

BRIC Tutorials

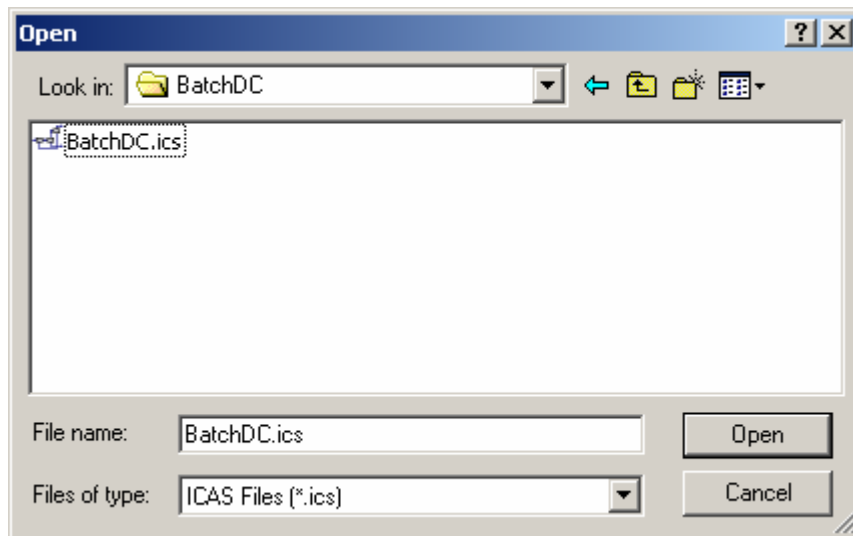
1. Batch Distillation
2. Reactive Flash

Example 1: Batch Distillation

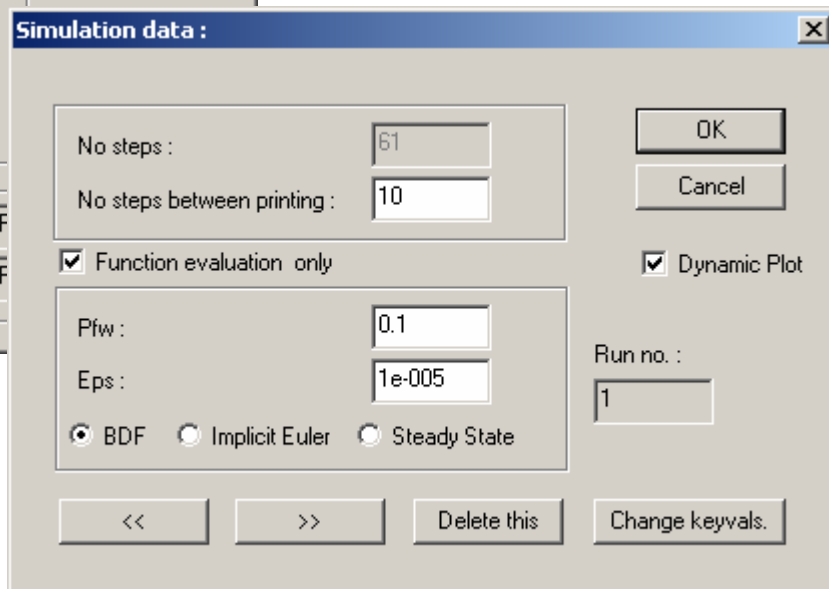
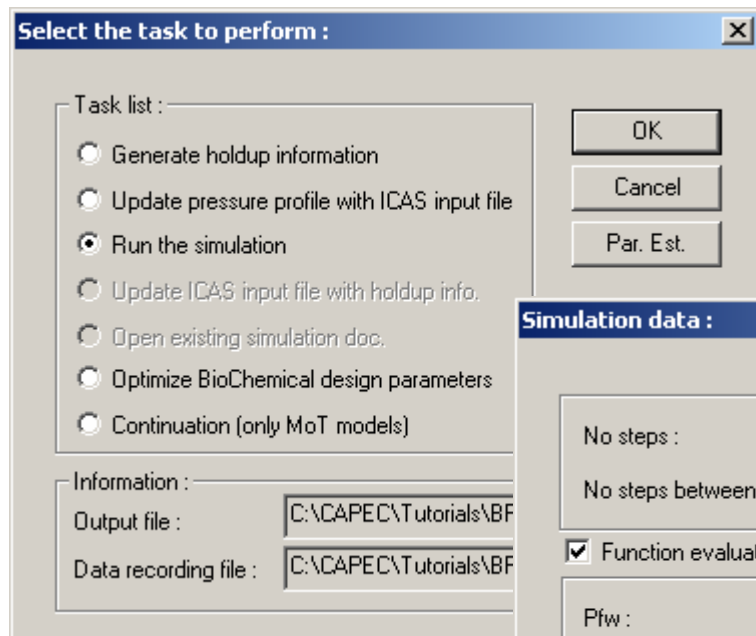
Purpose: To set up an operating sequence and validate it through dynamic simulation.

Problem Description: A charge of 45.4 kmol of 25 mole% benzene (B), 50 mole% monochlorobenzene (MCB) and 25 mole% of ortho-dichlorobenzene (DCB) is to be distilled. Desired product purity 99% and yield (amount of product) 95%

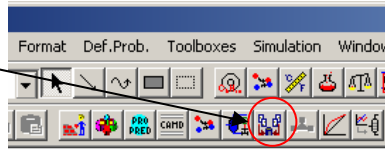
A. Open file BatchDC.ics from ICAS



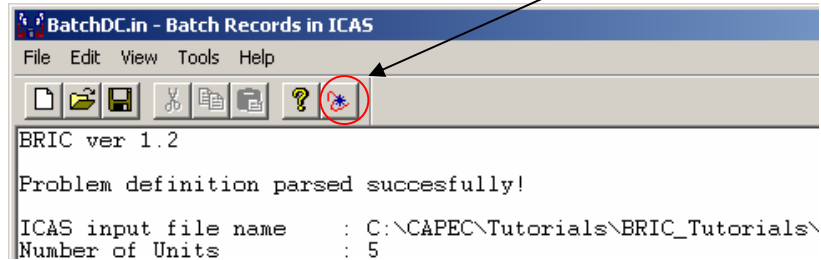
B. Run the Dynamic simulation from ICAS (Dynsim) in the Function Evaluation Only mode



C. The operating steps and conditions need to be specified in BRIC. From the ICAS screen, click the BRIC button.



One can specify operating steps and conditions, by clicking on the Show Runs button in the main BRIC screen.

