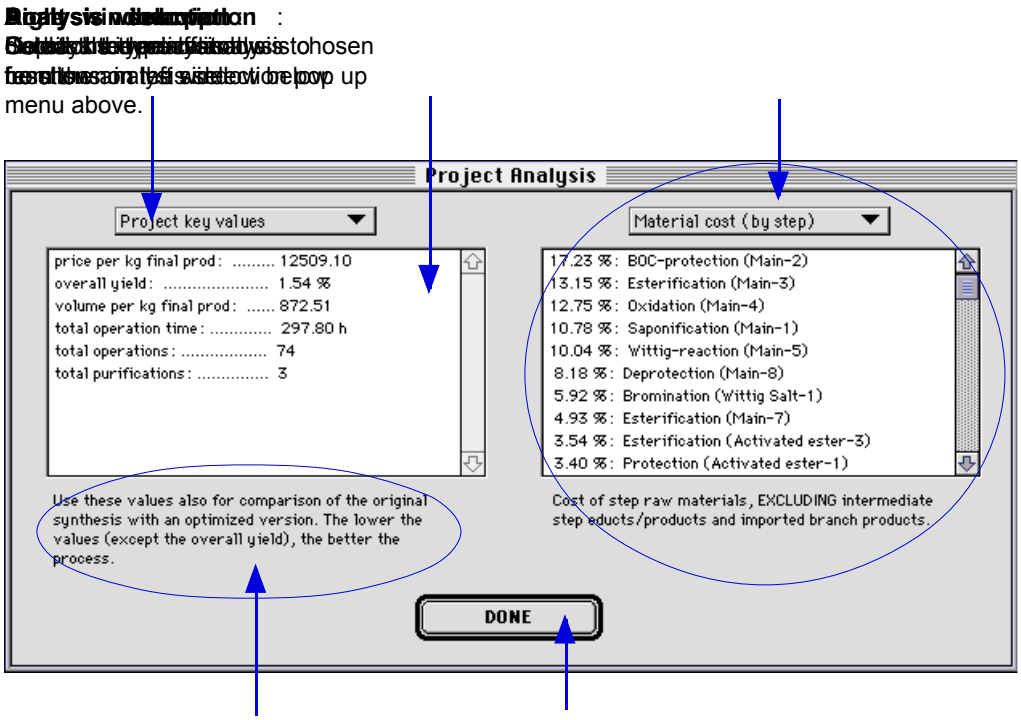
The Project Analysis Window

This window provides you with essential information for the improvement of your project from the economic point of view. Such analyses are particularly valuable to process research chemists. The window provides an online description of each analysis type selected.

The analyses provide exact values for material amounts and costs, but relative data for operating costs, such as the complexity of a step, the required volume or the required time. Such data are well suited for the comparison of different projects *without the need to know their actual operating costs*. The higher the complexity, the larger the volume and the longer the required time, the higher the operating costs of a project relative to another one. This approach is in most cases sufficient to identify the project with the lowest prospective overall costs.

The left and right side of the project analysis window are identical in their functions. This enables side by side comparisons: you could e.g. display a list containing the most expensive steps on the left side and check on the right side for the most expensive material of each of these steps.

The analysis result lists start with the “worst” item on top, “improving” downwards. You can print these analyses from the MAIN window by clicking the “Print Reports” button and selecting “Project Analyses” from the appearing “Reports” window (see previous page). Only the 10 most significant items of each list are printed.



- *Click “DONE” to go back to the main window. - This concludes part one of the quick tour (viewing a project). The second part will deal about creating data and editing them.*

Part 2

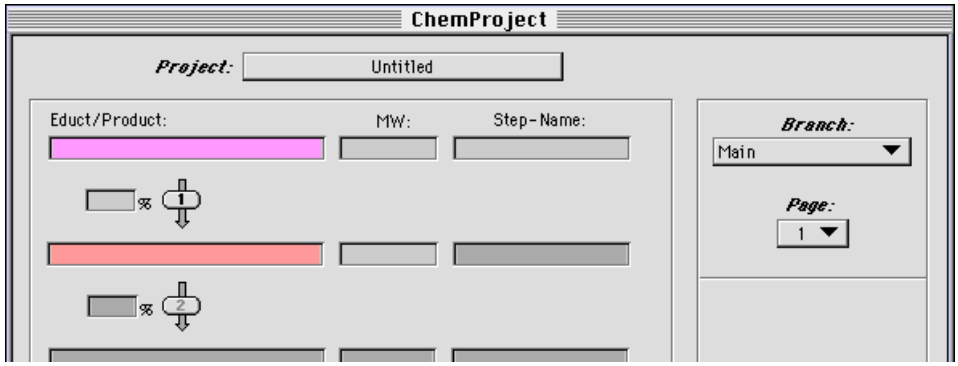
CREATING & EDITING THE PROJECT

The Main Window (Entering Step Data)

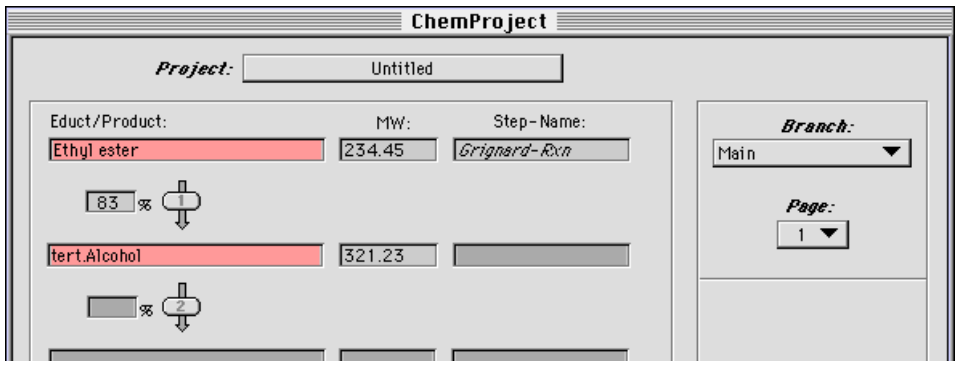
To create a NEW project, select **New** from the **File** menu. If no project is currently open, e.g. immediately after launching the program, you can proceed without this menu command. The window should look as shown below. Enter all data required by the first step, using either the ENTER, RETURN or RIGHT ARROW key to move to the next entry.

