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BATCHREACTOR APPLICATION EXAMPLE

SYNTHESIS REACTOR OF THYMOL

EXAMPLE PURPOSE
The main interest of this example is to use a reactive calculator generated by Simulis Kinetics after the identification of the reaction scheme of the thymol synthesis. Consequently, the components, the thermodynamic model and the chemical reactions are automatically provided in the BatchReactor simulation. The cooling device of the reactor is specified.

ACCESS	☑ Free Internet	☐ Restricted to clients	☐ Restricted	☐ Confidential

CORRESPONDING BATCHREACTOR FILE	*BATCHREA_EX_EN - Thymol.pbpr*

Reader is reminded that this use case is only an example and should not be used for other purposes. Although this example is based on actual case it may not be considered as typical nor are the data used always the most accurate available. Fives ProSim shall have no responsibility or liability for damages arising out of or related to the use of the results of calculations based on this example.

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1. INTRODUCTION

Thymol is a phenol contained in the thyme oil and in the volatile essential oils of other plants. It takes the form of colorless crystals with a specific aromatic smell. It is soluble in alcohols, in fat and oil, but slightly soluble in water. It is notably used for its antiseptic action, its antibacterial properties and its antifungal effect, as well as to stabilize the pharmaceutical preparations.

This example deals with the thymol synthesis. The operating mode involves two steps. During the first step, one of the reactants is fed, and, during the second step, the reaction is continued with no feed.

This example is the second example of a set of three, dealing with the synthesis and the purification of thymol. The first example: “SIMKIN_EX_EN – Thymol” allows to identify the chemical reactions parameters. The third example: “BATCHCOL_EX_EN – Thymol” deals with the thymol purification after its synthesis.

2. REACTION MECHANISM

The reaction mechanism for the thymol synthesis from m-cresol is as follows:

$$m\text{-}cresol + propylene \rightarrow thymol$$

Namely:

$$C_7H_8O + C_3H_6 \rightarrow C_{10}H_{14}O \quad \text{(R1)}$$

Three competing reactions are taken into account:

- ✓ 3M2P synthesis :

$$m\text{-}cresol + propylene \rightarrow 3M2P$$

Namely:

$$C_7H_8O + C_3H_6 \rightarrow C_{10}H_{14}O \quad \text{(R2)}$$

- ✓ 3M5P synthesis:

$$m\text{-}cresol + propylene \rightarrow 3M5P$$

Namely:

$$C_7H_8O + C_3H_6 \rightarrow C_{10}H_{14}O \quad \text{(R3)}$$

- ✓ 3M4P synthesis :

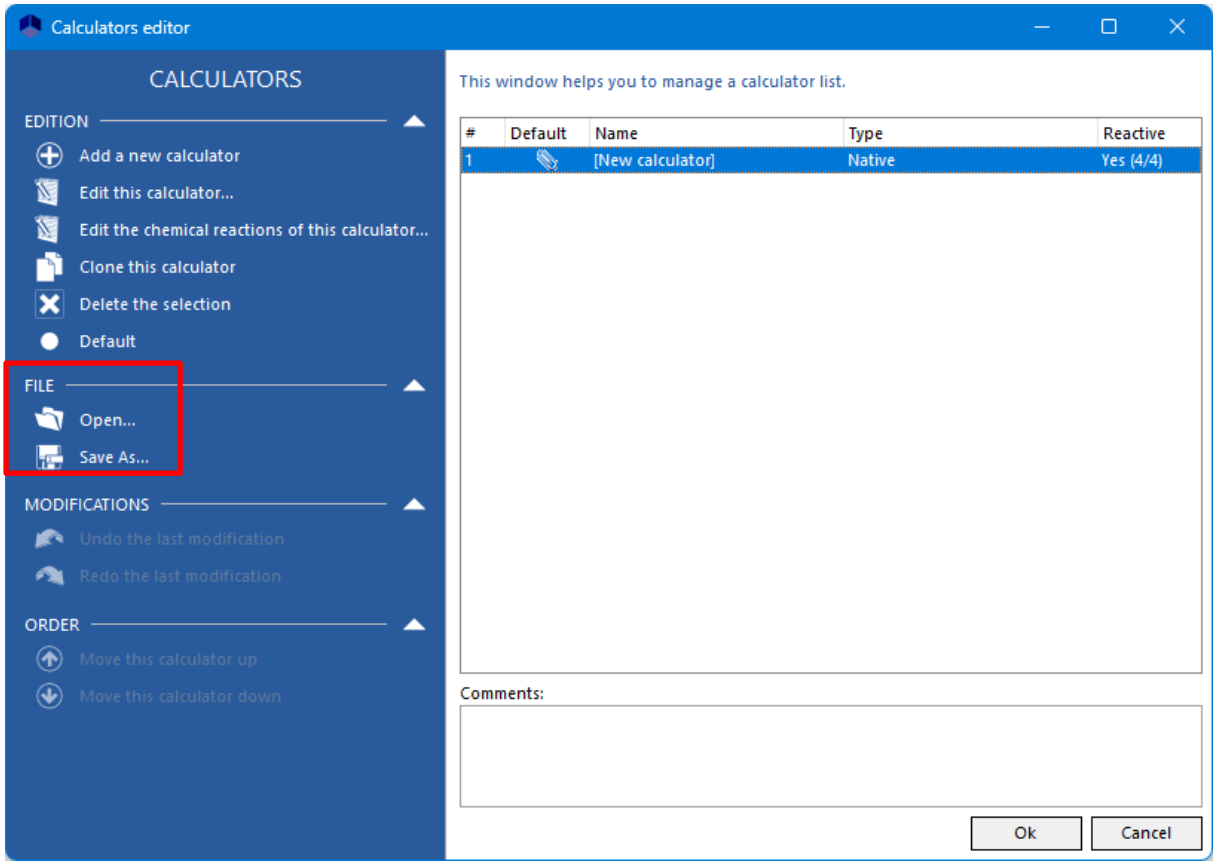
$$m\text{-}cresol + propylene \rightarrow 3M4P$$

