Getting started with Simulis Reactions®

Use Case 1: Features overview

Software & Services In Process Simulation

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ProSim

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Introduction

This document presents the main features of Simulis Reactions. This tool is associated to a thermodynamic calculator and enables to specify chemical reactions. Three types of chemical reactions can be defined:

- Instantaneous reactions
- Equilibrium reactions
- Reactions controlled by the kinetic

To illustrate, Simulis Reactions is used to model the reaction of production of thymol from m-cresol. The steps are the following:

- Step 1: selection of the compounds
- Step 2: selection of the chemical reaction type
- Step 3: configuration of the reaction model

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Description of the reaction model

The reaction of production of thymol from m-cresol is the following:

$$m\text{–}\,cresol + propylene \rightarrow thymol$$

This reaction is controlled by the kinetic and can be modeled using the Arrhenius law:

$$r = k^0 \times e^{\left(-E_a/RT\right)} \times C_{propylene} \times C_{m-cresol}$$

with:

Model parameters	Definition	Value
k^0	Frequency factor	197478 L.mol^{-1}.h^{-1}
E_a	Activation energy	10266 cal.mol^{-1}
C_i	Concentration of the component « i »	Process variable (mol.L^{-1})

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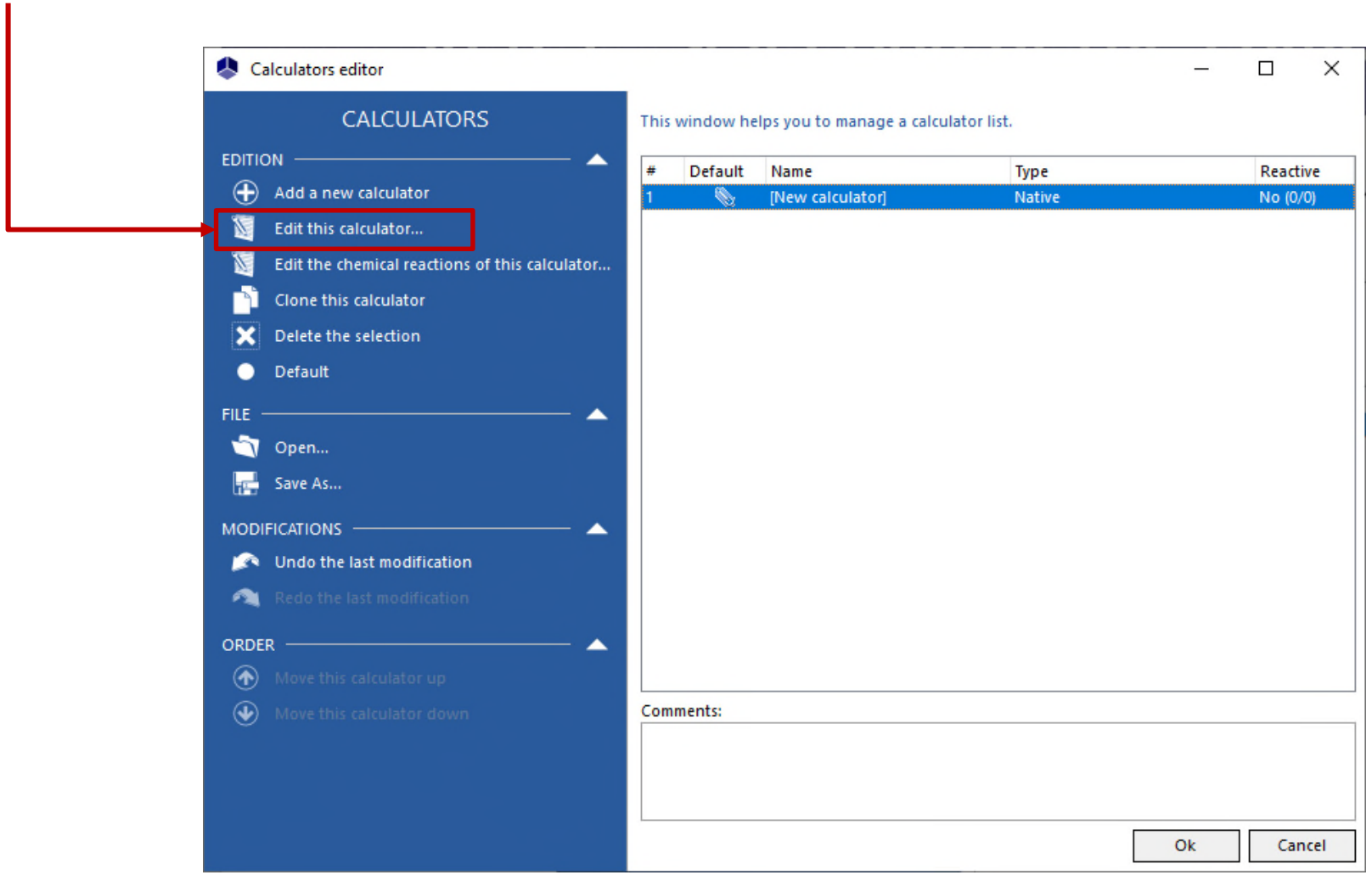
Step 1: selection of the compounds