When all step data are complete (don't forget to press e.g. RETURN after the last entry!), the "Operation" window automatically opens for operation material input (see next page).

- *Select **New** from the **File** menu, if your project is not already empty and untitled, as shown below:*



- *As an example of a new step, please enter the data as shown below. Use either the ENTER, RETURN or RIGHT ARROW key to move to the next entry. Please note, that at this stage only the fields of the first step are activated.*



- *When all step entries are complete (don't forget to press e.g. ENTER after the last entry), ChemProject checks their validity. If there is any validity problem, you will be prompted to correct it. Otherwise a new set of windows opens, as shown on the next page.*

The Operation Window

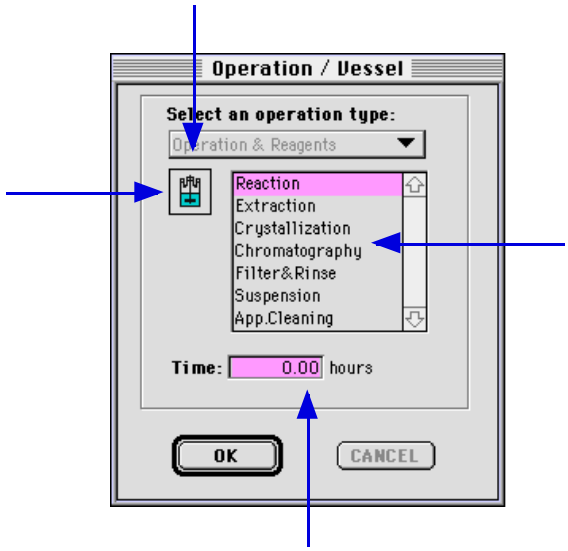
ChemProject divides each step of a synthesis into separate operations for better overview, structuring and analysis. A typical step might consist of a reaction, followed by an extraction, evaporation and crystallization. Two operation types are distinguished:

- **Operation & Reagents**: operations, in which external materials are consumed. The first operation of a step must always be of this type. The currently supported types are: *Reaction, Extraction, Crystallization, Chromatography, Filter&Rinse, Suspension, App.Cleaning.*

- **Operation Only**: operations, in which no external materials are consumed. They cause operating costs and add to the complexity of a step. The currently supported types are: *Evaporation, Distillation, Drying, Filtration.*

As rule of thumb, whenever the product-(mixture) is transferred to another vessel or apparatus, a new operation has to be defined. The first operation of a step is usually a reaction.

Operation Selection Specifies the type of operation. The list below (“Operation & Reagents” or “Operation only”).
click.



The "operation type" pop up menu is inactive when defining the first operation of a step, exclusively offering "Operation & Reagents" type operations (as shown in the picture).

As all operation times increase with the scale of the reaction, their time assignments should be redimensioned on significant reaction scale up.

- *Click on the different operation names in the operations list to view their symbols.*

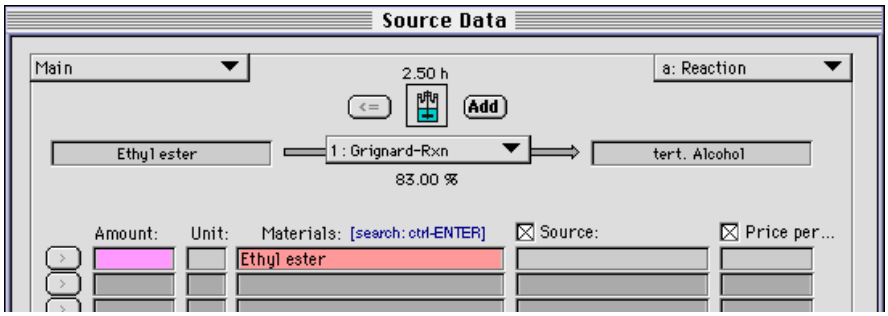
- *Select “Reaction” as your first operation and type in an operation time of 2.5 hours. Press RETURN or click OK.*

The Source Data Window (Entering Data)

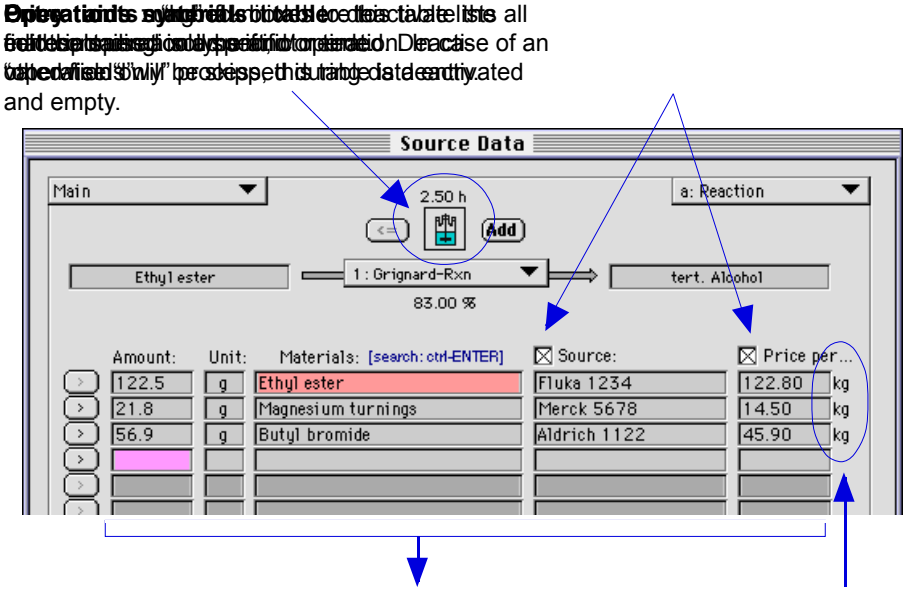
This window specifies all materials consumed in a specific operation, if of the “operation & materials” type.