Namely:

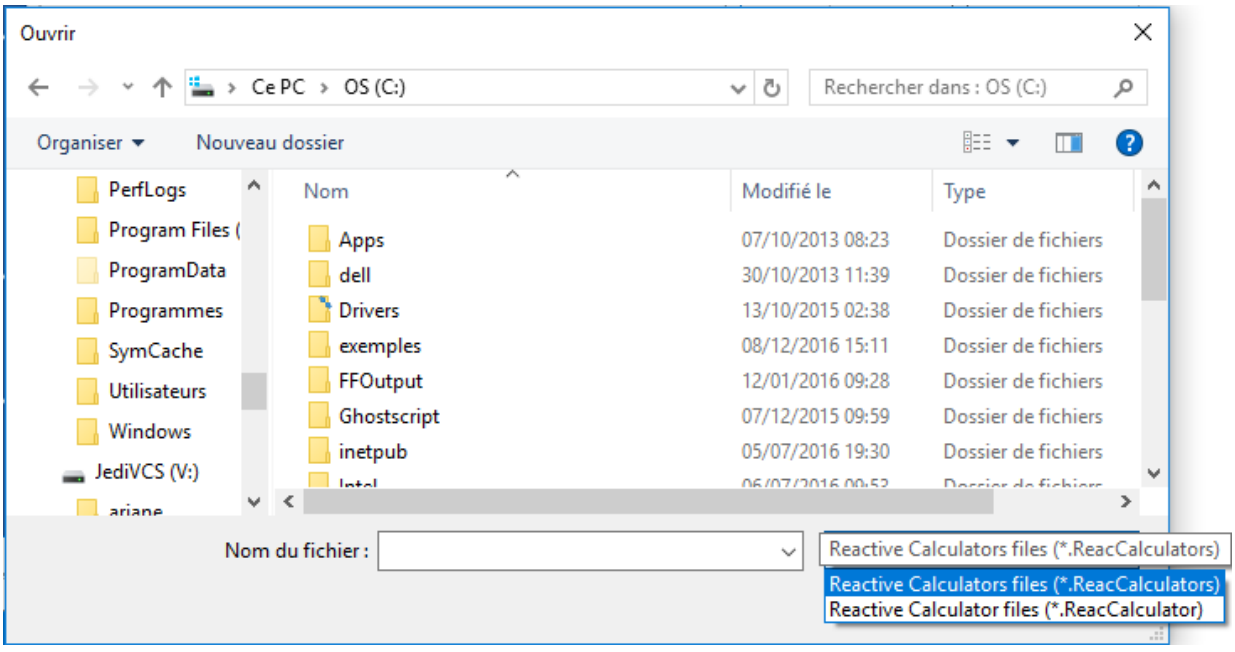
$$C_7H_8O + C_3H_6 \rightarrow C_{10}H_{14}O \quad \text{(R4)}$$

3. COMPONENTS, THERMODYNAMIC MODEL, REACTION MODEL

The components, the thermodynamic model and the reaction model (reaction scheme and reactions parameters) will be loaded directly from the “ReacCalculator” file generated at the end of the “SIMKIN_EX_EN – Thymol” example. In the calculators editor, delete the default calculator, then click **File/Open**.