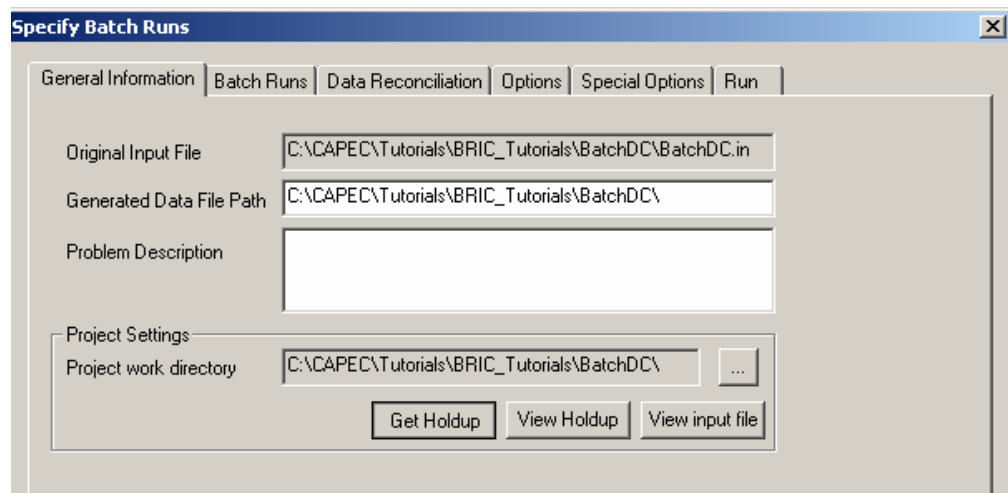


The main operation step specification dialog which appears consists of 6 sub-items. The items are described in the table below.

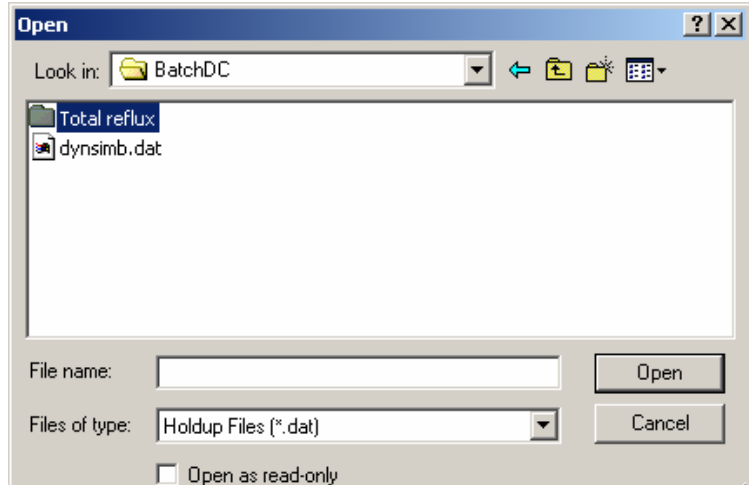
General Information	Shows where the process input file is located, where the data will be stored and can hold a brief description of the problem
Batch Runs	Defines the number of operation steps and the stopping conditions for each step. A condition profile can also be generated
Data reconciliation	For each operation step it can be specified how much information should be gathered and at what frequency it should be gathered
Options	For each operation step feed streams can be activated or deactivated, divider fractions can be changed or a new holdup can be generated.
Special options	For each operation step the method of solution can be changed, thermodynamic model can be changed, certain unit (CSTR & distillation) parameters can be changed
Run	Initiates the simulation runs and specifies how the runs should compile the information gathered, set scaling values and print frequency

C.1 Define initial process and conditions

Select the general information tab to view the initial process and starting conditions. BRIC will use the input file from ICAS as default initial process. Make sure that the input file contains the correct initial process conditions.



Press the Get Holdup button to specify the initial holdup. Select/open the holdup file (dynsimb.dat) corresponding to total reflux from the related directory .

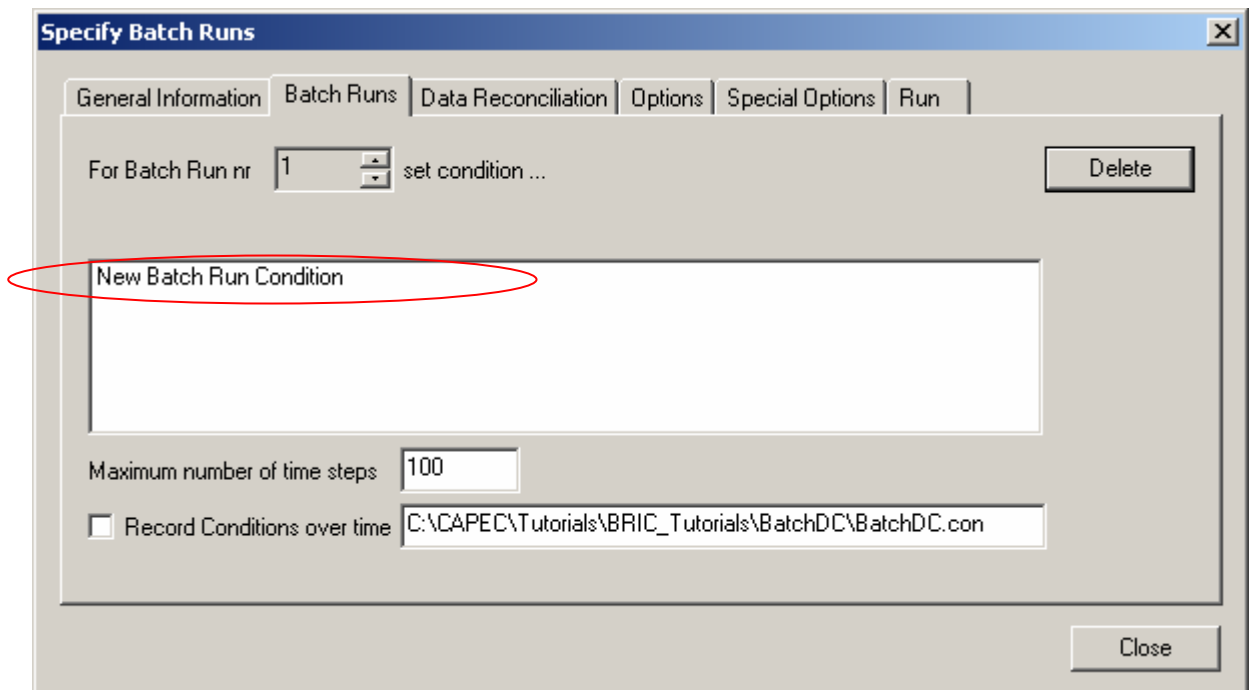


C.2 Define operation step 1

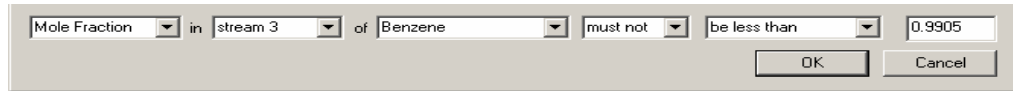
The steps for defining a desired operating sequence will be identified in the BRIC file. The desired operating sequence for the distillation column example is described in the following table.