The material **price** is either based on one kilogram or one liter of the material, depending on the unit specified in the **unit** field. In case of a solid material unit like “mg”, “g”, “kg” or “t”, it is by definition based on one kilogram, otherwise on one liter. If a solid material unit is changed to a liquid one, or vice versa, the corresponding price is immediately recalculated according to the material density .

- *In our example, after leaving the operation window, the screen below appears. The step educt, the reaction name and the step product are copied from the corresponding main window data, along with the step yield, the operation symbol and the operation time.*



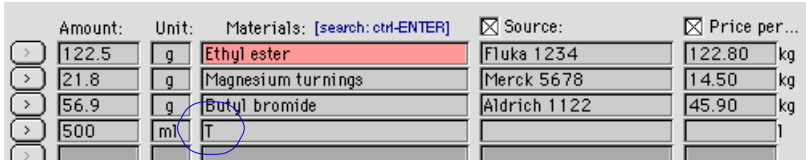
- *Enter the example data below using the ENTER, RETURN or RIGHT ARROW key to move to the next field. The step educt name is placed in a non-edit field, so the cursor jumps over it. After leaving a unit field, note the appearance of the corresponding price unit (kg or l) to the right of the “Price per...” field. When the end of a row is reached, the row below becomes activated.*



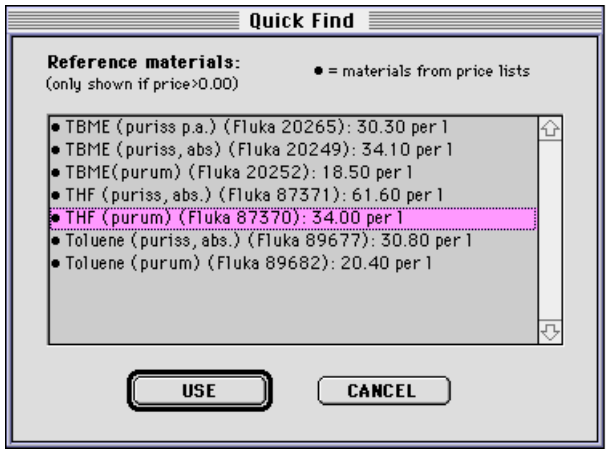
Quick Find: High Speed Data Entry

Data input can be speeded up enormously by just entering the first character(s) of a material in the **materials** field, followed by pressing CTRL-ENTER. This brings up the “Quick Find” window, which contains a selection of materials starting with above character(s). This selection is based on all materials used so far within the **current project**, as well as on all materials ldefined in the current **price list(s)** (see page 26). After double clicking the desired entry, all data is automatically entered into the corresponding material entry fields.

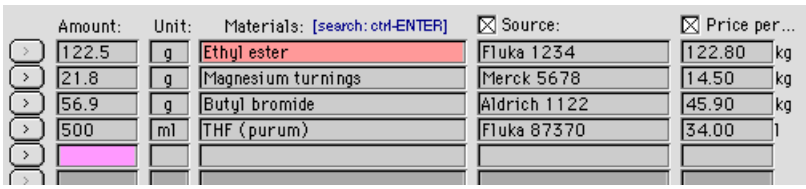
- *In the fourth row, first enter the amount and unit as given below. In the materials field, just type a “T” or “t” (not case sensitive). Your materials table should look like this:*



- *Now press the CTRL and the ENTER keys simultaneously (this command sequence is also indicated on top of the materials column): the “Quick Find” window appears.*



- *Suppose you’d like to enter THF(purum). Double click the corresponding entry in the "Quick Find" window which subsequently disappears to reveal the current material entry filled with all the required data.*



- *If you enter “TH” or “THF” instead of just “T” into the materials field, Quick Find accordingly narrows down its selection*

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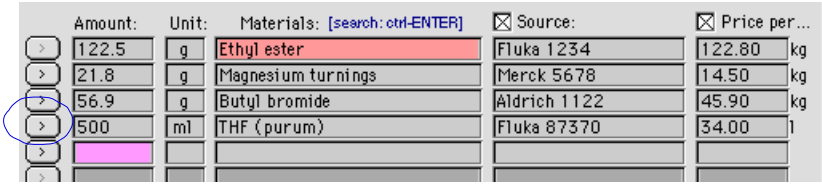
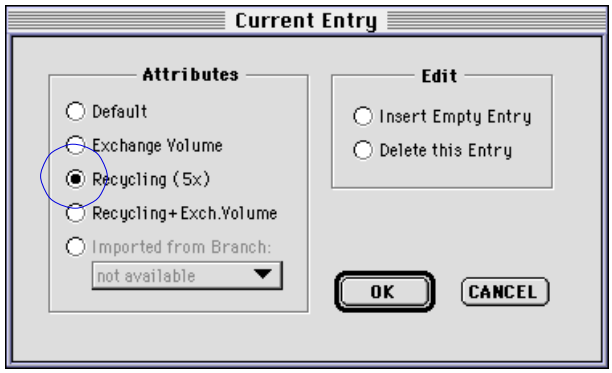
Assigning Material Attributes

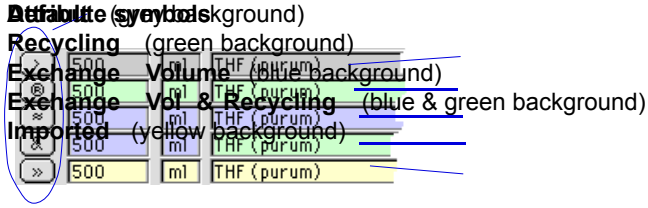
Each material can have a specific property (an attribute): it may be recyclable, an exchange volume, or imported from another branch (see definitions below). Use the materials entry button to access such definitions in the"Current Entry" window.