From the "*Calculators editor*" window, select "*Edit this calculator*"



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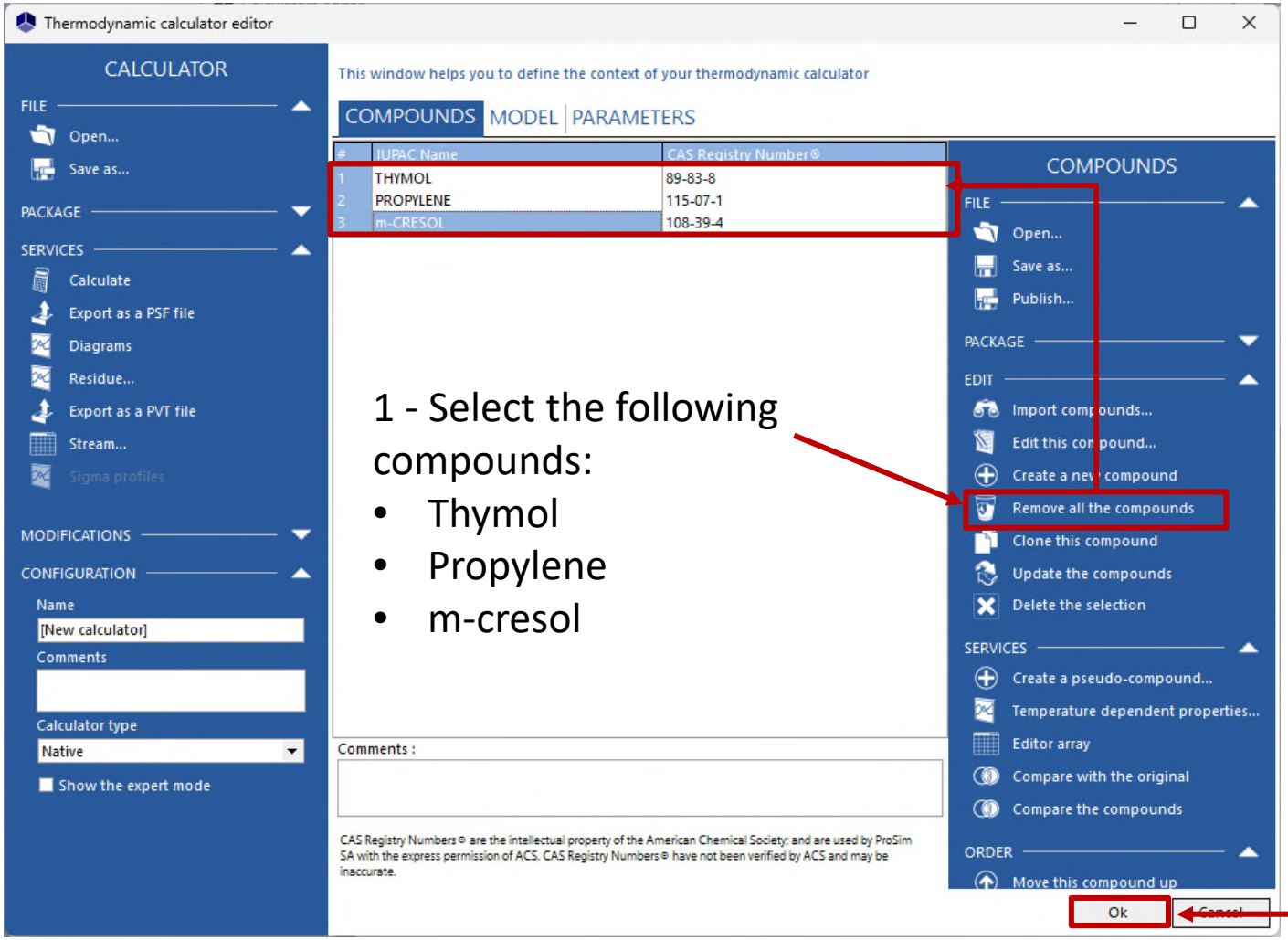
Step 1: selection of the compounds



