



$\mathcal{M}_3^{\text{PRO}}$

Membrane Module Modelling^{PRO}

$\mathcal{M}_3^{\text{PRO}}$ software has been developed at the Separation Processes Group (Laboratoire des Sciences du Génie Chimique, UPR CNRS 6811 – Nancy, France) in order to simulate multicomponent gas separation processes by membrane modules. Four different types of hydrodynamic conditions are taken into account: perfect mixing, cross plug flow, co-current plug flow, counter current plug flow. For each case, $\mathcal{M}_3^{\text{PRO}}$ enables the following variables to be computed as a function of the component mole fractions:

- membrane surface area and stage cut for a fixed pressure ratio,
- membrane surface area and pressure ratio for a fixed stage cut,
- stage cut and pressure ratio for a fixed membrane surface area

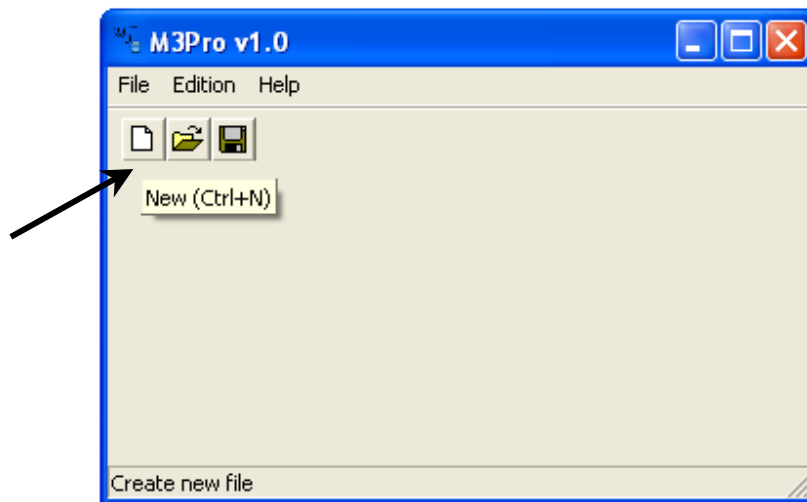
In a first step, the gas mixture to be treated, the type of hydrodynamic conditions, the operating parameters and the type of simulation are specified. After the computation has been performed, the results are automatically saved by $\mathcal{M}_3^{\text{PRO}}$ in different text type files.

Additionally, a membrane permeability property data bank is also included in $\mathcal{M}_3^{\text{PRO}}$ which can be gradually modified and extended. Membrane / gas type and the associated permeability value can be entered and saved. An automatic permeability unit converter is also included.

General presentation of \mathcal{M}_3^{PRO}

After the software has been started, the following window appears. There are two possibilities in order to start the application :

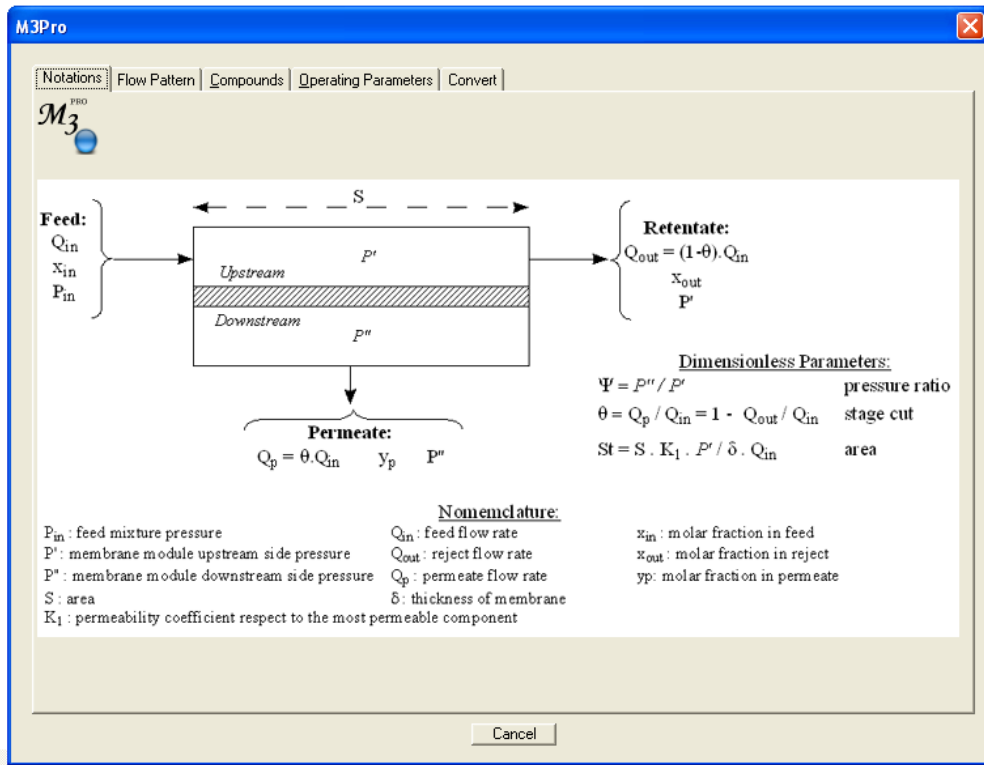
- click on « File/new file »
- click on « New » icon



A new window opens with 5 different items in the menu bar :