Period nr	Reflux ratio	Vapour boilup rate	Period time (hr)
1	1.294	100	0.0919
2	1.969	100	0.0441
3	2.65	100	0.0597
4	3.865	100	0.0618
5	6.654	80	0.0993
6	11.962	80	0.0954

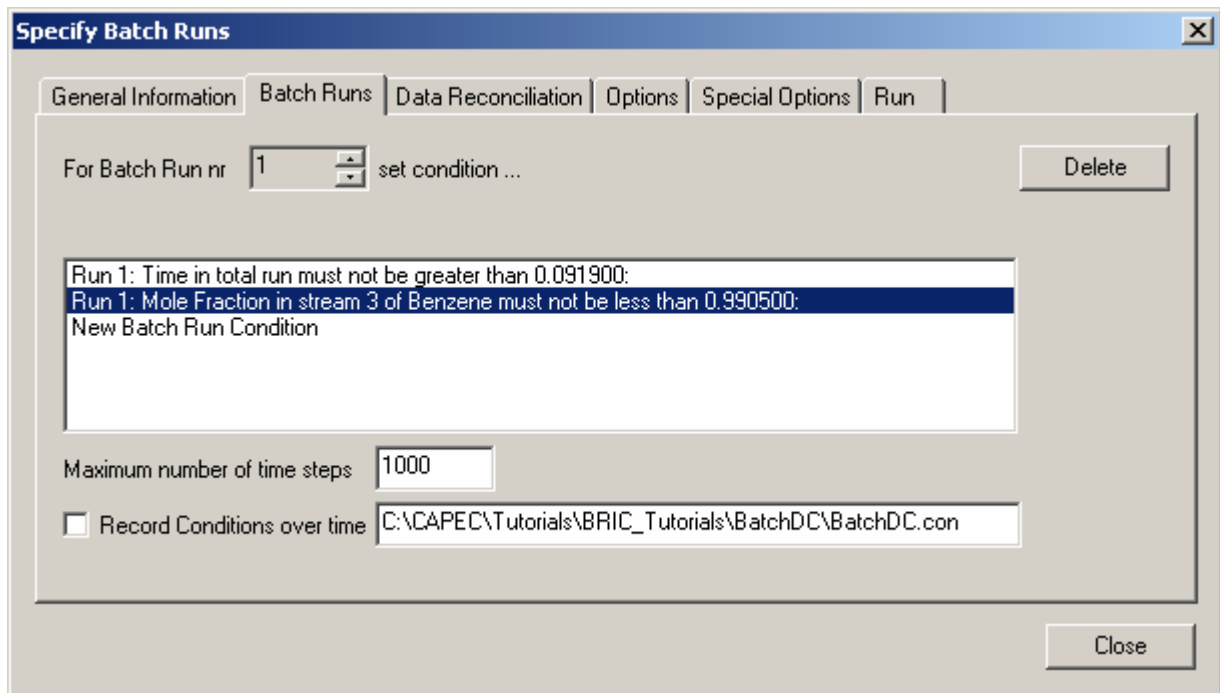
In operation step 1, we need to set the conditions for the termination of this run as well as the data reconciliation level. It is not necessary to change any stream parameters (options tab), since the initial process conditions in the input file are the same for the desired period nr 1. In the Batch runs tab, verify that the current batch run is set to 1 and double click on the New batch run condition line. This is shown in the screen shot below.



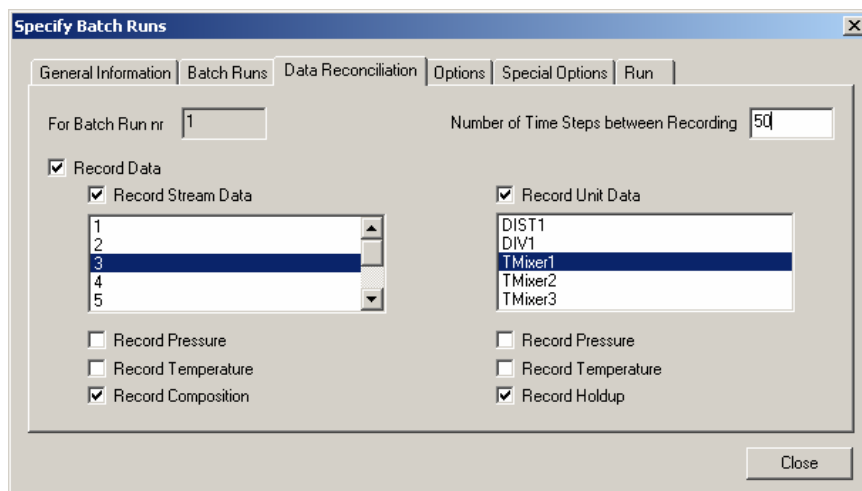
Double clicking on the New Batch Run Condition, displays the condition definition dialog. Different end criteria for the same run can be chosen. Additional end criterion for each period (except the time) can be the distillate purity.



The Batch Runs tab for the first run is shown below:

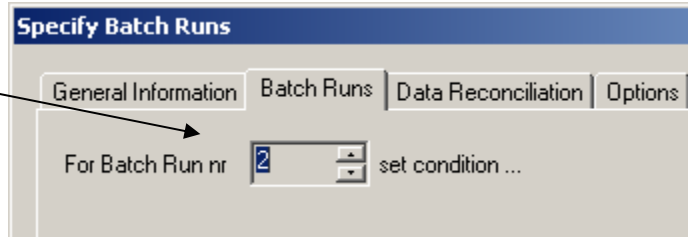


Next we will specify the amount of information to gather in this step. The Data Reconciliation tab is selected and the information to specify is marked. For a Distillation problem, useful information could be the distillate's composition profile (stream 3) and product tank's holdup profile (Tmixer 1).



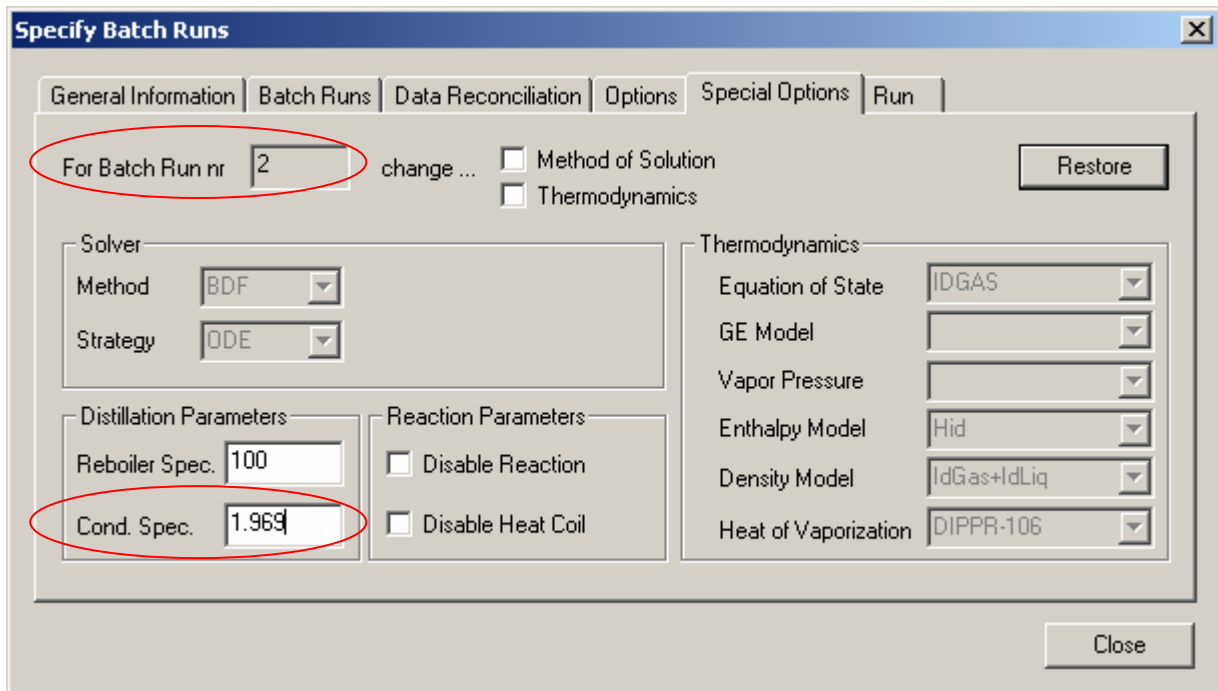
C.3 Define operation step 2 to the last step

Specifying a new operation step is made in the Batch Runs tab where the For Batch Run nr is increased, as shown below.