- *In our example, let's suppose we decided to recycle THF. Thus, click the THF-entry attribute button. In the appearing "Current Entry" window, click on the "Recycling (5x)" box .*



The "Current Entry" dialog offers options for different material attributes, as well as for inserting or deleting an entry in the source data window. By default, materials contain no attributes. When materials are assigned an attribute, their entry becomes marked accordingly in the source data window:



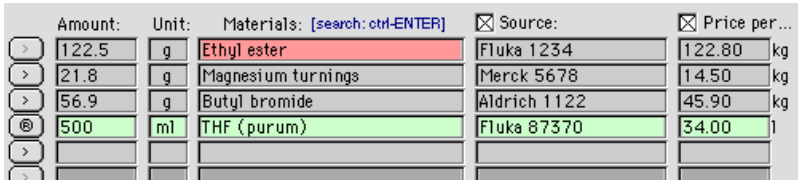
Exchange Volume (≈): Material which is added and successively removed during a single operation (mostly used for extractions). Only the LARGEST of several exchange volumes is added to the total volume of an operation, thus providing the MAXIMUM volume reached.

Recycling (®): Material which can be recycled. While its source price per unit remains the same, its calculated chemcost (=> results window) is reduced by the recycling factor. A fixed overall recycling factor of 5 is assigned (average *approximation*). Please make sure that a recycling is actually feasible, especially when dealing with solvent mixtures.

Import («): Material which is imported from other branches of the project. This attribute in fact CONNECTS different branches with each other. The pop up menu offers a choice of branches actually available for connections, i.e. which are present and not already connected to other branches (page 25).

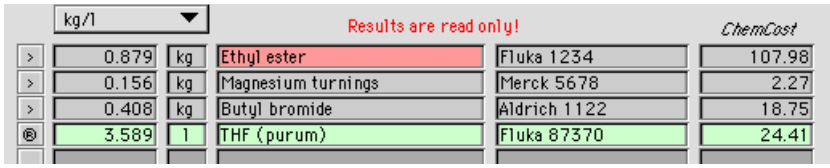
continued...

- *Click OK. The attribute window disappears, the THF entry in the source window has obtained a light green background, and its button symbol is "®" , which defines it as a recyclable material.*



- *Note that although THF is being recycled now, its source price per liter remains the same as before. This is obvious, since the supplier price remains unaffected by your recycling. However, the material's chemcost (=> RESULTS window) is reduced by the recycling factor after project calculation:*

- *In order to check the effect of the recycling attribute, click the "Show Results" button. This brings up the RESULTS window, which shows the material requirements and costs of this operation calculated for 1 kg final product.*

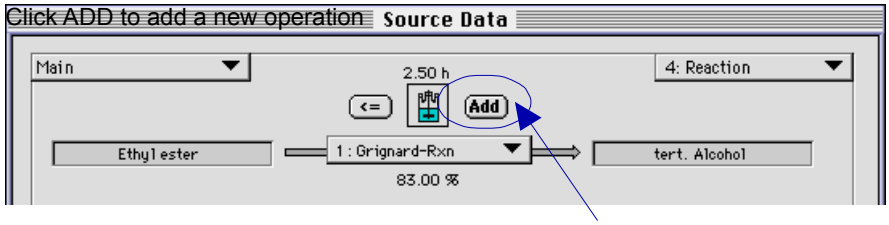


- *Without recycling, 3.588 liters of THF would cost 3.588 x 34.00 = 121.99 currency. The indicated chemcost of 24.41 currency corresponds exactly to one fifth of this value (the recycling factor).*

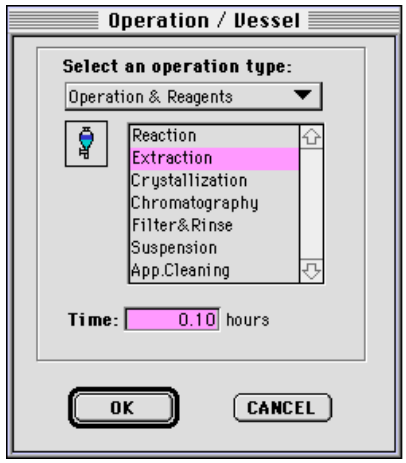
- *Click the "Edit Source Data" button to switch back to the source data window.*

Adding A New Operation

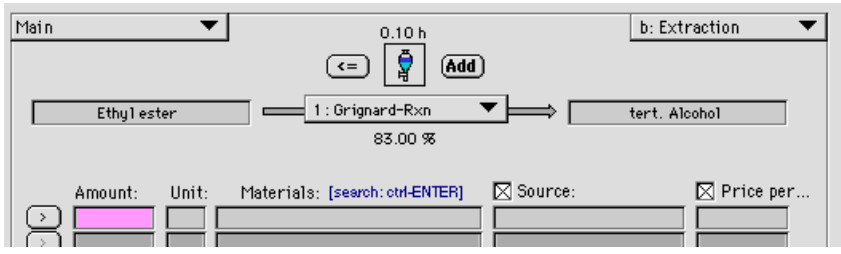
When moving to the LAST operation of a step, the right arrow button symbol changes from “=>” to “Add”. Click it to append a new operation to the current step.