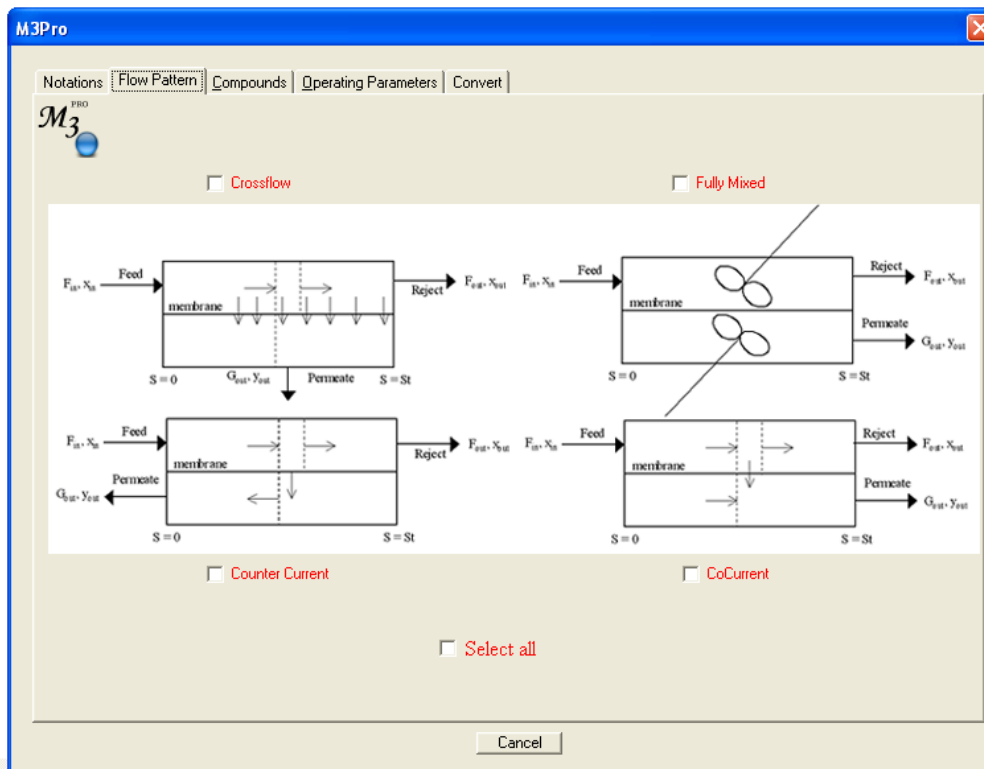
1. « Notations »

Describes and explains the different variables and symbols used



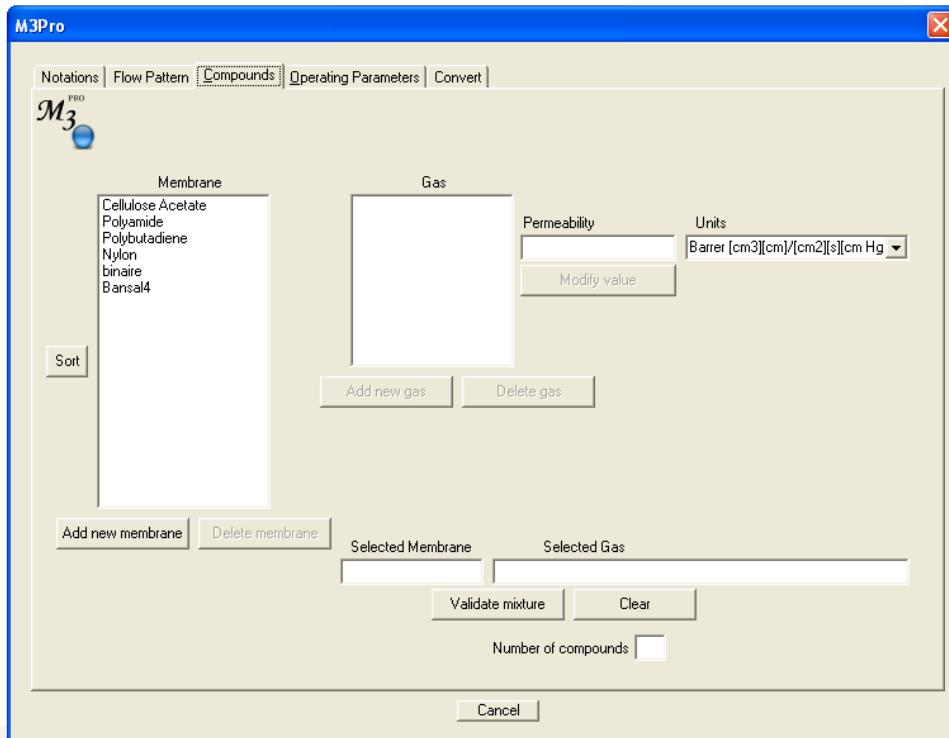
2. « Flow pattern »

Gives an overview of the four types of hydrodynamic conditions which can be selected



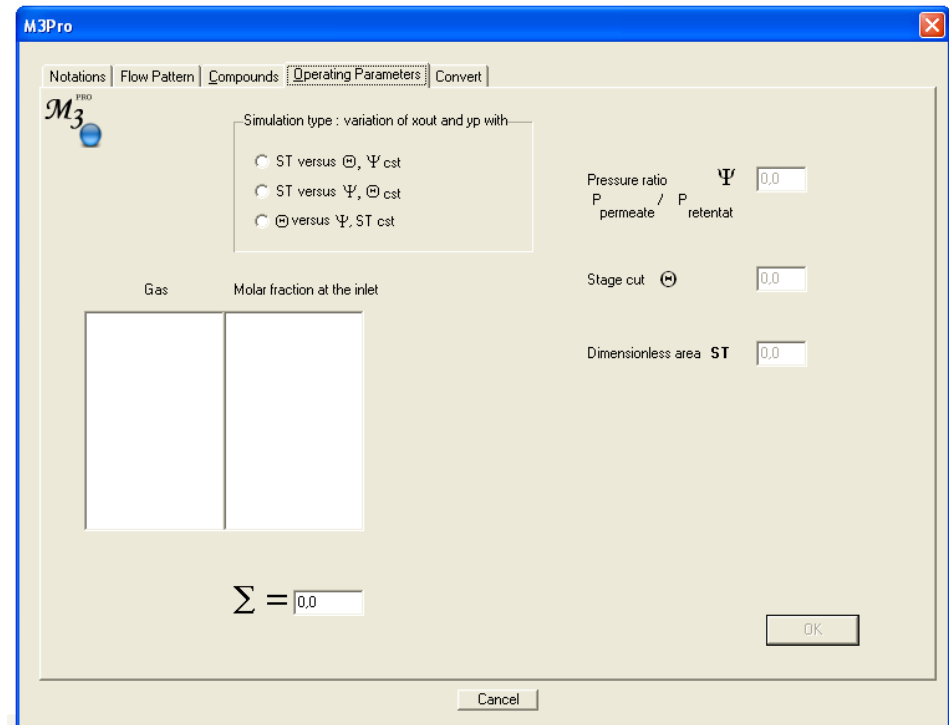
3. « Compounds »

Opens the permeability data base and has to be used in order to select the gas mixture to be used for computation.