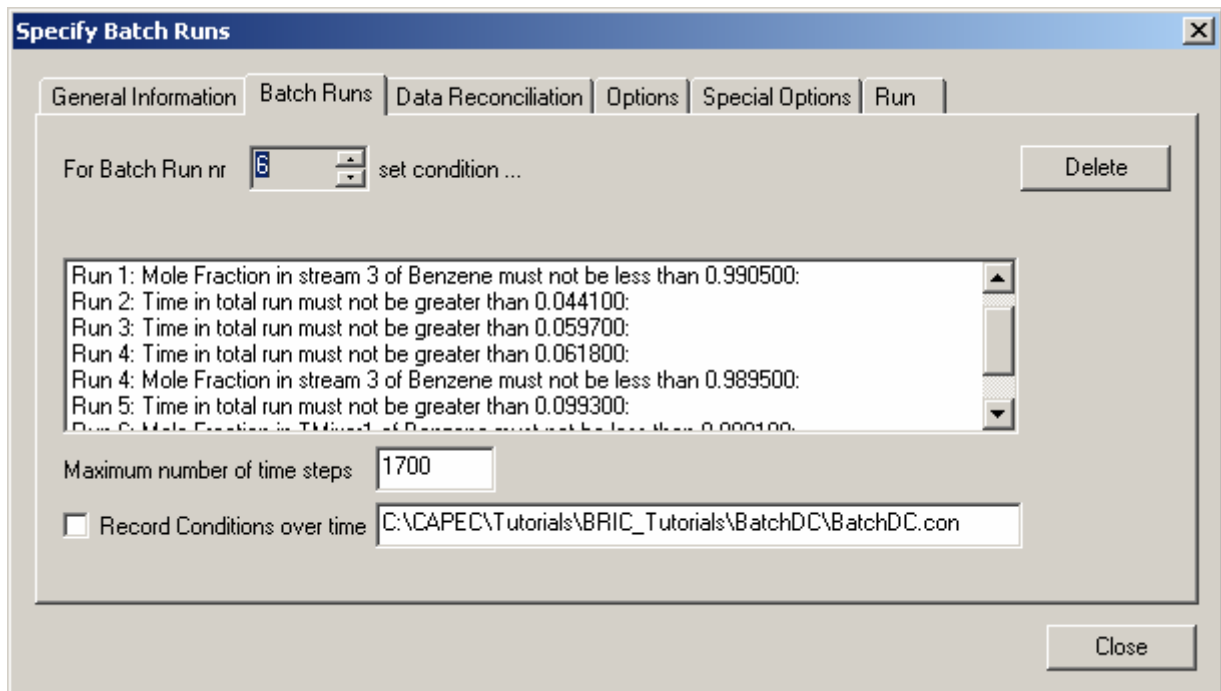
As in operation 1, the new run end criteria are specified in the **New Batch Run Condition** and the data is gathered in the **Data Reconciliation**. However, now one has the possibility to change parameters either of the streams or of the units. So, for example, changing the reboiler's and condenser's parameters is possible.

For the second operating step (corresponding to period 2 in the sequence), we need to change the reflux ratio to 1.969 from the value of 1.274 that was specified for operating step 1.



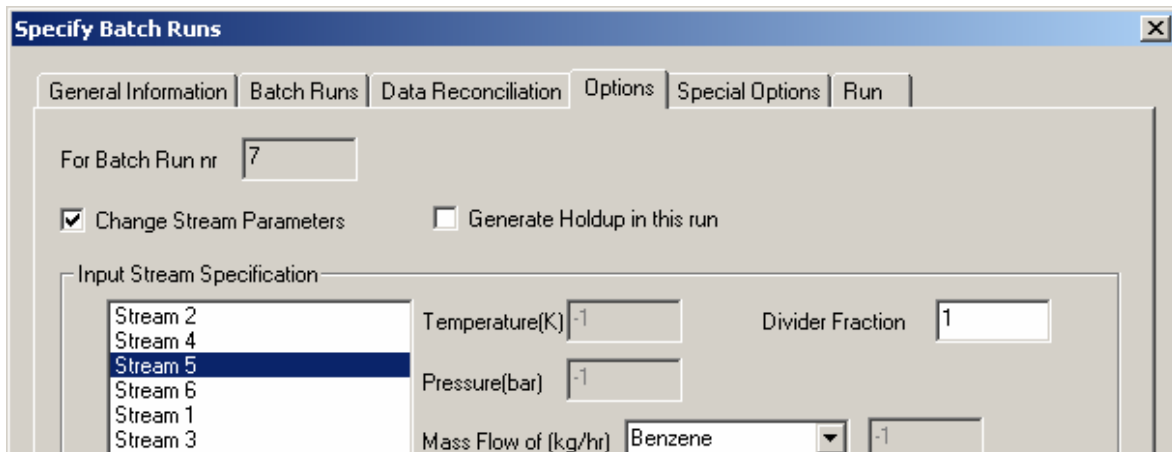
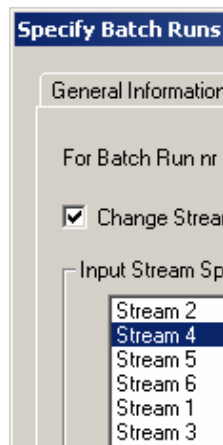
The procedure is repeated until all the operating steps are defined, the information to be gathered specified and the appropriate changes in the unit (distillation) parameters made.