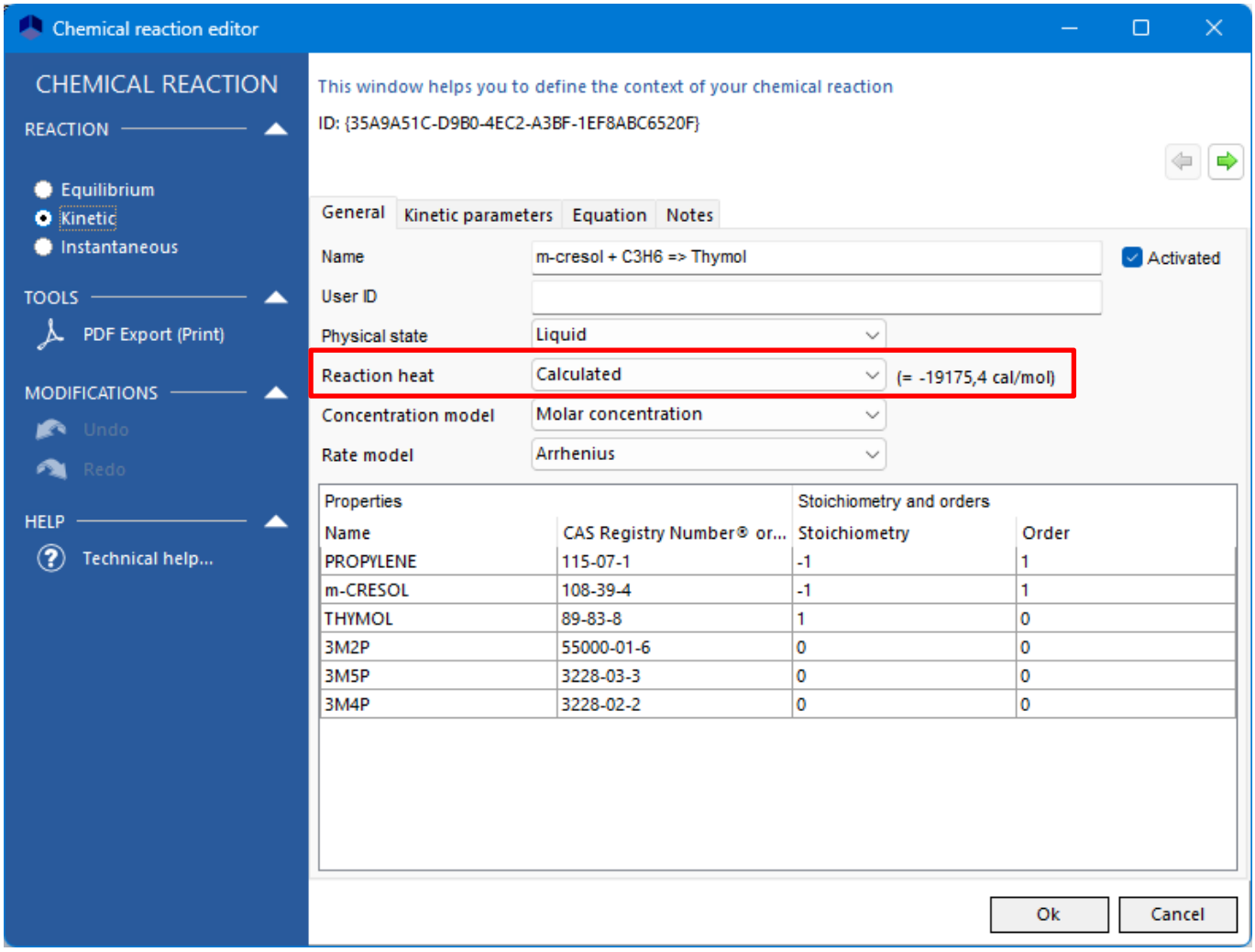


In the **Open** window, select a Reactive calculator file (.ReacCalculator) as file type.



In the example “SIMKIN_EX_EN – Thymol”, the reactions enthalpies have not been identified nor provided. It is then necessary to indicate that they will be calculated using the standard enthalpies of formation.

To do this, click on the item “Edit chemical reactions of this calculator”, then select the first reaction and click on “Edit this reaction”. In the field “Reaction heat” chose the option “Calculated”. Do this for each of the reactions.