4. « Operating parameters »

Can be used in order to define the entrance gas mixture composition, as well as the type of computation to be performed.

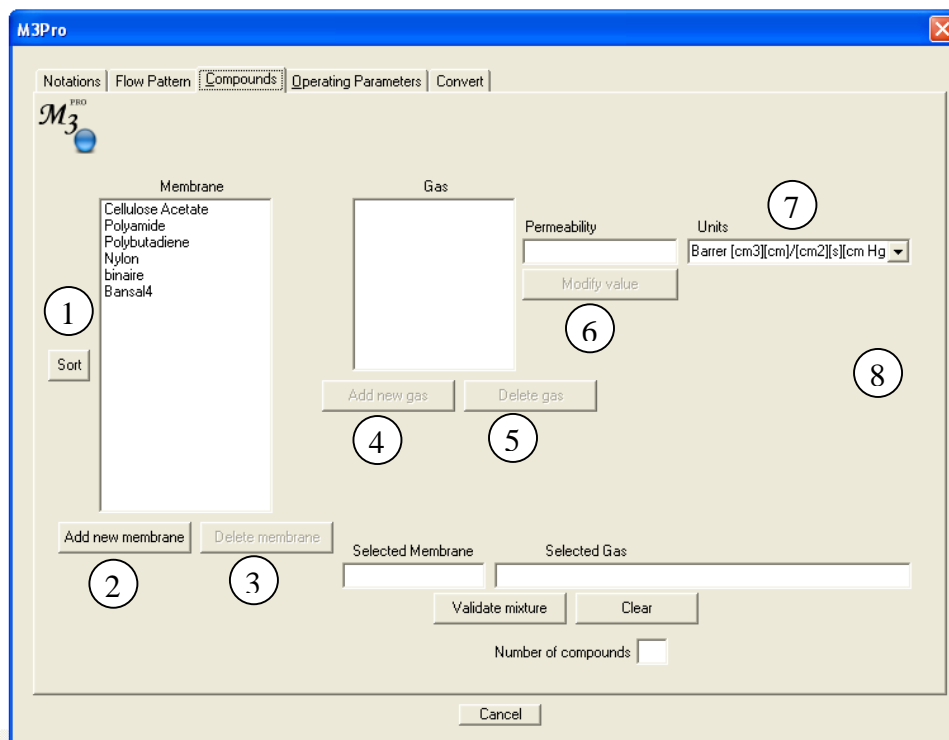


5. « Convert »

In the 1.0 version, this page is not active.

Working with the membrane permeability data base

This operation can be performed through the « compounds » section.

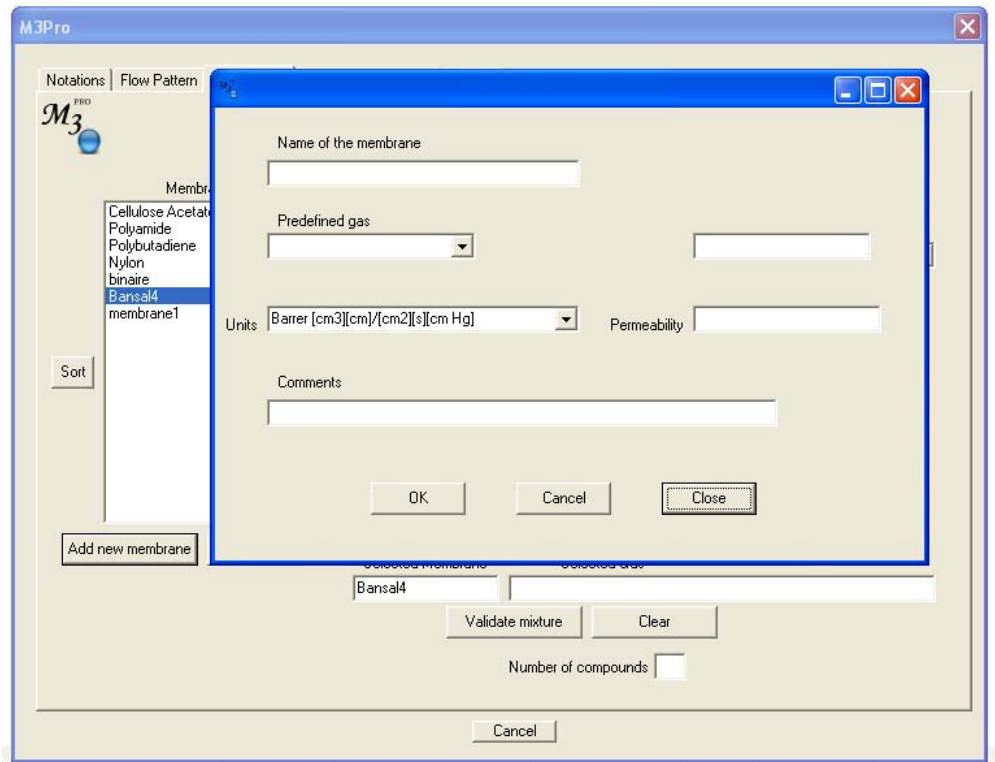


The following actions, identified by a number on the above figure, can be activated:

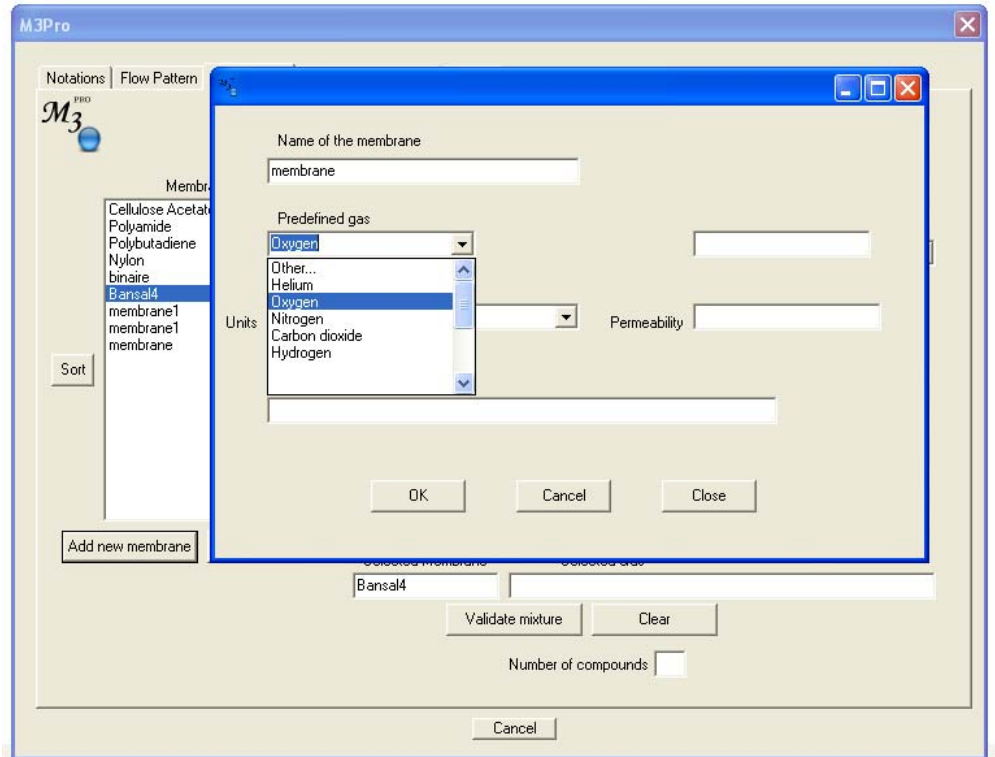
1. « Sort » : automatic alphabetically sorting of the membranes names which have been saved. The last saved membrane name automatically appears at the end of the list before this function is activated.
2. « Add new membrane » : opens a window where a new membrane type and its associated gas permeability data can be saved
3. « Delete membrane » : efface une membrane enregistrée et des gaz associés à cette membrane,
4. « Add new gas » : enables a new gas type to be associated to a previously saved membrane type
5. « Delete gas » : deletes a gas which is associated to a given membrane,
6. « Modify value » : modification of a given gas permeability value associated to a given membrane
7. « Units » : offers a given type of permeability unit to be selected
8. « Save » : after modification of permeability data, this function automatically appears and can be activated.

Adding a new membrane

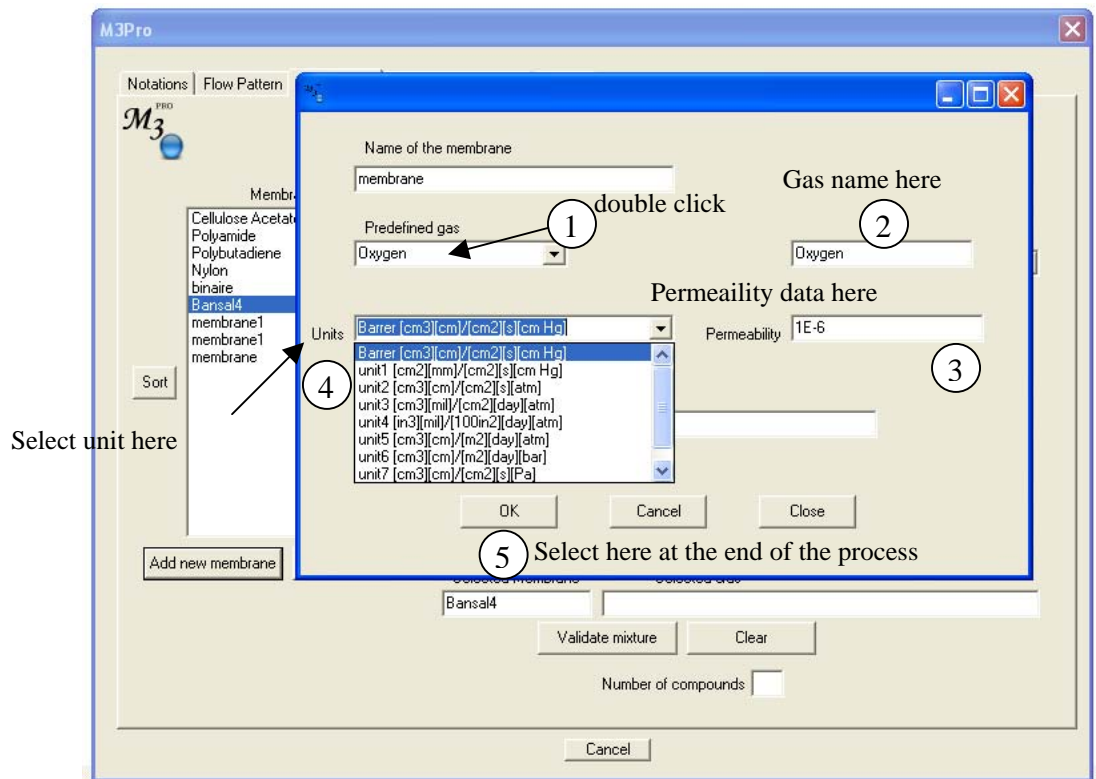
When clicking on « Add new membrane », the following window appears.