The final Batch Runs tab is like that:

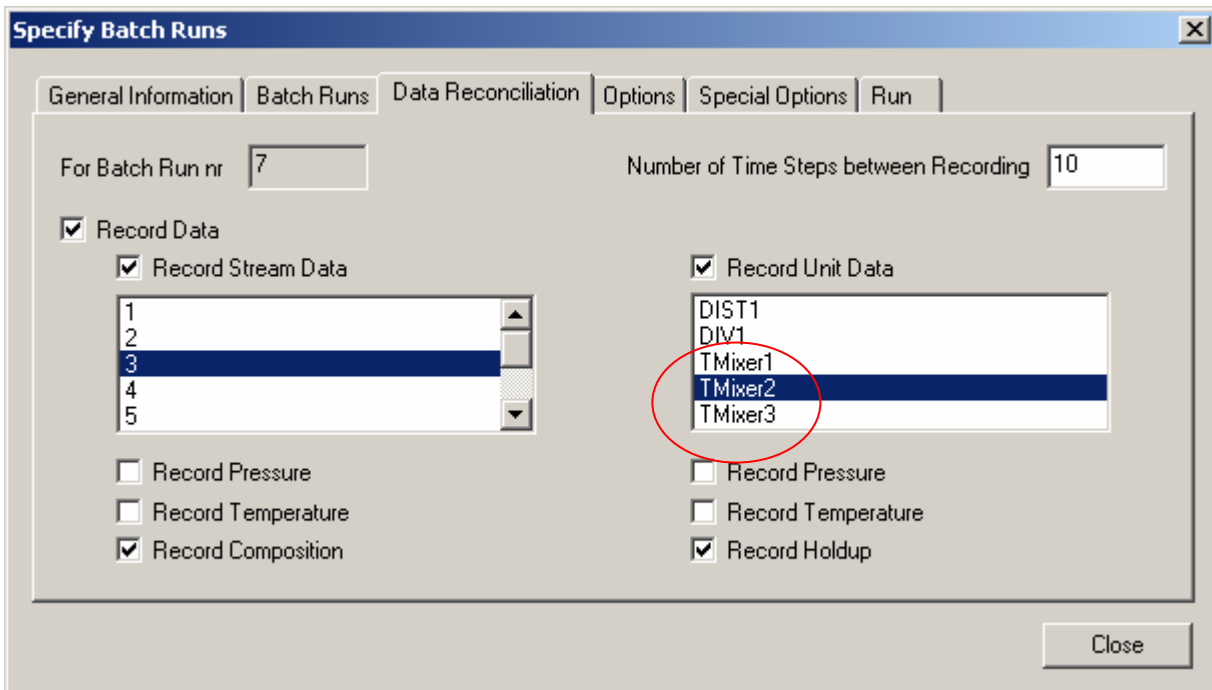


Additionally, when the objectives (purity and yield) for product 1 (benzene) are satisfied, we can collect an off-cut product in the second product tank (Tmixer2).

We need to specify an extra batch run (nr 7), where the stream parameters are changed. In this run, the valve to Tmixer1 is closed and the one for Tmixer2 is opened. This is done by changing the divider fraction for streams 4 and 5 from 1 and 0 to 0 and 1 respectively.



Note that the data gathered for this run will need to change. We will need to collect data for the second product tank (Tmixer2).

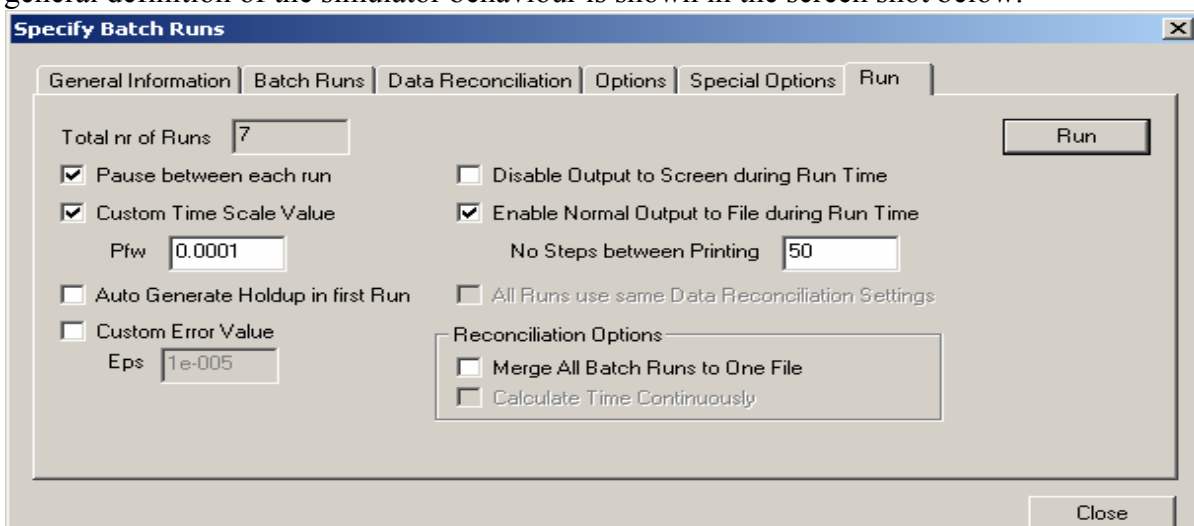


The final step is to define how the simulation should be performed.

C.4 Define general problem information for BRIC

The Run tab is used to define the behaviour of the simulation engine and other specific simulation engine values. The Custom Time Scale Value is defined in this tab. A value of 0.1 is usually sufficient for a CSTR problem, while for distillation problems this could go down to 0.0001. The Pause between each run option is also checked. This will stop the simulation engine between each step and report which condition, if any, was fulfilled.

If the time step is scaled down (as in the case of a distillation column), then in order to have a faster simulation, the print frequency should be reduced (to 20-100, rather the default value 10). The general definition of the simulator behaviour is shown in the screen shot below.



C.5 Run the batch simulation

Pressing the Run button will initiate the simulation engine. Before starting the simulation engine it is recommended that a copy of the ICAS input file (*.in) and the holdup file (dynsimb.dat) is made (and kept at a different folder than the work directory). If an operation step fails for some reason, all the steps following will be corrupted. The error must be corrected and all steps must be redone.

C.6 Simulation results

BRIC will output the following files. [process] refers to the name the process is saved as in ICAS.

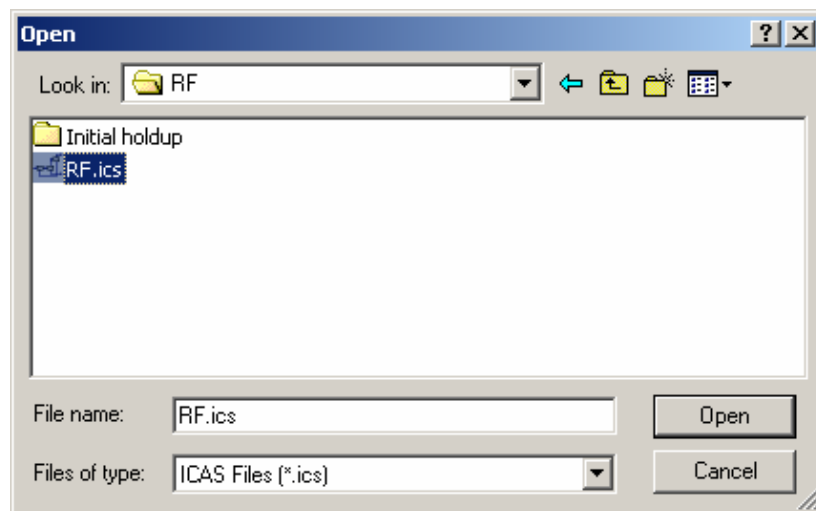
- Run0.csv
- Run1.csv
- ...
- Run(n-1).csv, n being the number of runs specified (Run6.csv in this case)
- [process].out (in this case BatchDC.out)

Example 2: Reactive Flash

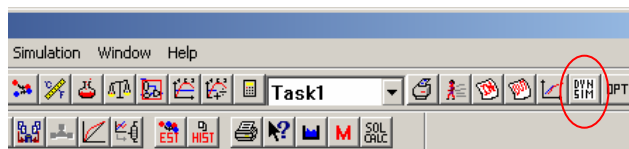
Purpose: To set up an operating sequence, where the heat input to the reactor can change from run to run (additional feature of BRIC), and validate it through dynamic simulation.