1 - Select the following compounds:

- Thymol
- Propylene
- m-cresol

2 - Click on « *Ok* »

For more information about the compounds selection, please refer to *"Getting started with Simulis Thermodynamics, use case 1"*

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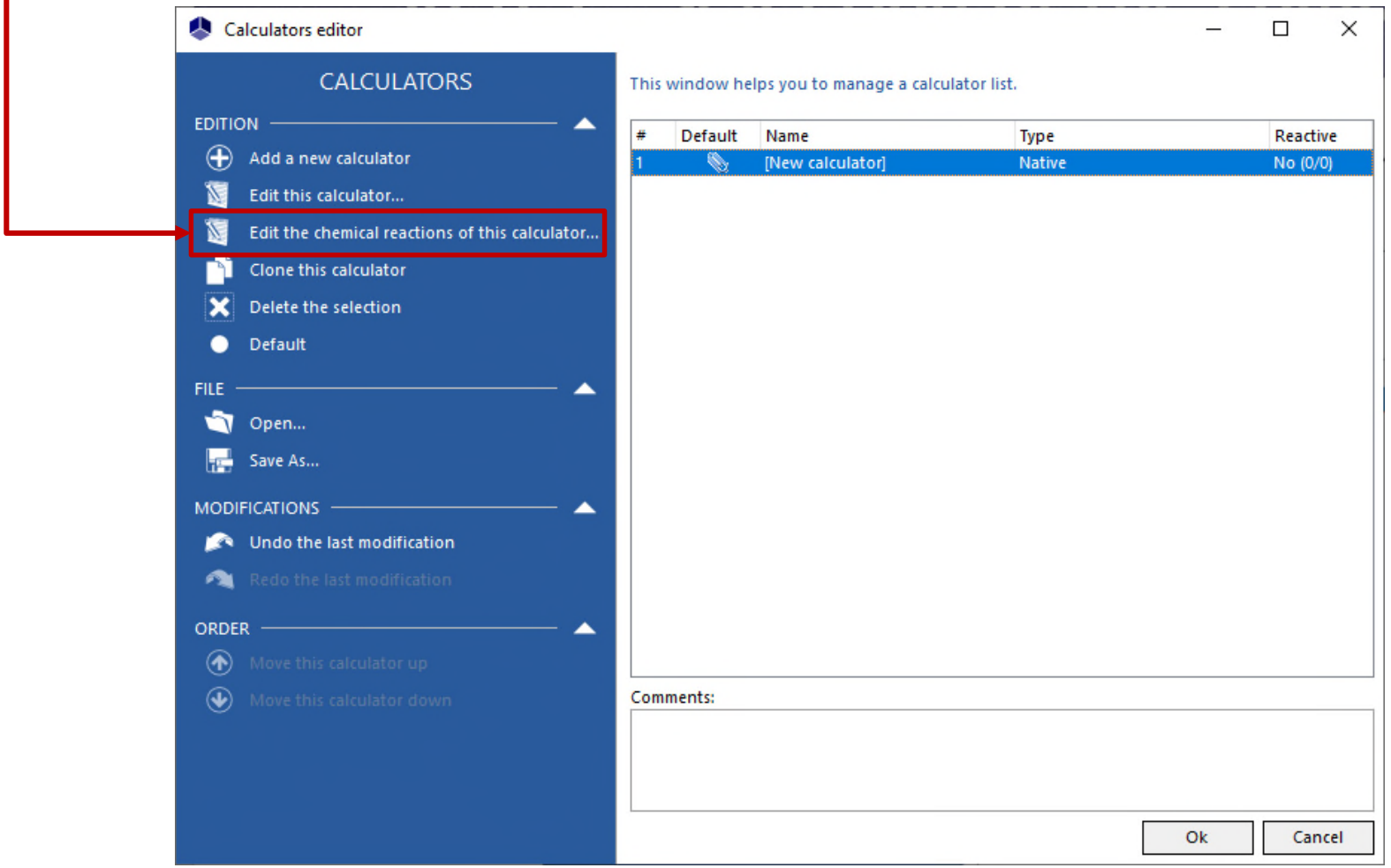
Step 2: selection of the chemical reaction type