4. SIMULATION

4.1. Process description

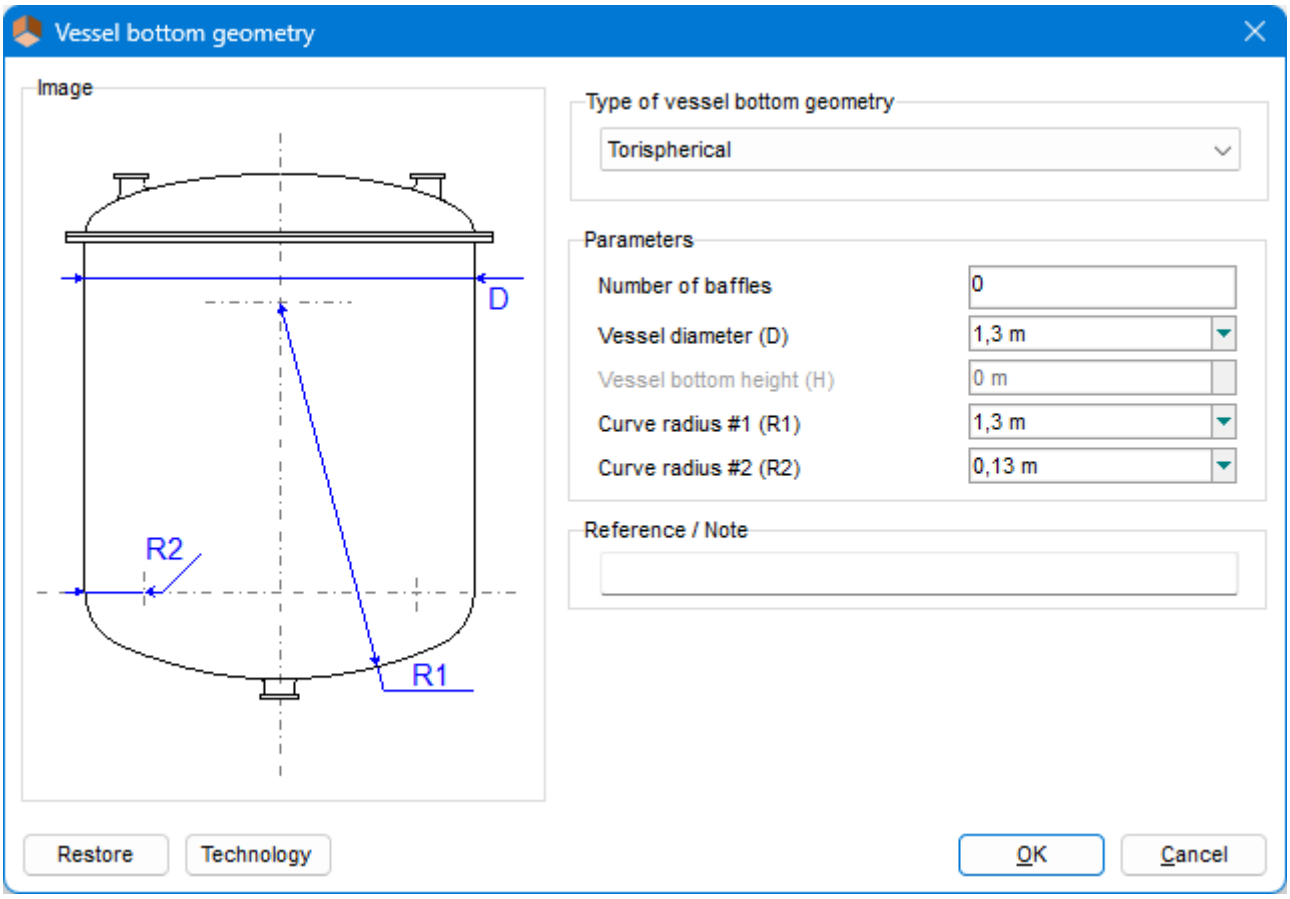
4.1.1. Reactor

The reactor used for the thymol synthesis is a monophasic liquid reactor.