Problem definition: A 2-phase reaction system, where reaction is taking place in the liquid phase but vapour is also present.

- A. Open file RF.ics from the ICAS screen.



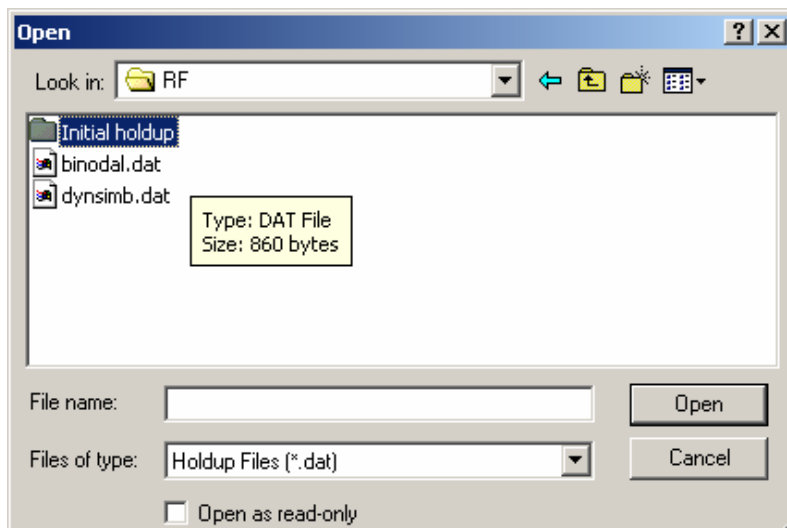
- B. Run the Dynamic simulation from ICAS (Dynsim) in the Function Evaluation Only mode



- C. Go to BRIC as described in section C of the Batch Distillation example.

C.1 Define initial process and conditions

In the general information tab, the input file can be viewed (checked that it is correct) and the initial holdup can be selected. The holdup file is selected from the folder (Initial holdup) where a copy of dynsimb.dat is kept. One can also view the Holdup to check whether the right file was selected.



C.2 Define operating steps and conditions

The desired operating sequence for the reactive flash example is as follows:

	Heat input	
	+ 400 MJ/hr	$P \leq 1.5$ atm
	0 MJ/hr	1hr or $P \leq 1.8$ atm
	+ 100 MJ/hr	$P \leq 2.1$ atm
4	0 MJ/hr	$P \leq 2.3$ atm

In operation step 1, we need to set the conditions for the termination of this run as well as the data reconciliation level. It is not necessary to change any stream parameters (options tab), since the initial process conditions in the input file are the same for the desired period nr 1. In the **Batch runs** tab, verify that the current batch run is set to 1 and double click on the **New batch run condition** line.

Pressure(bar) in FLASH1 of [] must not be greater than 1.5

OK Cancel

Since, there is no flow out of the flash (neither vapour nor liquid flow out), in order to observe the effect of the vapour in the pressure, interesting/useful data to reconcile are the temperature, pressure and holdup of the flash.

Specify Batch Runs

General Information | **Batch Runs** | Data Reconciliation | Options | Special Options | Run