- *Click the “Add” button.*
- *Select the “Extraction” entry from the appearing operation window, enter an operation time of “0.10” hours and click the “OK” button.*



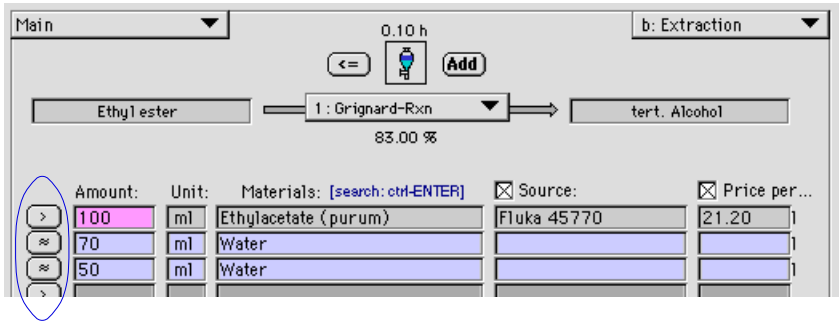
After defining the operation type and time (the latter being optional except for “reactions”), the empty source data window appears, ready for your input.



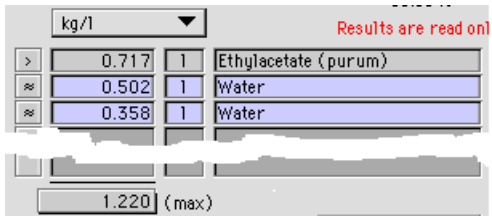
continued...

- *Enter the materials shown below. When you move to the price field after entering "Fluka 45770", the price is filled in automatically, since above source specification was found in a price list. Please note that you may skip source specifications and prices, like in the case of water in this example.*

- *Since we want this operation to describe the organic phase being washed with two portions of water, specify both water entries as "exchange volume" by clicking their respective entry buttons and assigning the corresponding attributes (see page 15).*



- *To see the effect of this "Exchange Volume" definition, click the "Show Results" button and examine the operation volume field (below the material amounts). Only the LARGEST exchange volume is added to the total volume. The "(max)" indication appears as an additional reminder.*

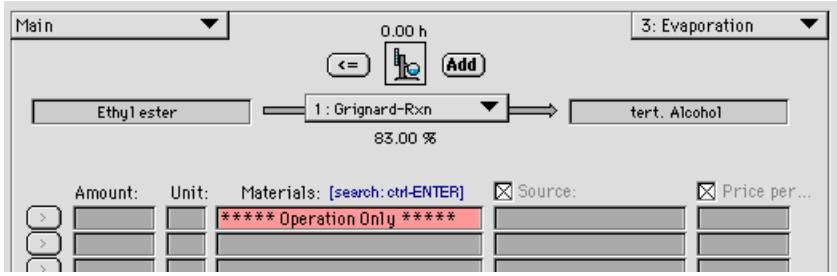


- *Click the "Edit Source Data" button to return to the source data window.*

- *Click the "Add" button, which will bring up the operation window. This time select "Operation Only" from the pop up menu and "Evaporation" from the list. Without entering an optional time, click "OK".*

continued...

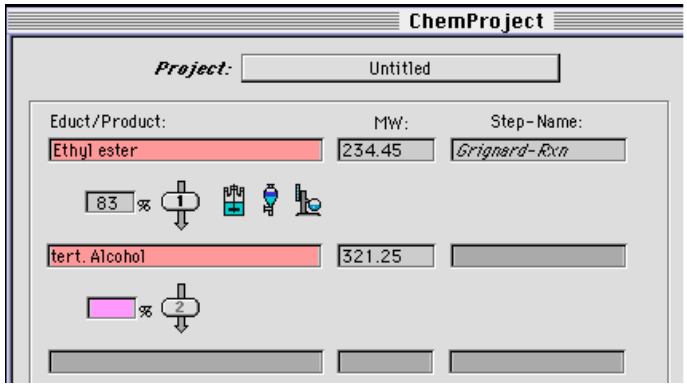
After the definition of an “Operation Only” type operation, all material entries are in the source data window become disabled and empty (see below). Although such an operation does not contain any material information, it is causing operating costs and adding to the complexity of the step.



- *Move back and forth between the three operations you just entered, using either the arrow buttons or the operations pop up menu in the top right corner of the window.*
- *When finished, click “DONE” to go back to the main menu, where the three newly created operation symbols have appeared within the first step.*

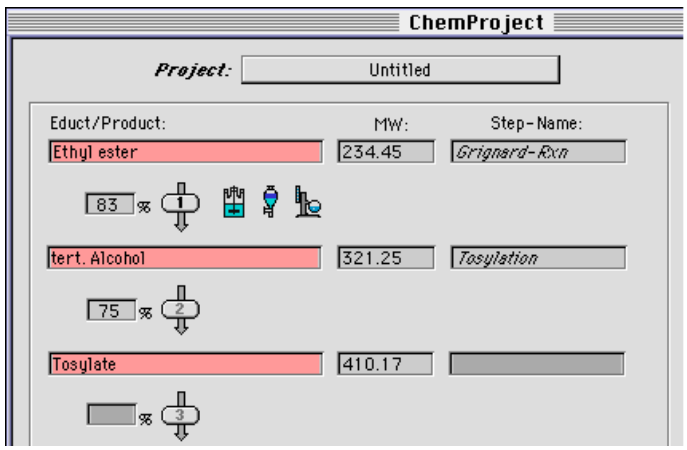
Adding A New Step

After having entered the first step, the main window looks like this:



Now fill in the data fields of the next step. After entering the step yield, the initially disabled fields become activated. When done, the operation window opens, followed by the source data window, as discussed on the previous pages.