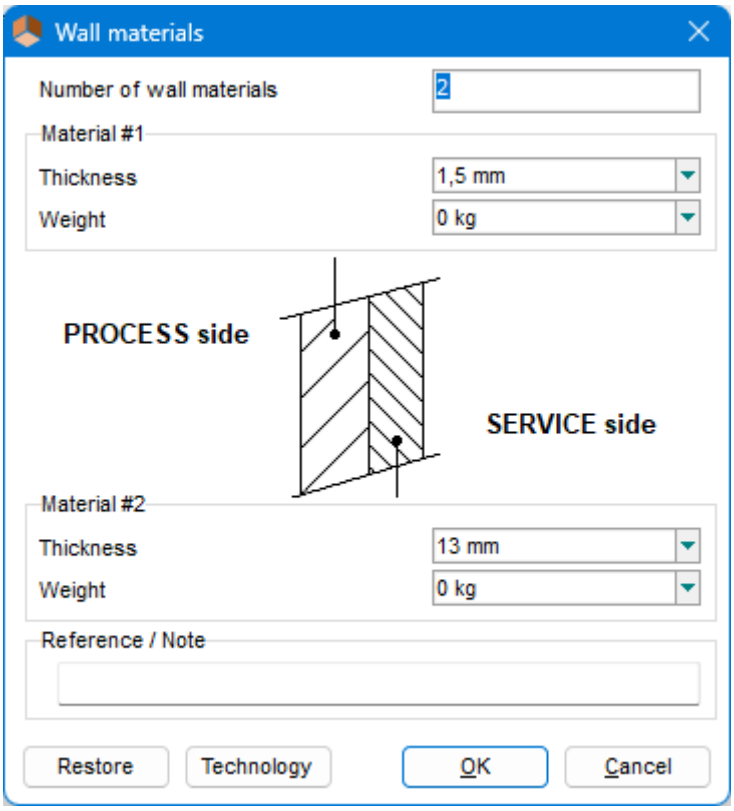
The initial conditions are presented in the following table:

Initial conditions	
Temperature	25°C
Pressure	12 atm
Initial load	
Total load	1 486 kg
Propylene	2% mass
m-cresol	98% mass

The vessel bottom geometry is described hereafter:



The reactor is made up with glass-lined steel.



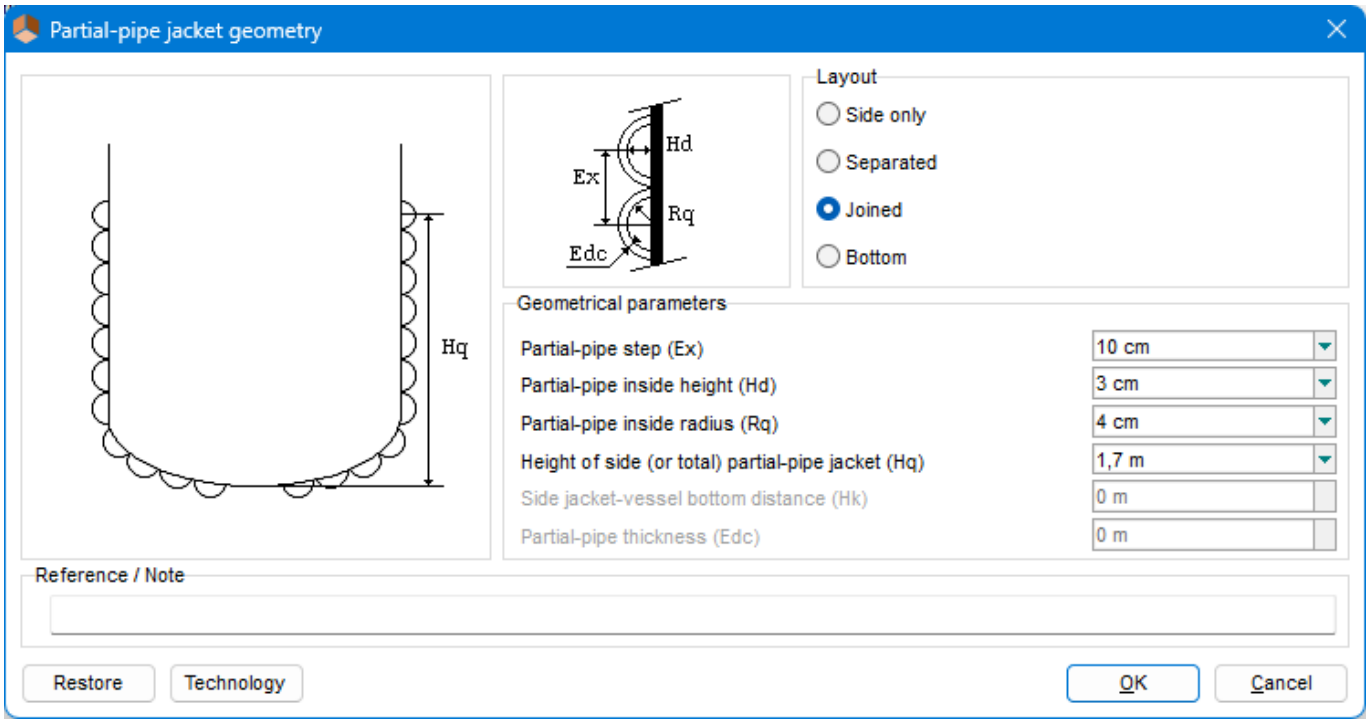
The steel thermal conductivity (material #2) is considered to be equal to 52,25 $W.m^{-1}.K^{-1}$ and the enamel thermal conductivity (material #1) to 1,161 $W.m^{-1}.K^{-1}$. The thermal conductivities are specified for each operating step.