For Batch Run nr: 1 Number of Time Steps between Recording: 10

Record Data

Record Stream Data Record Unit Data

1
2
3 FLASH1

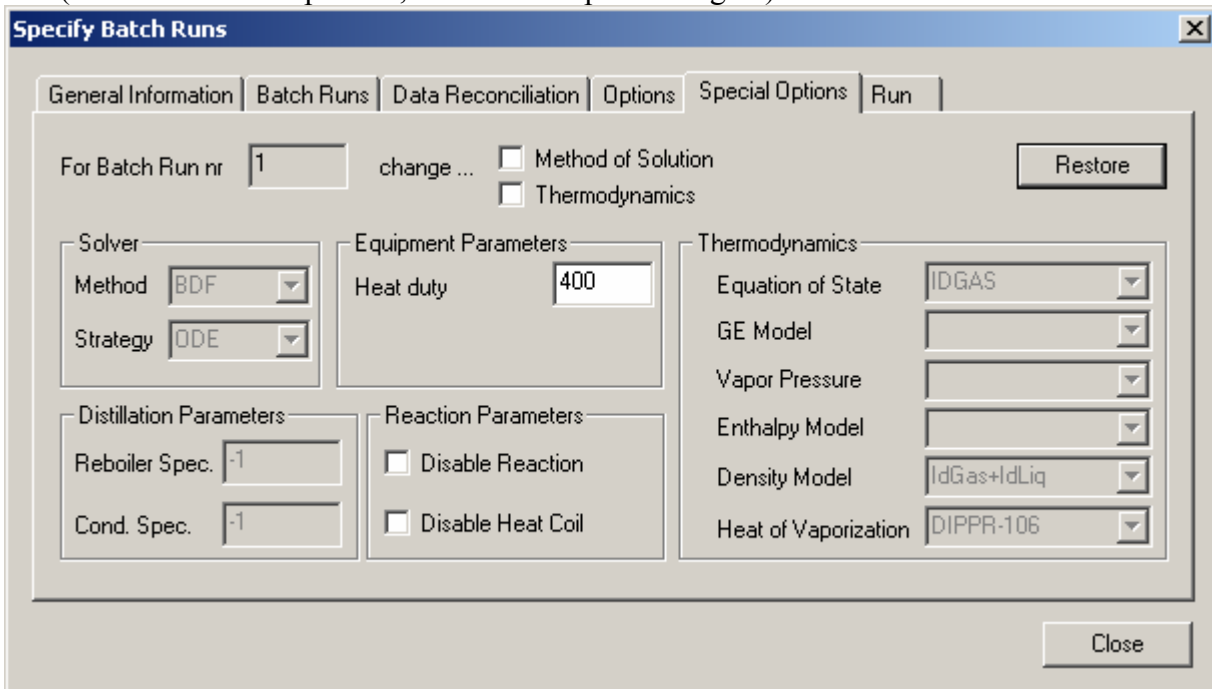
Record Pressure Record Pressure

Record Temperature Record Temperature

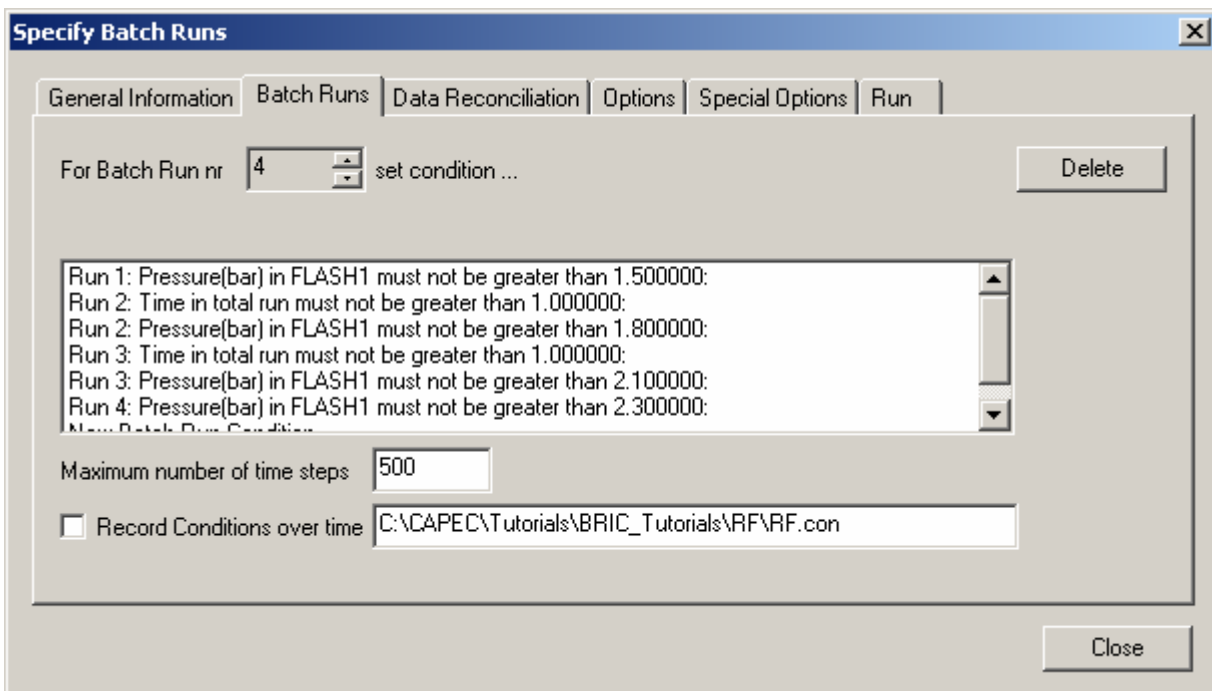
Record Composition Record Holdup

Close

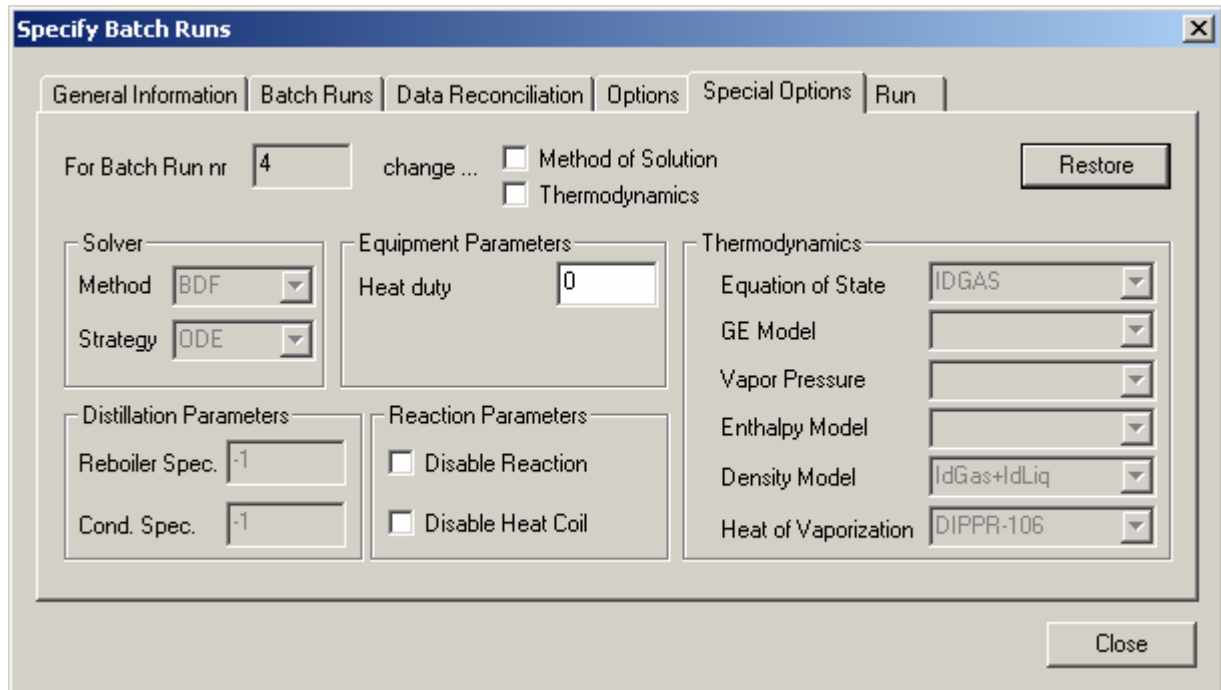
The heat duty for the reactor (reactive flash) should be defined for **each** run in the Special Options tab. (Even if the heat input is 0, it should be specified again)