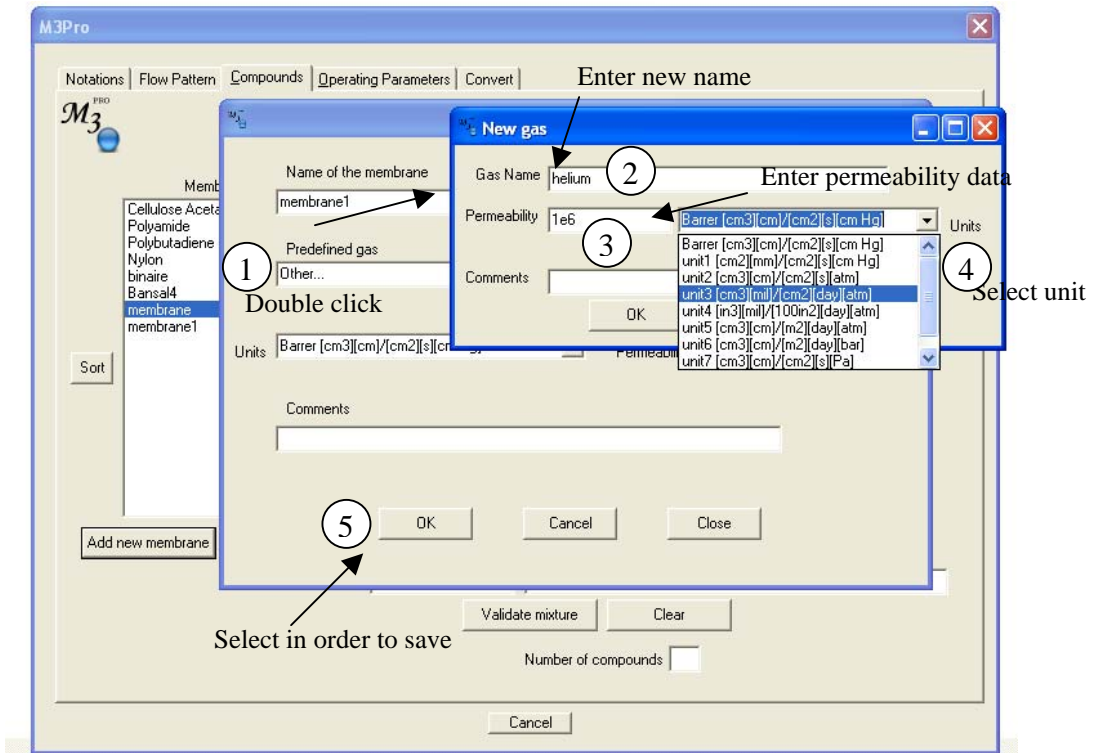
Type the membrane name and click on « Predefined gas ». If the name of the gas that you want is already included in the list, select it:



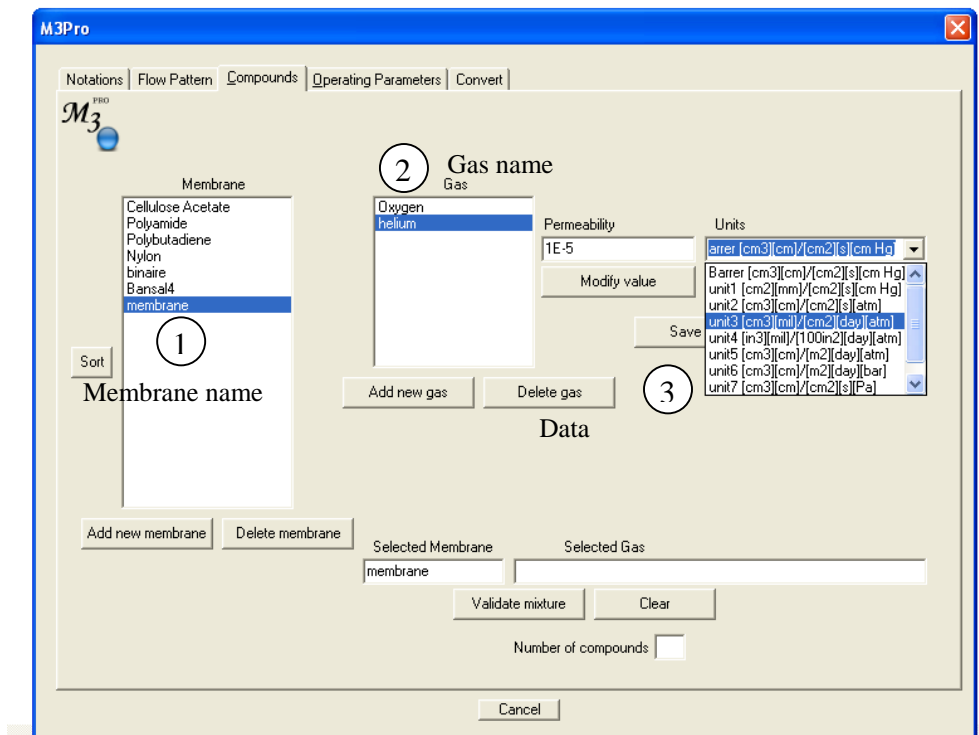
Double click on the name, so that a permeability figure can be entered. The number is written in the « Permeability » section and the corresponding unit is indicated in « Units », Click on « OK » in order to save this data.