The alarms are as follows:

	Volume	Temperature
Minimum	1 l	0°C
Maximum	3 m^3	40°C

4.1.2. Cooling device

The reactor is equipped with a wall heat exchanger (partial-pipe jacket), with the following characteristics:



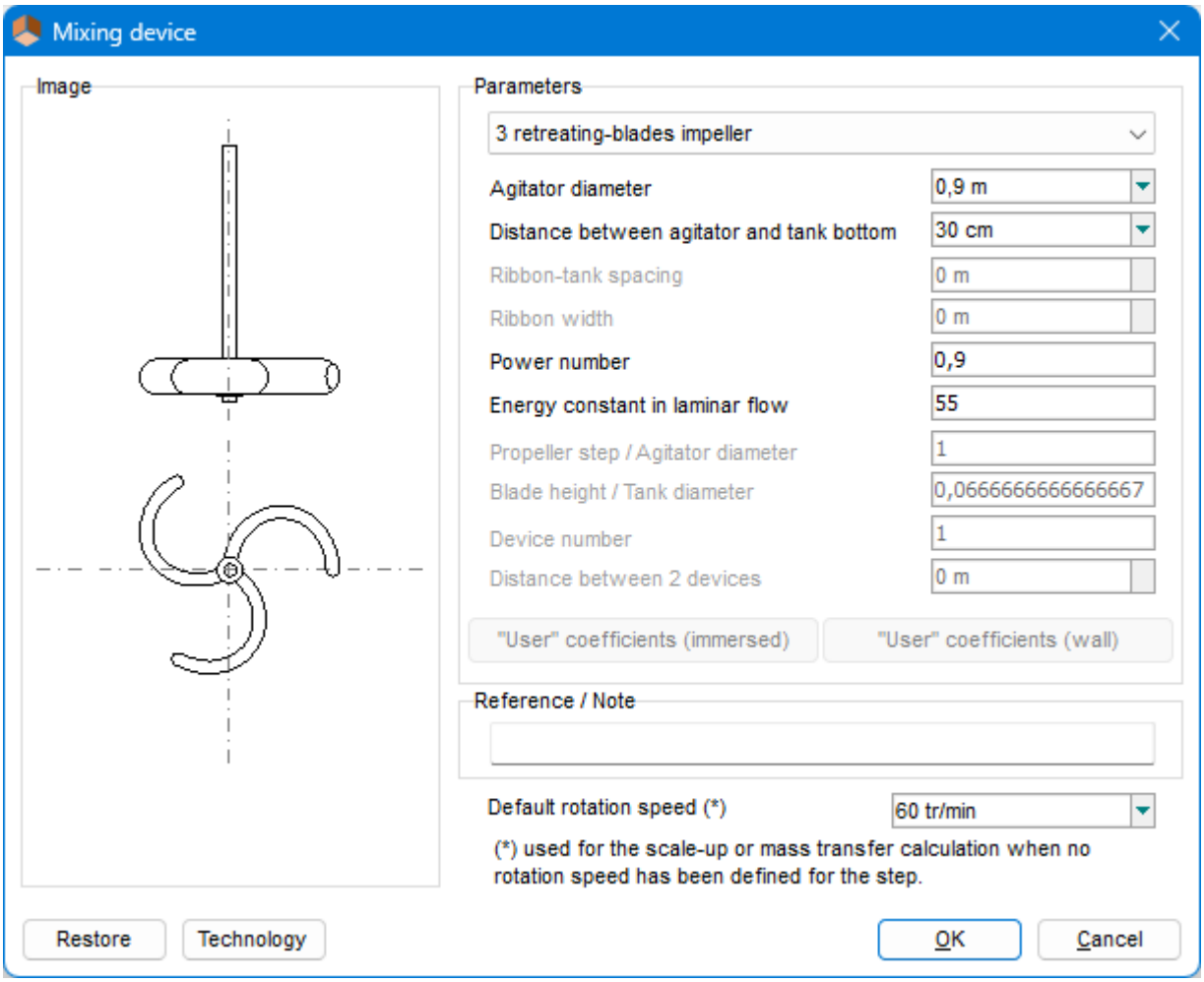
The thermal fluid used is the same for the two operating steps:

Heat transfer fluid (the same for the two steps)	
Type	Water
Mass flowrate (initial value)	1 500 kg/h
Inlet temperature	14°C

The water mass flowrate will be automatically adjusted in order to keep constant the reactor temperature as it has been defined in each operating step.