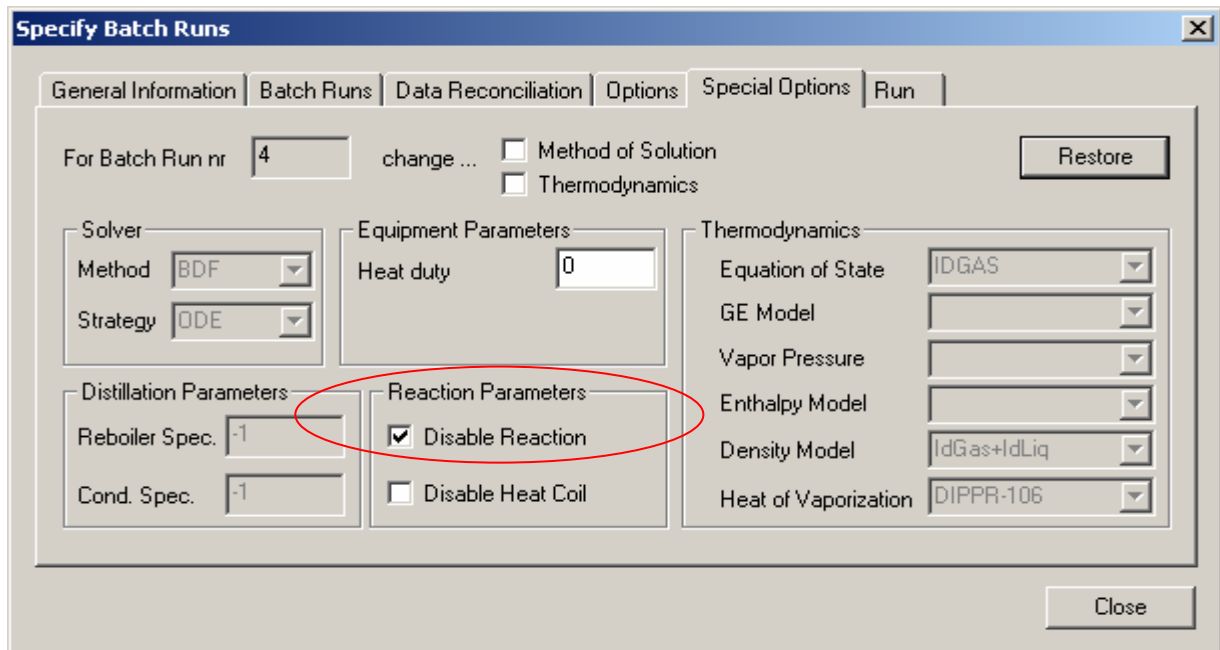
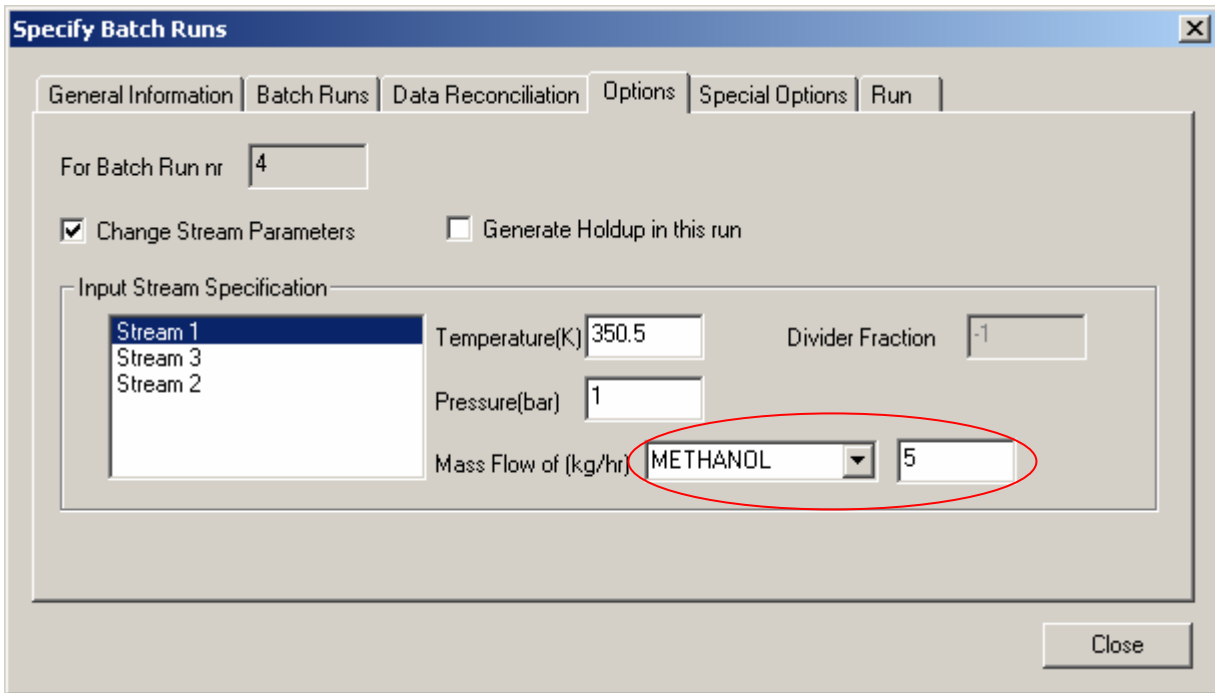
The other batch runs are specified in the same way (as shown in section C.3 of the distillation example). The Data Reconciliation is the same for all runs (Flash P, T and holdup). The end criteria for each run are specified according to the desired operating sequence. The final Batch Runs tab looks like the following:



The new feature of BRIC is that the heat input for the reactive flash can be changed from one batch run to the other in the same bric file. So, heat can be added for some time and then adiabatic operation can be applied, cooling, etc.



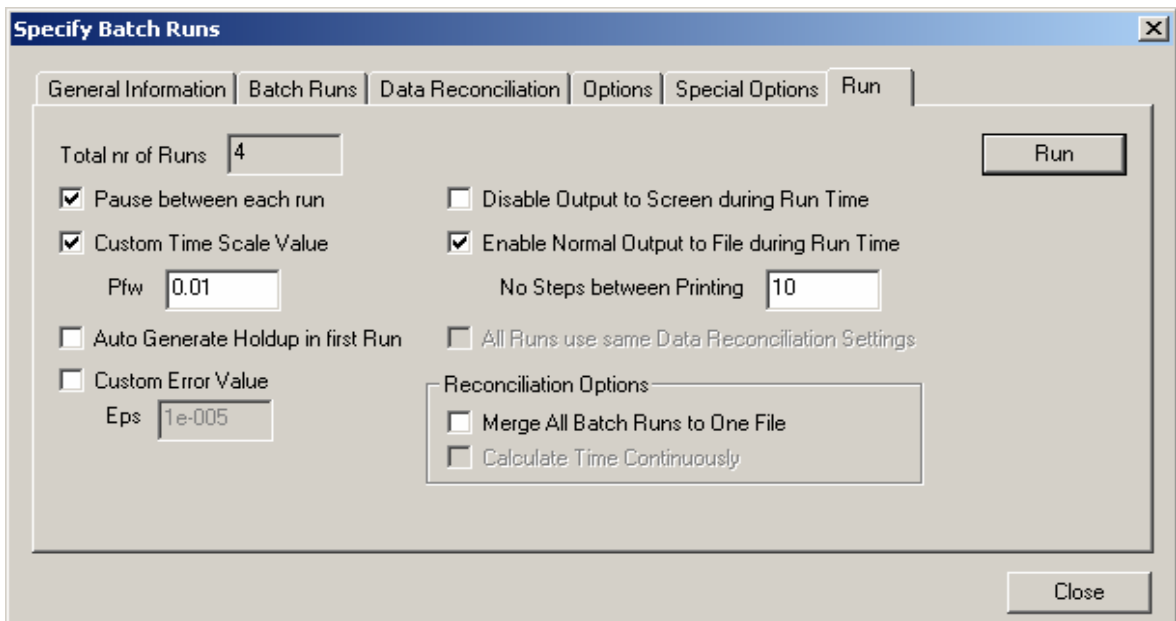
This study case is mainly a simple example to show the new capability of BRIC. Another feature (not shown in the bric file provided) of BRIC for reaction examples is that reaction can be enabled and disabled from one run to the other. Additionally, the addition of a reactant can be stopped or commenced or changed from one run to the other in the Options tab.



C.3 Define general problem information for BRIC

The Run tab is used to define the behaviour of the simulation engine and other specific simulation engine values. The Custom Time Scale Value is defined in this tab. A value of 0.01 is used for this reactive flash problem. The Pause between each run option is also checked. This will stop the simulation engine between each step and report which condition, if any, was fulfilled.

It is fine in this case to leave the print frequency to the default value 10, since the custom time scale value is not as small as it was for the distillation example.



C.4 Run the batch simulation

Similarly as for the distillation example.