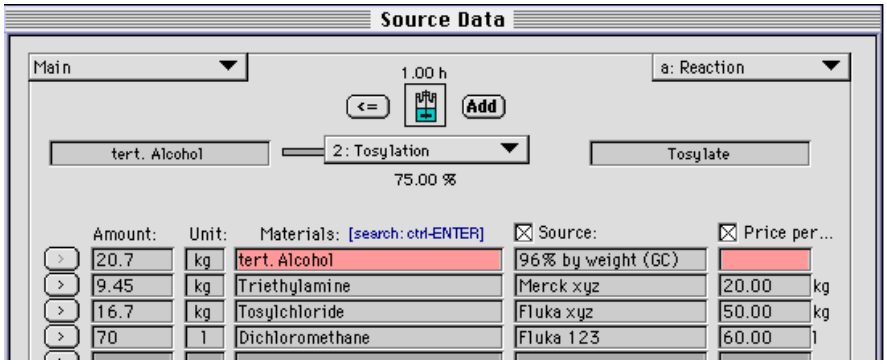
- *Fill the four data fields of the second step with the data shown below.*



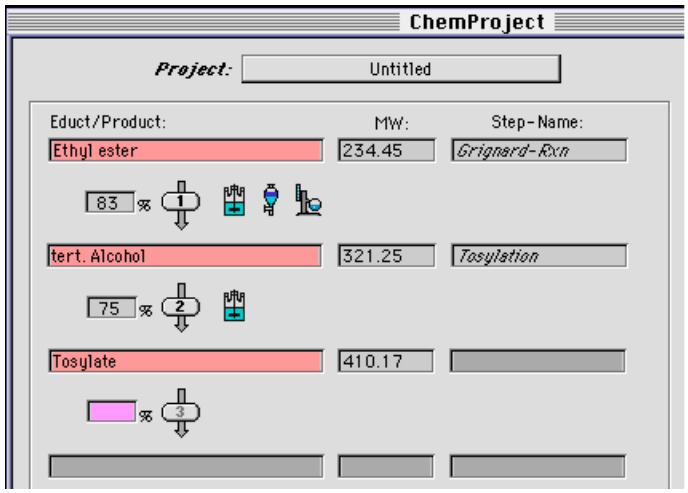
- *When all fields are entered, the operation window appears. Define the operation as "Reaction" and the operation time as 1.00 h. Click "OK".*

continued ...

- *Enter the data below in the source data window. Note that none of the materials are present in the supplied price list, nor have they been used in this project so far. Therefore, the CTRL-ENTER sequence of QuickFind (page 14) will not present any hits this case. Also note that this step is entered in kilogram-scale, while the previous one was entered in gram-scale. This is perfectly fine, since ChemProject scales all steps to fit each other on project calculation.*



- *At this point, you would usually click the "Add" button to enter more operations. However, since this is just a demonstration step, we will not add any more. Click "DONE".*

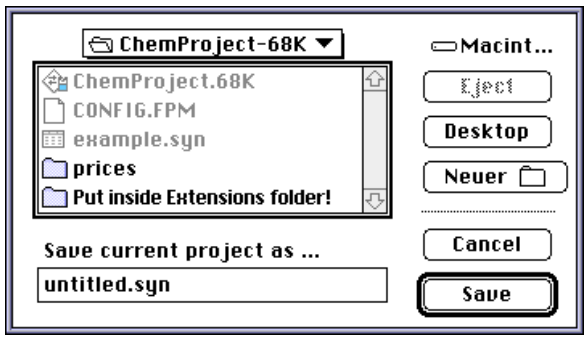


- *The reaction symbol for the second step has appeared in the main window, which is ready for the entry of more steps.*

Saving The Project

Use the **Save As...** command from the **File** menu to save the current project. This menu item is only available when the main window is the active window. It will bring up the file dialog:

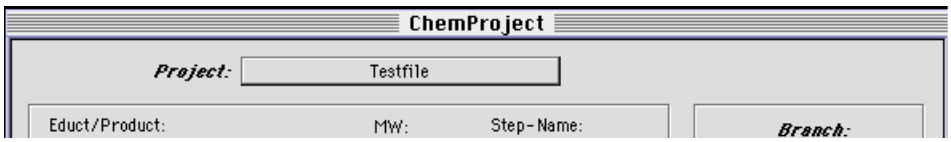
- *Select **Save As...** from the **File** menu.*



If the current project has not been saved so far, the title “untitled.syn” appears as a suggestion. Change this name to whatever you like. If you don't add the “.syn” appendix, it is automatically appended to the project name when the file is saved. Files without this appendix cannot be recognized by the program.

Note: Due to limitations of the programming environment, project file names are forced to lower case characters after processing.

- *Let’s call the example file “testfile.syn”. Enter this name in the name box, specify where you want to save it and click the “Save” button.*



The new project name now appears in the “Project” field of the main screen (without the “.syn” appendix).

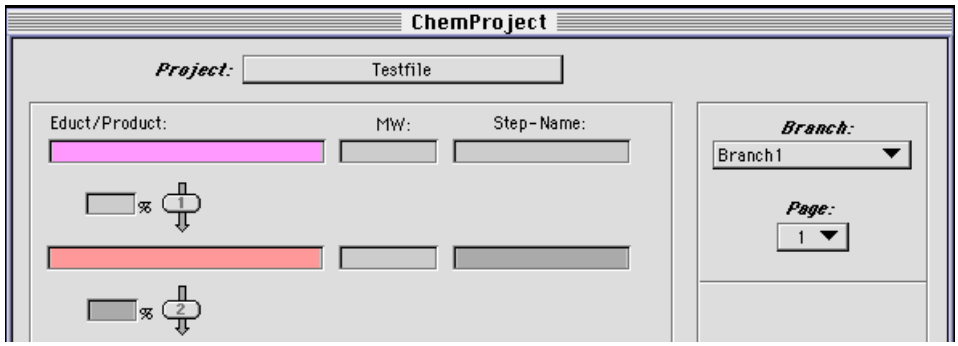
You can also RENAME your project with the **Save As**... command.

Creating, Deleting And Renaming A Branch

Create a new branch by selecting **Add New Branch** from the **Project** menu. Then enter the desired name in the appearing branch dialog.