4.1.3. Mixing device

The characteristics of the mixing device appear hereafter:



The rotation speed of the agitator (60 rpm) is defined in each operating step (same speed for the two steps).

4.1.4. Feeds

A continuous flow of propylene (reactant) is supplied during the first step:

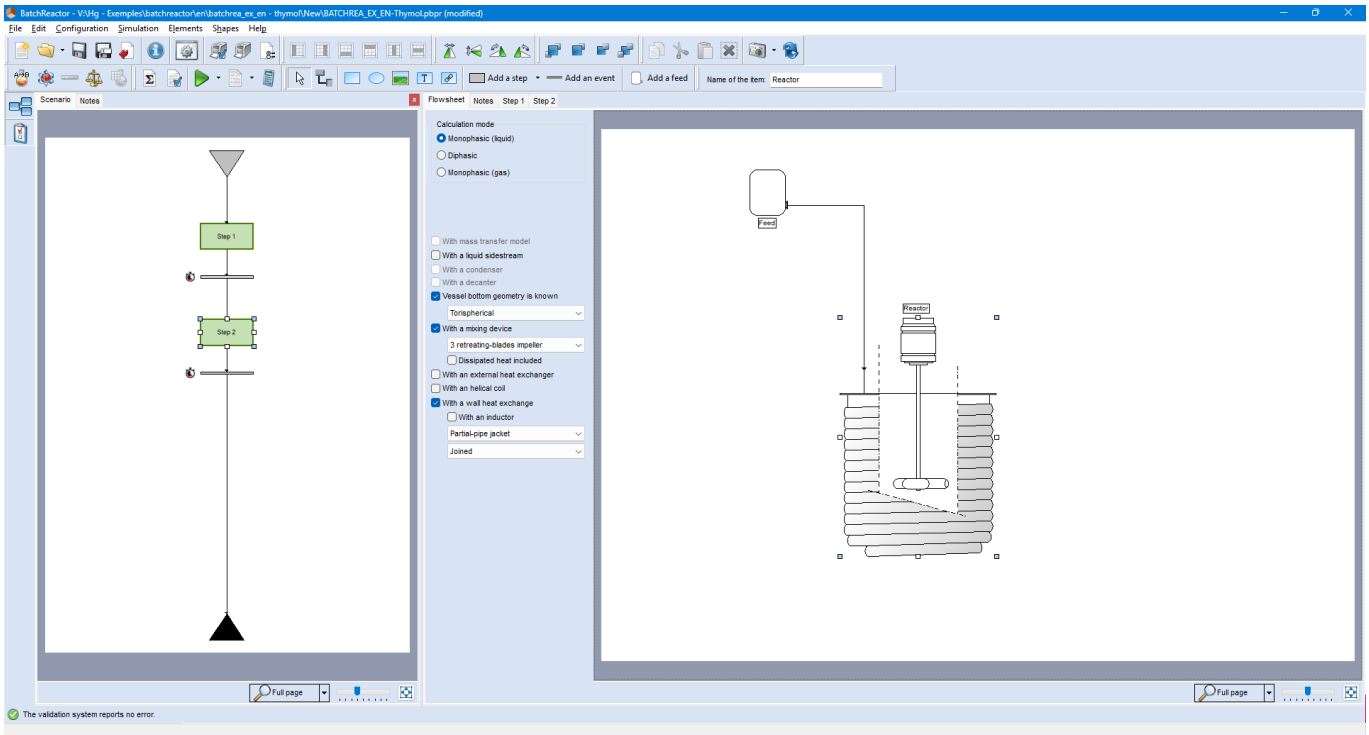
Temperature	25°C
Pressure	12 atm
Propylene flowrate	39 kg/h

4.1.5. Operating mode

The operating mode is made up with two steps. During the first step, the second reactant (propylene) is added. The reaction starts. During the second step, the reaction is carried out but without propylene feed. These two steps are carried out at constant temperature, by acting on the utility fluid flowrate. The operating parameters are given in the following table:

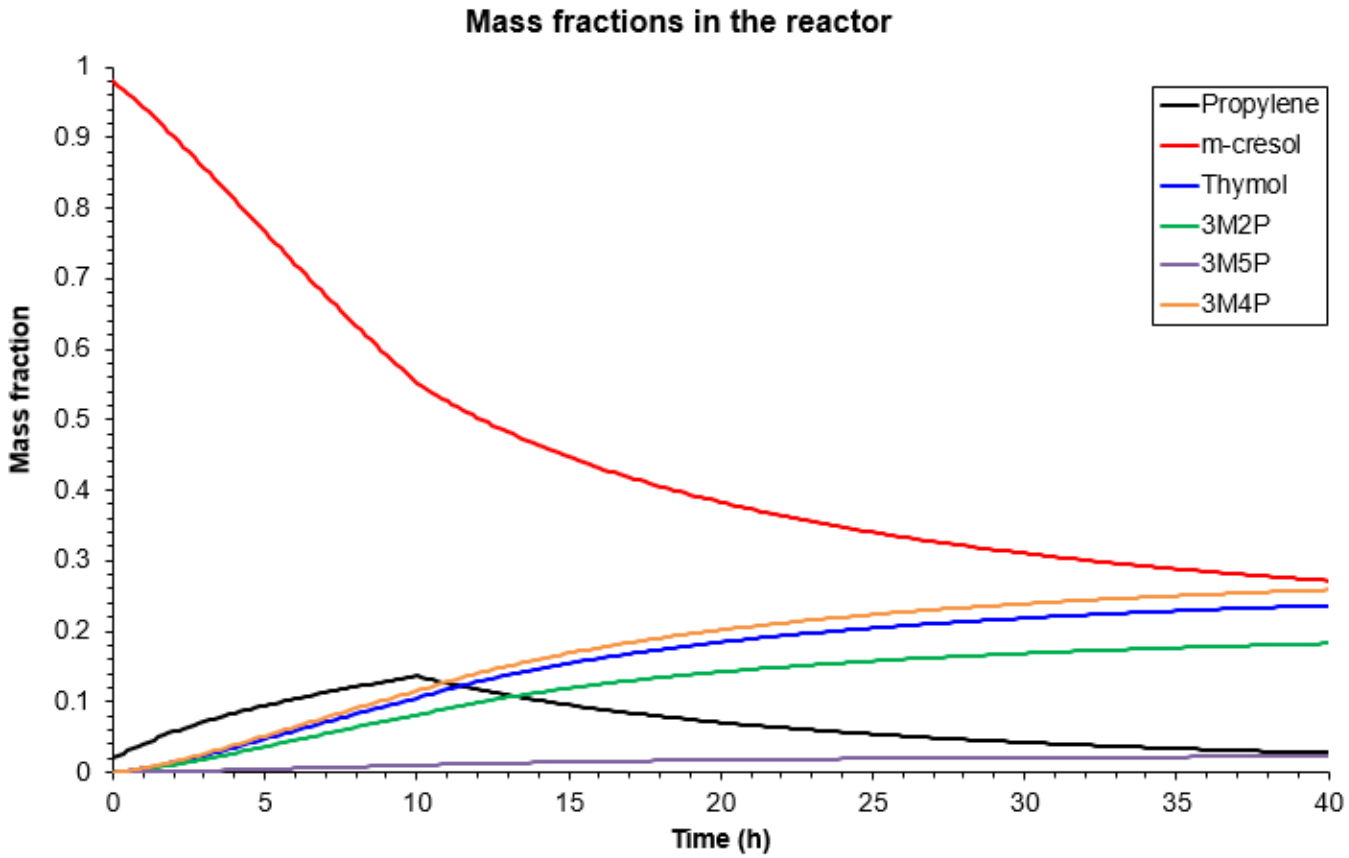
Parameter	First step	Second step
Type of step	Control of reactor temperature	
Reactor temperature	25°C	
Reactor pressure	12 atm	
Propylene feed	Open	Closed
Stop event	Time elapsed since the beginning of the step: 10 h	Time elapsed since the beginning of the step: 30 h

The scenario is presented on the left of the following screenshot and the flowsheet on the right part.



4.2. Results

The mass fraction of m-cresol decreases throughout the operation, as this reactant is present only in the initial load. The mass fraction of propylene increases during the first step (10h): as this reactant is fed with a flowrate that exceeds the quantity consumed, it then accumulates during this period. After the feed stops, it is consumed and disappears. The mass fractions of the reaction products (thymol, 3M2P, 3M5P, 3M4P) increase all along these two steps.



The following graph shows the evolution of the water flowrate necessary to keep the reactor isothermal at 25°C. For 7 hours, the necessary flowrate of utility increases as the reaction starts strongly due to the propylene addition. Then the flowrate decreases, as the m-cresol is consumed decreases, and the reaction slows down. At the beginning of the second step (i.e. after 10 hours), this change is faster as there is no longer propylene supply.