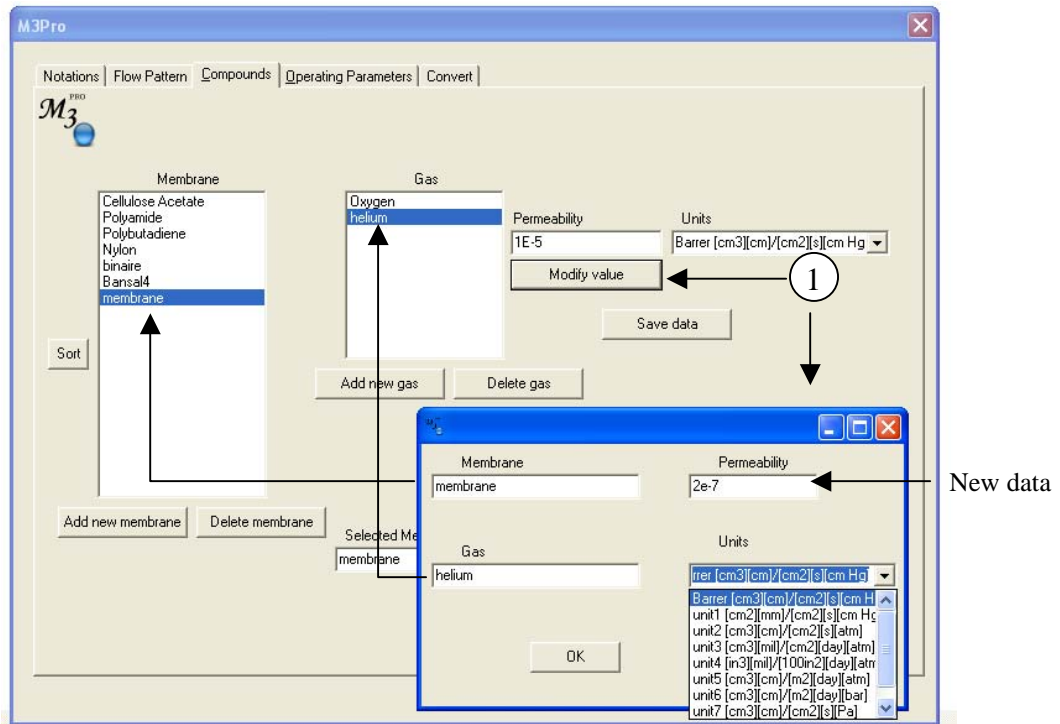
If the name of the gas that you want to select does not appear in the list, then click on « Predefined gas » and « Other ». A new window is created where the new gas name and the corresponding permeability data can be entered and saved.



Coming back in the « Compounds » section, the modifications that have been performed can be visualized.



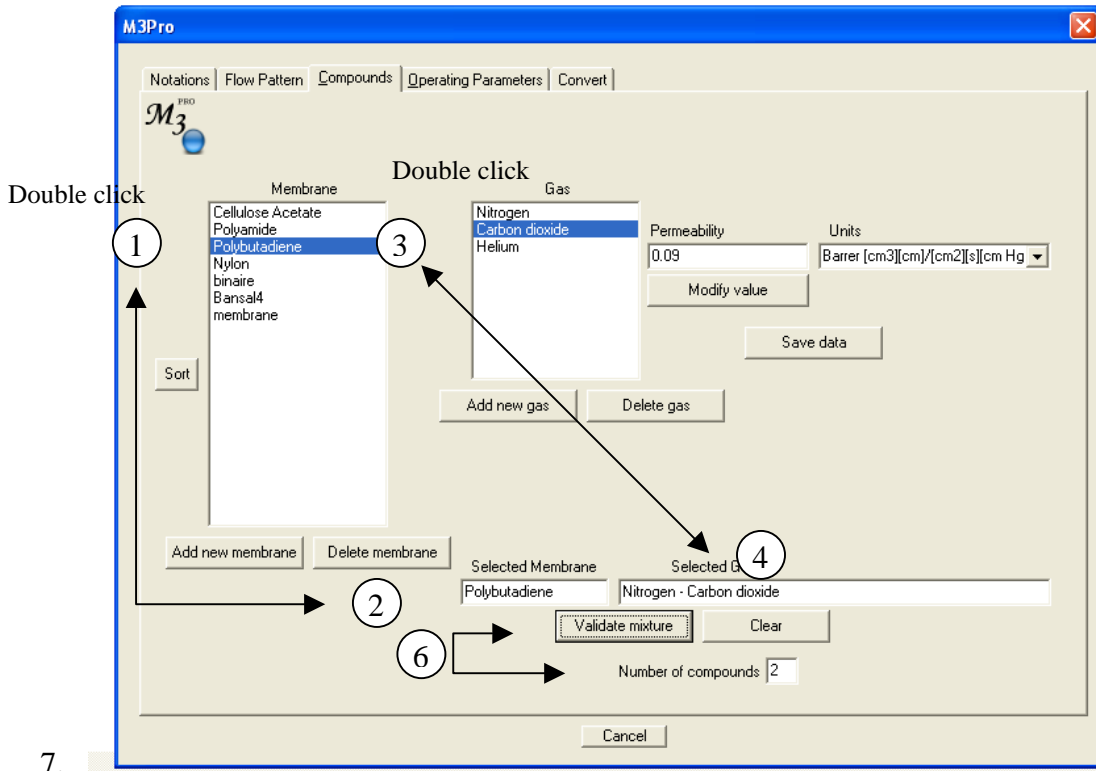
By clicking on « Modify value », the permeability data can be changed.



Selecting a multicomponent mixture

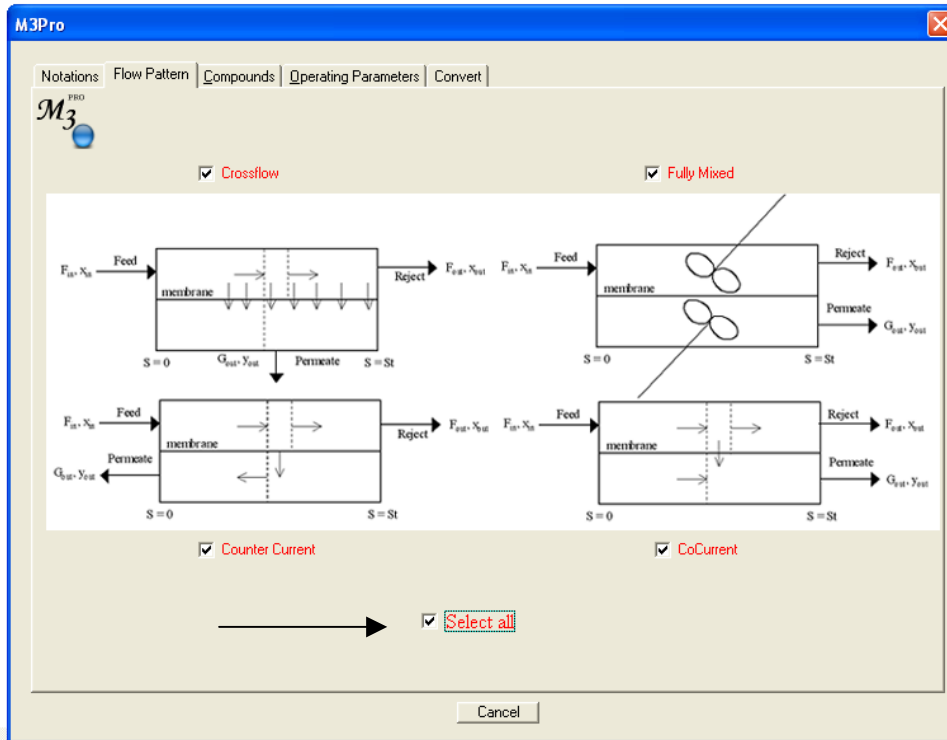
The following actions have to be carried out:

1. Select a membrane type
2. double click on the membrane name, which then appears in the « selected membrane » frame
3. Select a gas type
4. Double click on the gas name, which then appears in the « selected gas » frame
5. Repeat the process for each type of gas you want to include in the feed mixture
6. Click on « validate mixture ». The number of selected compound is shown so that the user can check the mixture number of compounds.



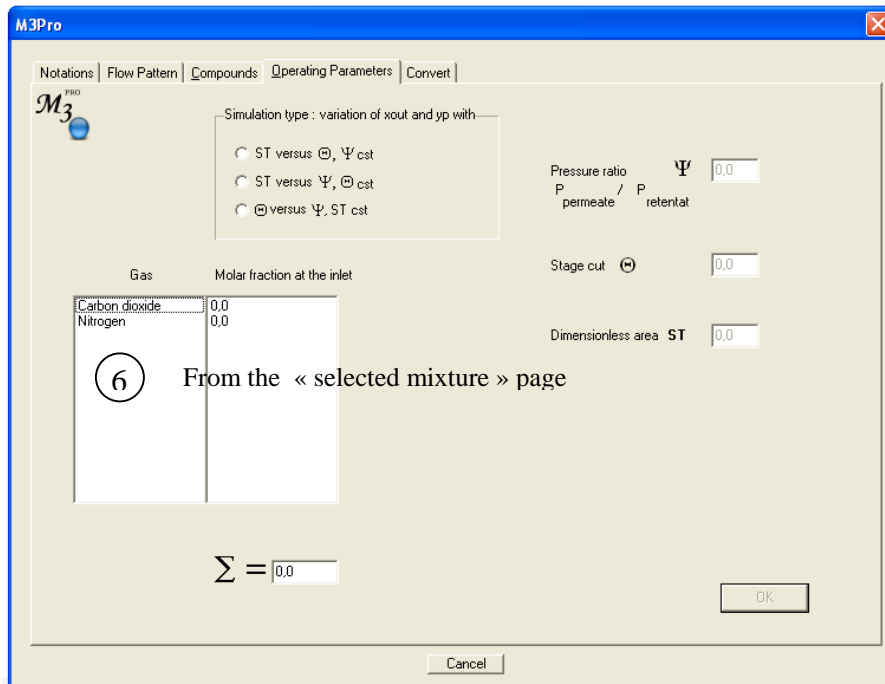
Select a hydrodynamic flow pattern

1, 2, 3 or 4 different hydrodynamic flow patterns can be selected, either by clicking on each pattern type which is chosen, or by clicking on « select all » if the four patterns have to be simultaneously computed.