- *Select **Add New Branch** from the Project menu. The branch dialog appears:*

- *Enter "Branch1". Of course, it could be given any other name.*
- *Click "OK".*



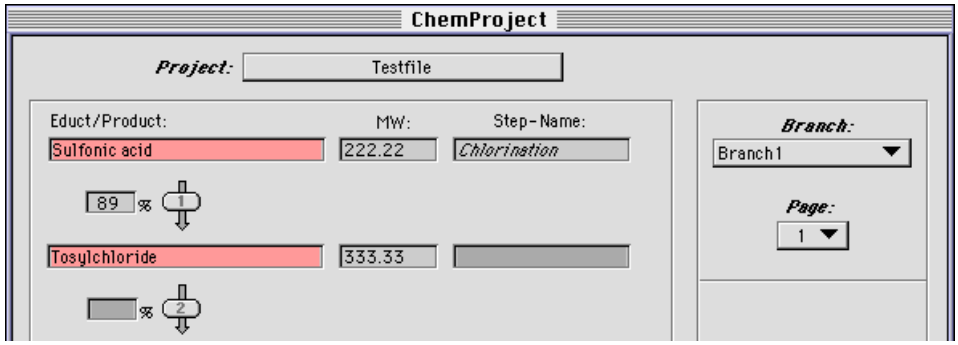
The main screen displays the name of the new branch in the branch pop up menu and is ready for the the new branch data.

From the **Project** menu, two other branch operations are available. They both act on the currently selected branch:

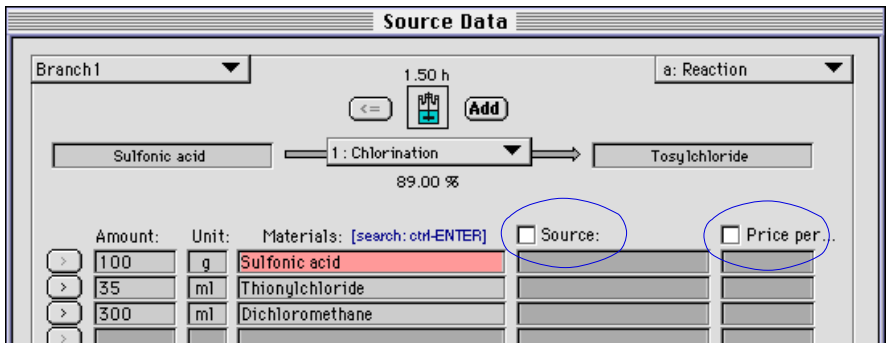
- **Rename Current Branch**: Brings up the branch dialog. Enter the new name and click "OK".
- **Delete Current Branch**: Deletes the current branch. Caution! All branch data will be lost.

continued ...

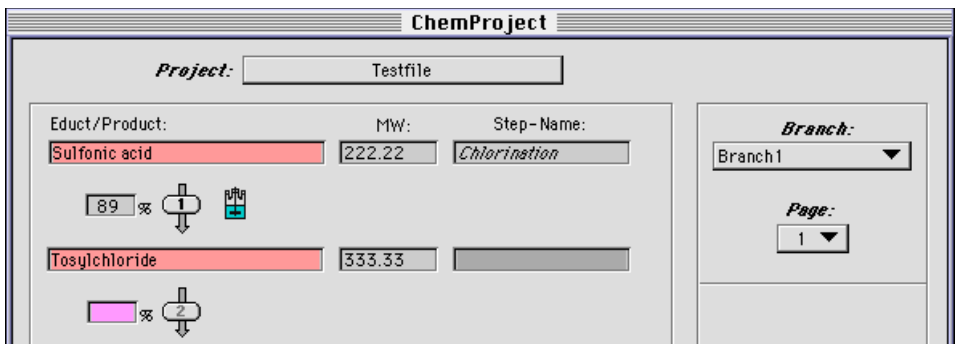
- *A very short step consisting of one single operation will be entered now for use in the next chapter. Please enter the data given below.*



- *Specify the operation type as "reaction" and the time as "1.50" h in the operation window. Then click "OK".*
- *Since we don't intend to enter any source descriptions or prices in this example, first uncheck the "Source"- and "Price per..." boxes in the appearing source data window: the cursor now conveniently skips these deactivated fields.*



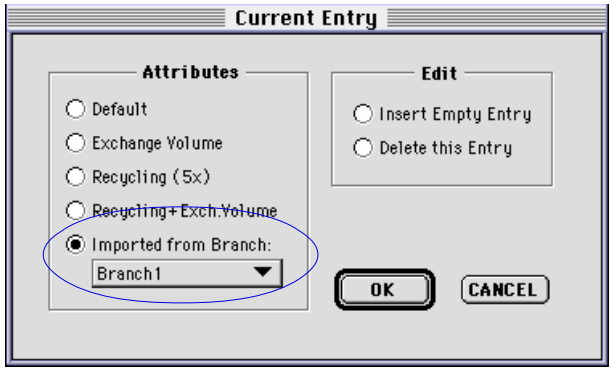
- *Enter the data above and click "DONE". This provides the shortest possible branch, consisting of one single step and operation. Of course, a branch will contain much more data in actual projects. The main window now should look as below:*



Connecting Branches

A synthesis usually consists of a main branch, possibly connected to one or more side branches. These, in turn, may be connected to yet other branches, thus building a synthesis tree. A connection between two branches occurs, when one branch uses (imports) the final product of another one. ChemProject allows the simultaneous use of up to 16 branches, which may be nested to any desired degree.