Back to the “*Calculators editor*” window, click on “*Edit the chemical reactions of this calculator*”



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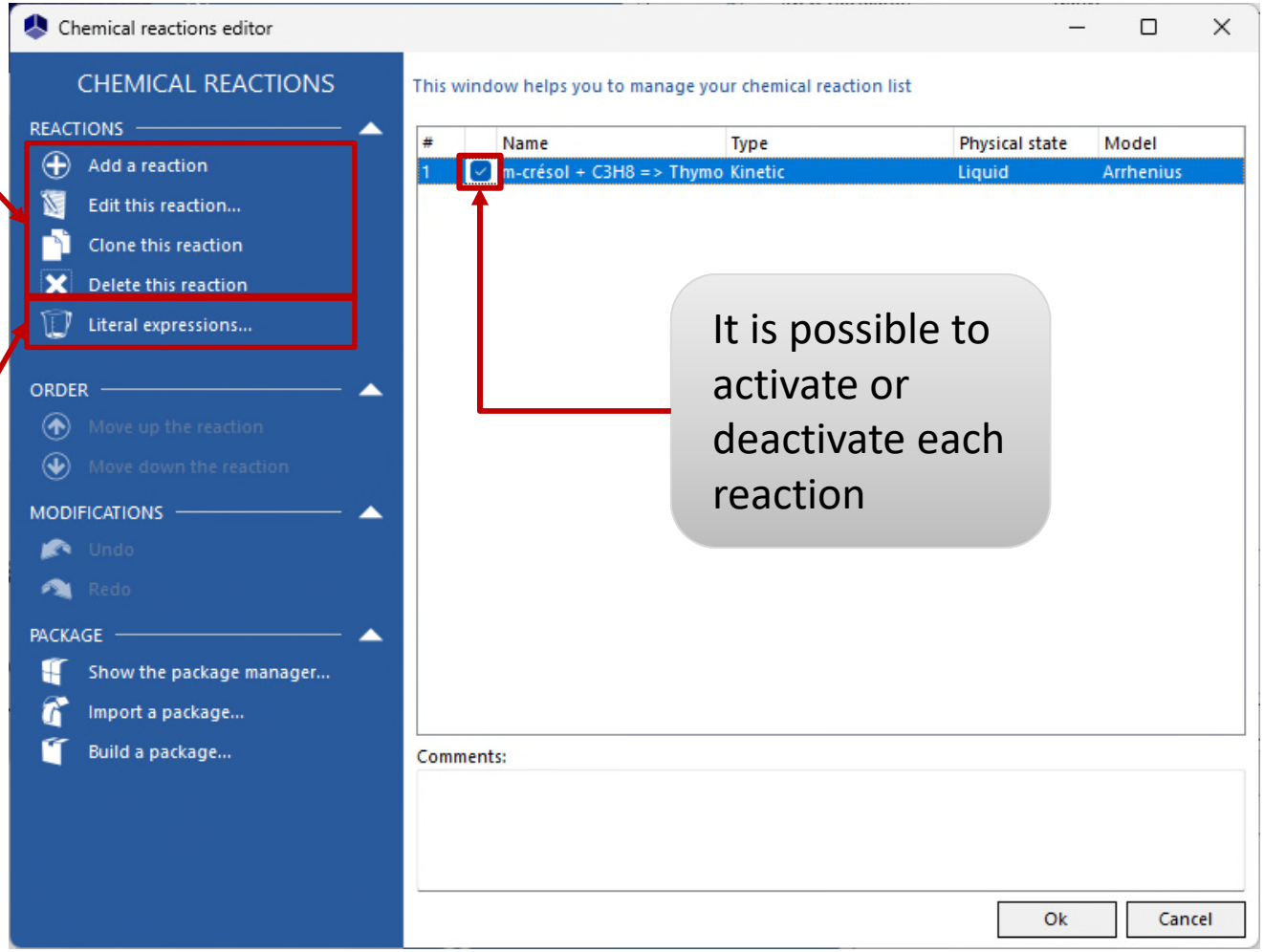
Step 2: selection of the chemical reaction type