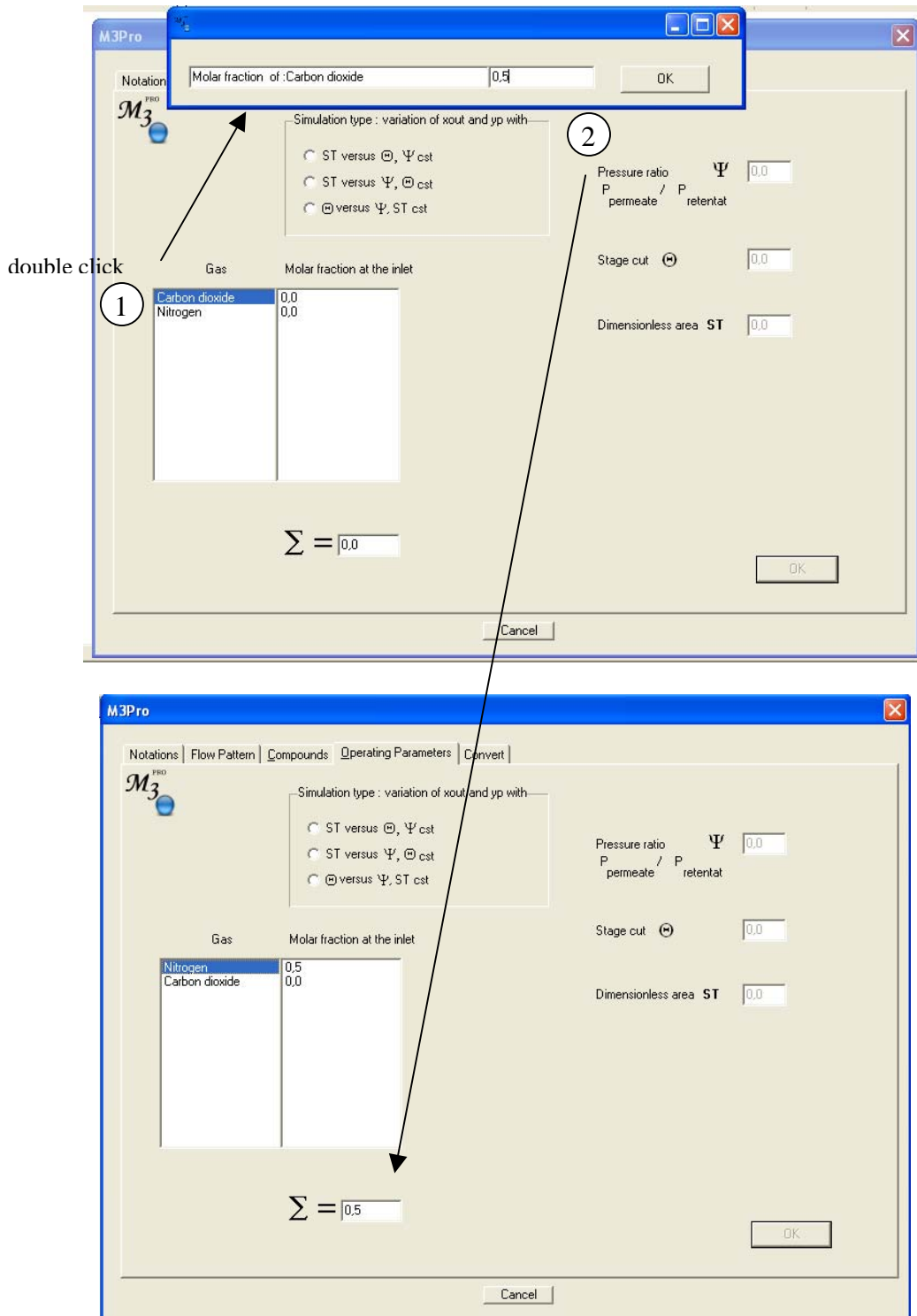


Defining the feed mixture conditions

Open the « Operating parameters » page. The mole fraction associated to each selected gas on the feed side appears.



In order to save the mole fractions data set, double click on a given gas name. Enter the corresponding mole fraction in the new window which has opened, and then click on « OK ». The sum of mole fraction is indicated in « Σ », so that you can check that the total effectively corresponds to 1 at the end of the process.

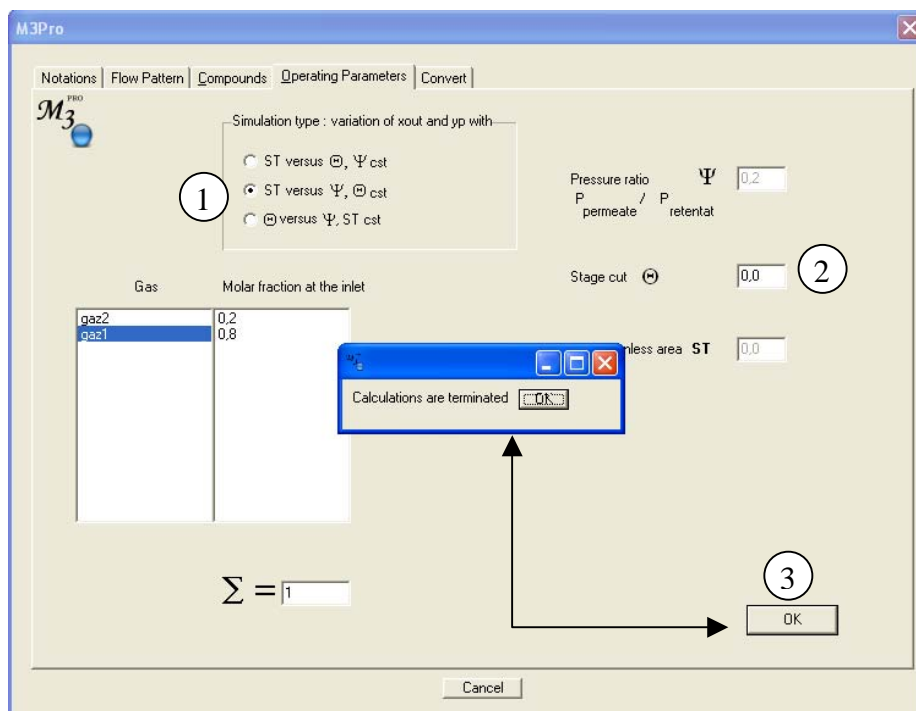


Computation type selection

$\mathcal{M}_3^{\text{PRO}}$ will compute the retentate and permeate compounds mole fraction as a function of:

- membrane surface area and stage cut for a fixed pressure ratio,
- membrane surface area and pressure ratio for a fixed stage cut,
- stage cut and pressure ratio for a fixed membrane surface area

For a given option, a series of information will be asked. When all the necessary information has been entered, « OK » is activated. The computation then starts and a message indicating the end of the process is shown.



Results

After the simulation has been performed, a series of text files is created, where the results are saved and the simulations conditions summarized (membrane name, gas names, mixture composition, permeability data associated to the gas/membrane pairs).

```
Cross Flow_psi - Bloc-notes
Fichier Edition Format Affichage ?

-----
-- version 1      Software M3 Pro      --
--              : Cross Flow         --
--              : LSGC                --
-- Roda bounaceur - Valerie warth - Eric Favre --
-----

Number of compounds = 2
Name of the membrane : binaire
Mixture :
Compound 1 : gaz2
Compound 2 : gaz1
Permeability of compound 1 : 0.10D+00
Permeability of compound 2 : 0.10D+01
Molar fraction of compound 1 : 0.20D+00
Molar fraction of compound 2 : 0.00D+00

  Psi      St      teta      X 1      X 2      Y 1      Y 2
0.0010  1.00E-05  1.99E-06  2.00E-01  0.00E+00  1.00E+00  0.00E+00
0.0110  1.00E-05  1.89E-06  2.00E-01  0.00E+00  1.00E+00  0.00E+00
0.0210  1.00E-05  1.79E-06  2.00E-01  0.00E+00  1.00E+00  0.00E+00
0.0310  1.00E-05  1.69E-06  2.00E-01  0.00E+00  1.00E+00  0.00E+00
0.0410  1.00E-05  1.59E-06  2.00E-01  0.00E+00  1.00E+00  0.00E+00

Ln 1, Col 1
```