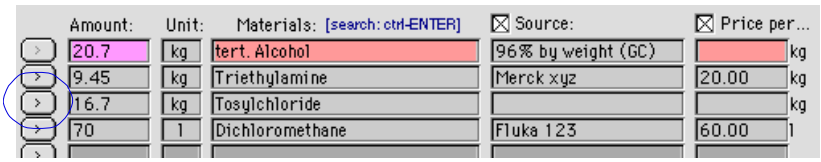
To define a material as being imported from another branch, click its material button in the source data window (second picture below). This brings up the “Current Entry” dialog:



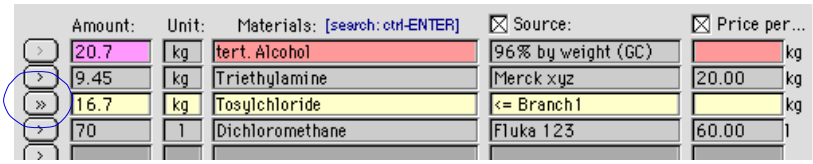
Check the “Imported from Branch” attribute. This entry is not accessible if no other branches exist within the project, or if all are already connected. Specify in the the branch pop up menu, which branch this material is imported from. For your convenience, only available (unconnected) branches appear in this menu. It is always the **final product** of the specified branch, which is imported. After clicking “OK” the newly defined material appears as a yellow entry in the source data window (see picture at bottom of page), with the “»” symbol on its button and the source branch specified in the “Source” field.

- *In our example, suppose we decided not to buy tosyl chloride, but to prepare it in a separate branch. We have just created this branch on the previous page. Now we want to connect it to the “Main” branch.*

- *Since the connection can only be defined from the receiving branch, first move to the main window of the “Main” branch, if not already there. Then click the reaction symbol of the second step. In the appearing source data window, click the button of the “Tosylchloride” entry:*



- *Click the “Imported from Branch” box in the appearing window (see picture on top of this page). Since only one branch (“Branch1”) is available, no other import choices are offered by the branch menu. Otherwise you would have to specify the branch you want import from. Then click “OK” to complete the connection.*



- *The newly connected branch will now be included in all project calculations. Look at different report previews (see page 8) to verify this.*

Price Lists

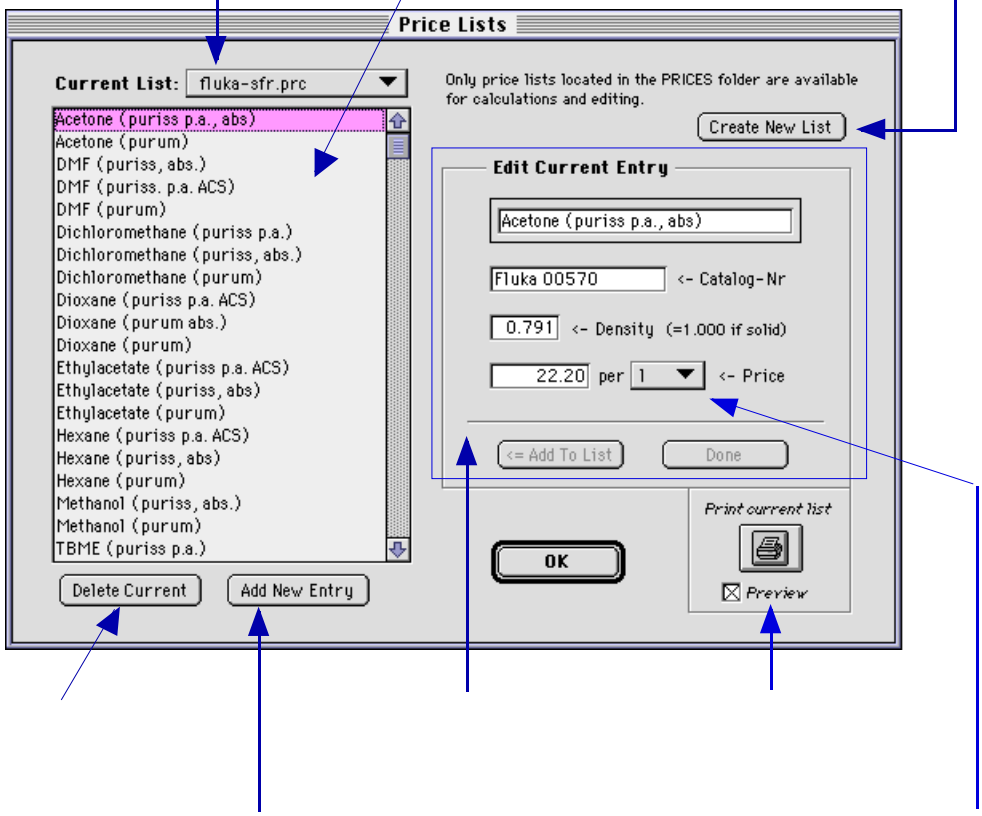
Price lists are databases containing prices and densities of materials. Invisible to the user, they provide QuickFind (page 14) with prices and other details of a requested material. The demo price list delivered with this program (“Fluka-SFr”) is a very small one, containing prices and densities of a few common solvents. In practice, you will have to build your own price lists, tailored to your needs, suppliers and local language & currency. *Keep them at a size of no more than a few hundred items for easy maintenance and optimum speed*.

Only price lists located inside the “prices” folder and ending with ".prc" can be accessed. You could e.g. create a price list for small order prices and one for bulk prices or different price lists for different suppliers for easy maintenance. In any case, all price lists within the “prices” folder are internally merged to a single database when ChemProject launches. If you don’t need specific price lists, move them outside this folder BEFORE starting ChemProject. The “prices” folder can hold any number of price lists.

Specify a name in the appearing name

ems in the “Edit Current Entry” area.

item to the price list. Click “Done” when done with entering new items to reactivate items list.



Use the RETURN key to move to the next field in the “Edit Current Entry” area. The material density entry is required for solid/liquid recalculations. Also note, that the current list is automatically saved before printing it or selecting another list.

Credits

I would like to thank following colleagues at Hoffmann-La Roche Basel for their support :

Dr. Paul Spurr (proof reading of the manual, discussions)
Dr. Hans Hilpert (testing, discussions)

This program was written almost entirely in my spare time . Therefore special thanks to my wife Maren for her patience and support, and especially for not teaching my Mac how to fly through closed windows.