It is possible to add, edit, clone or delete reactions

It is possible to generate the literal expressions of the reactions



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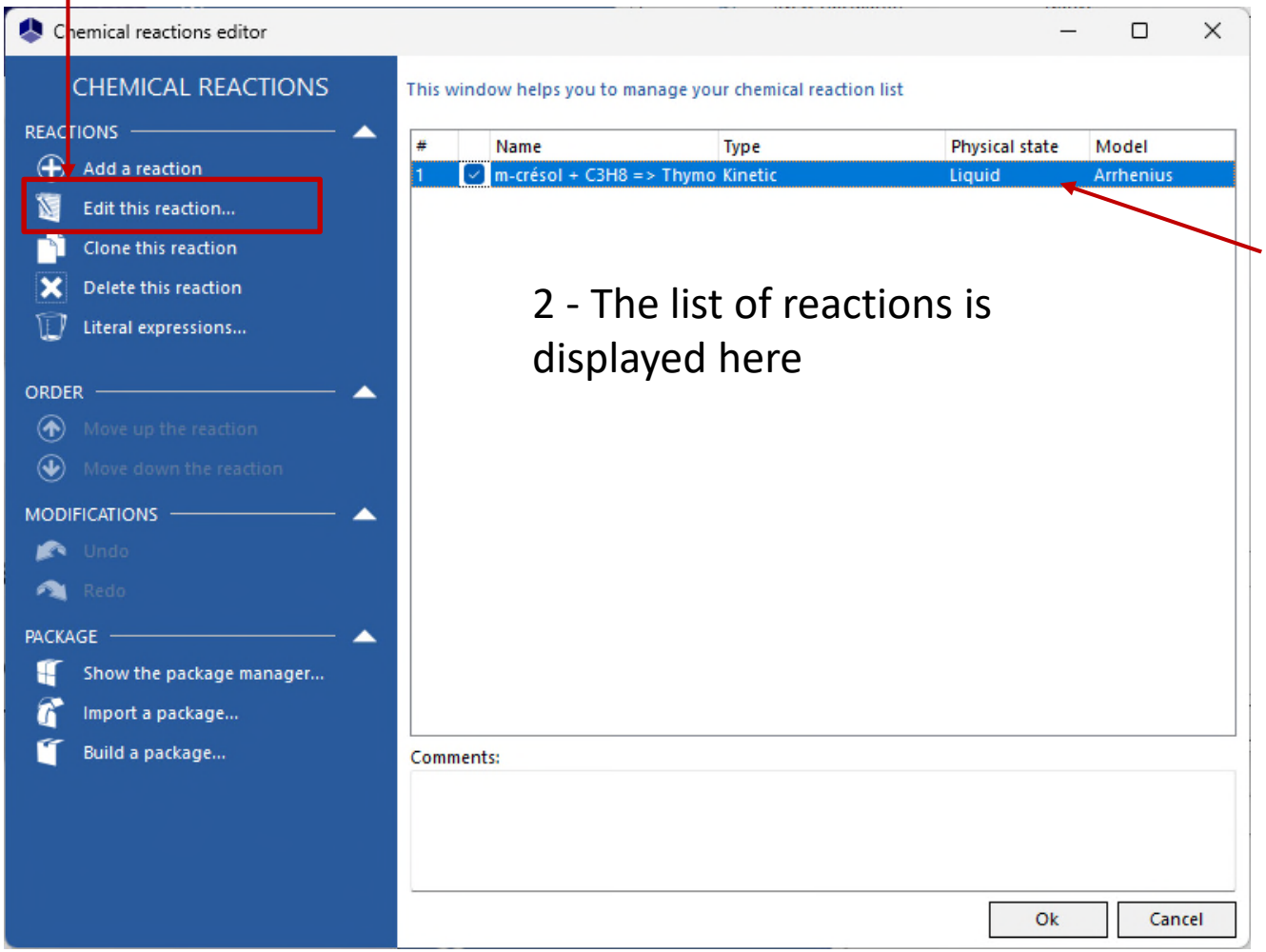
Step 2: selection of the chemical reaction type

1 - Click on "*Add a reaction*"



3 - Double click on the new reaction to configure it

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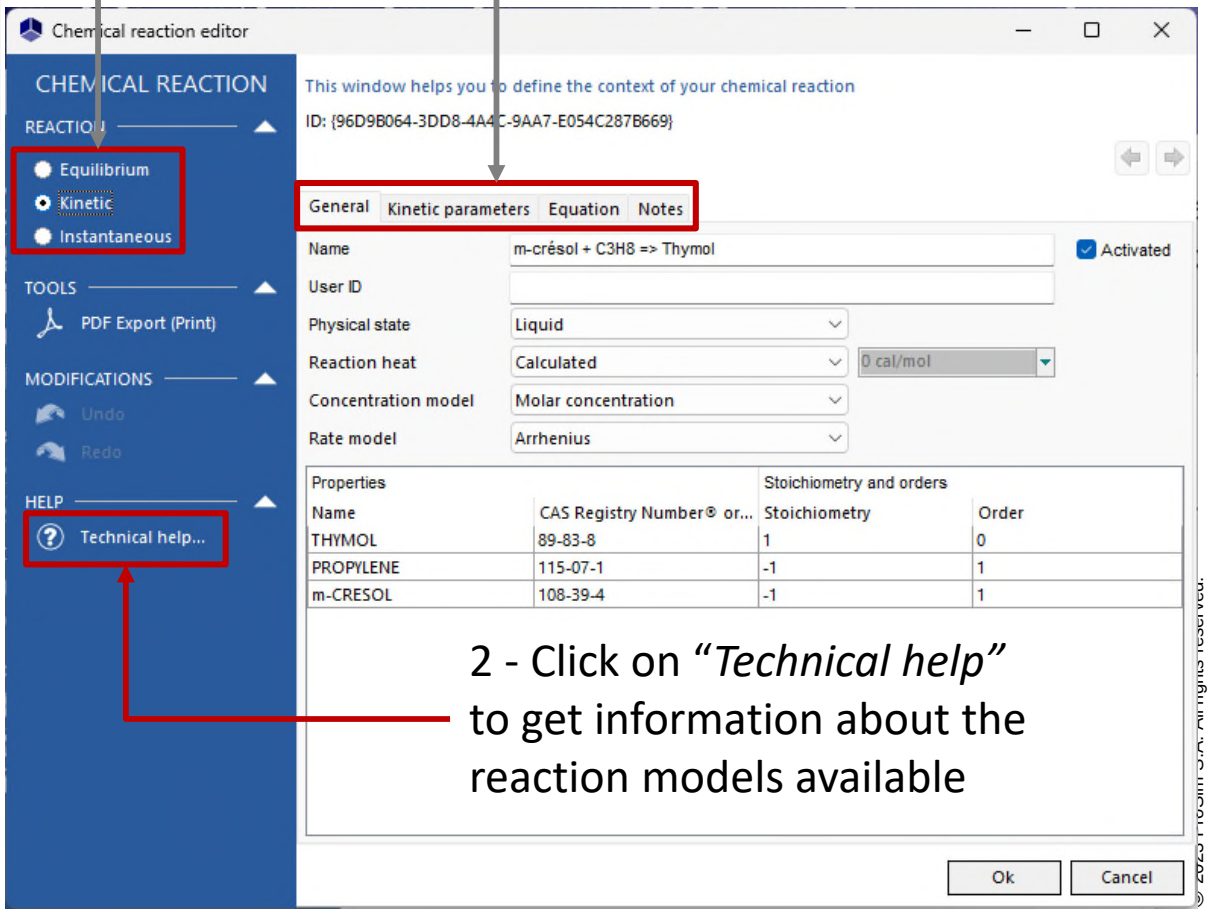
Step 2: selection of the chemical reaction type

3 types of reactions are available:

- Equilibrium
  $A \Leftrightarrow B$
- Controlled by the kinetic
  $A \Rightarrow B$
- Instantaneous
  No accumulation of reactants

Tabs used to define the parameters of the reaction model



1 - Select the chemical reaction type: "*Kinetic*"

2 - Click on "*Technical help*" to get information about the reaction models available

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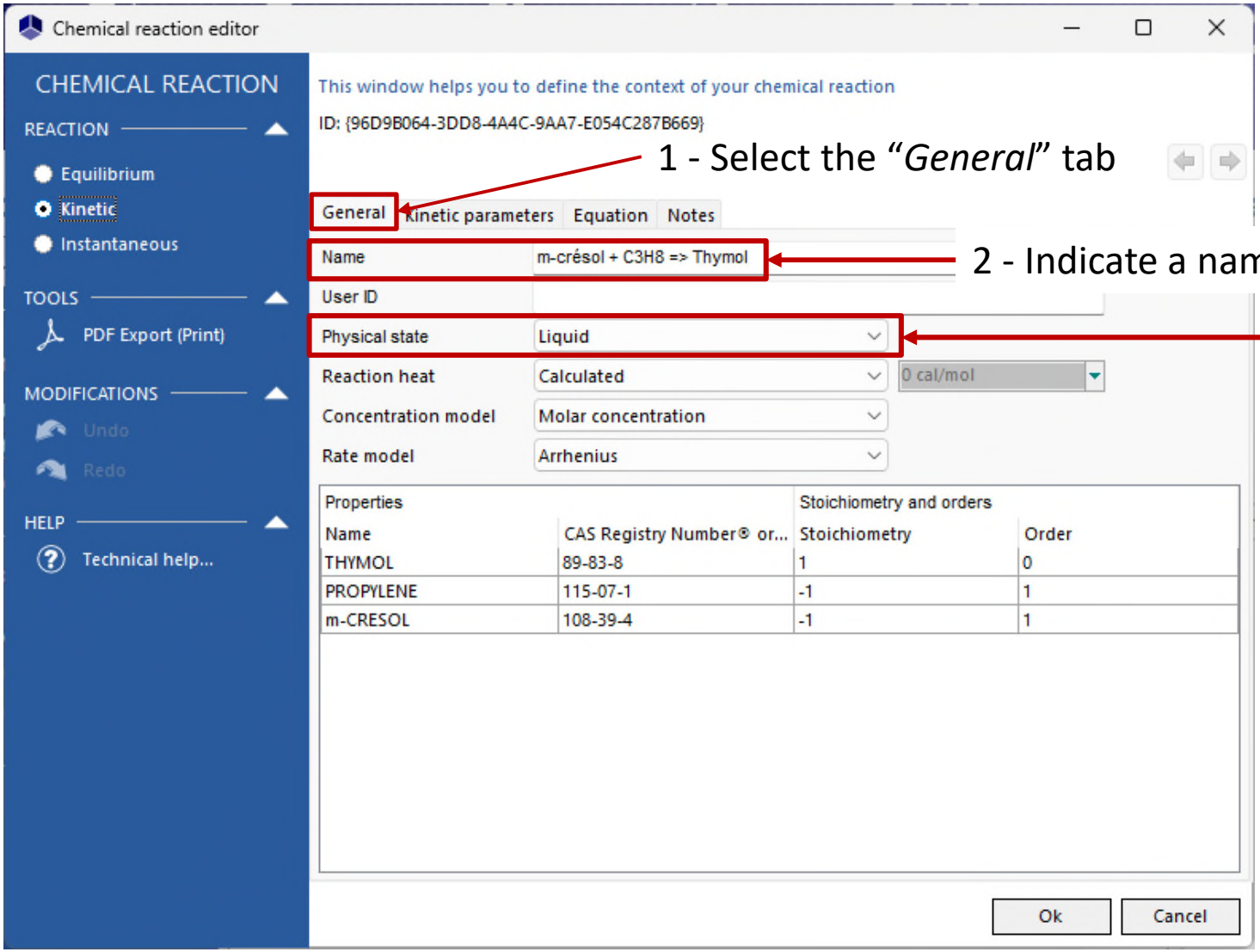
Step 3: configuration of the reaction model

Once you have selected the reaction type, specify the parameters of the reaction model:



3 - Indicate the reactive phase (vapor or liquid)

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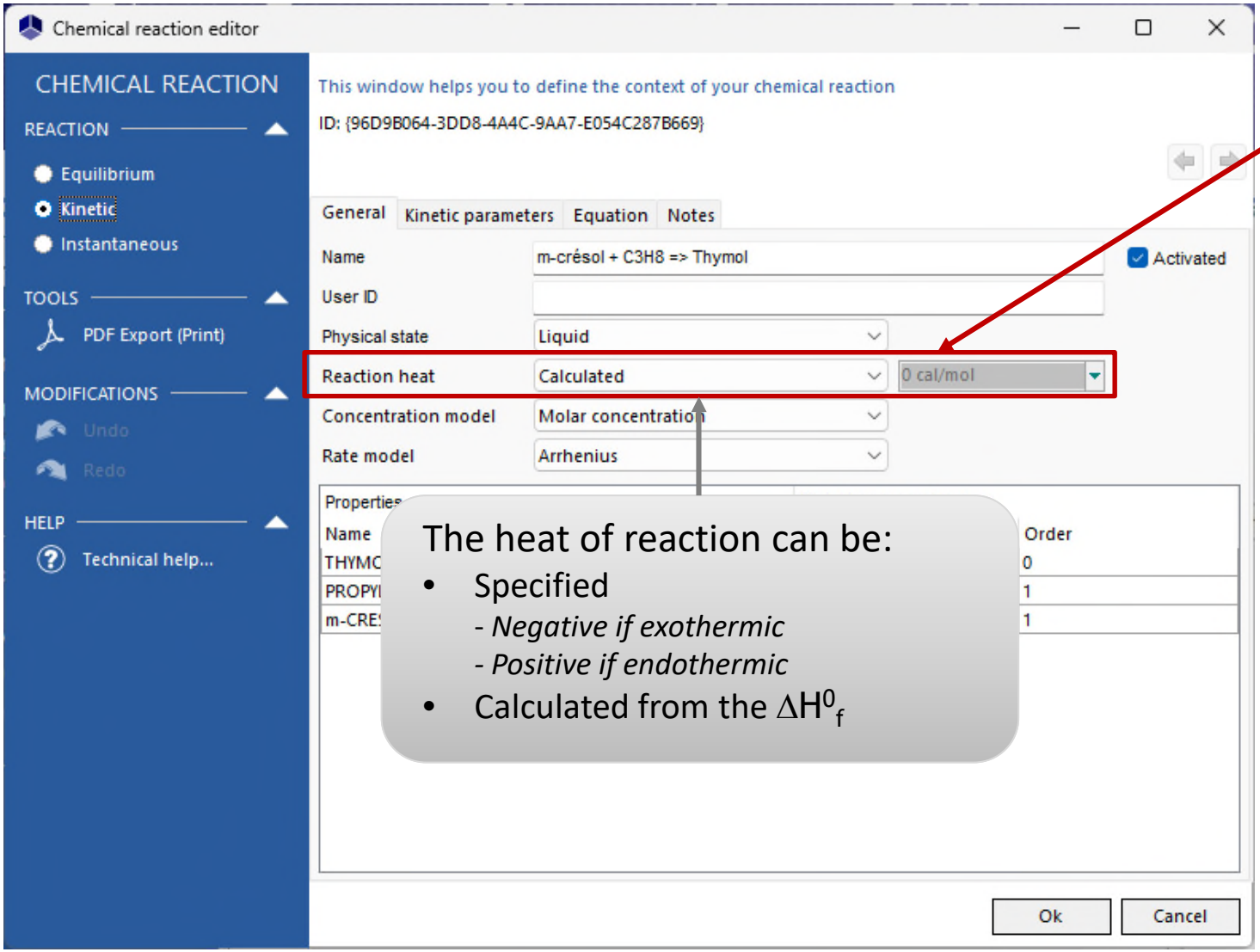
Step 3: configuration of the reaction model

Once you have selected the reaction type, specify the parameters of the reaction model:



The heat of reaction can be:

- Specified
  - *Negative if exothermic*
  - *Positive if endothermic*
- Calculated from the ΔH^0_f

4 - Indicate that the "*reaction heat*" is calculated from the ΔH^0_f

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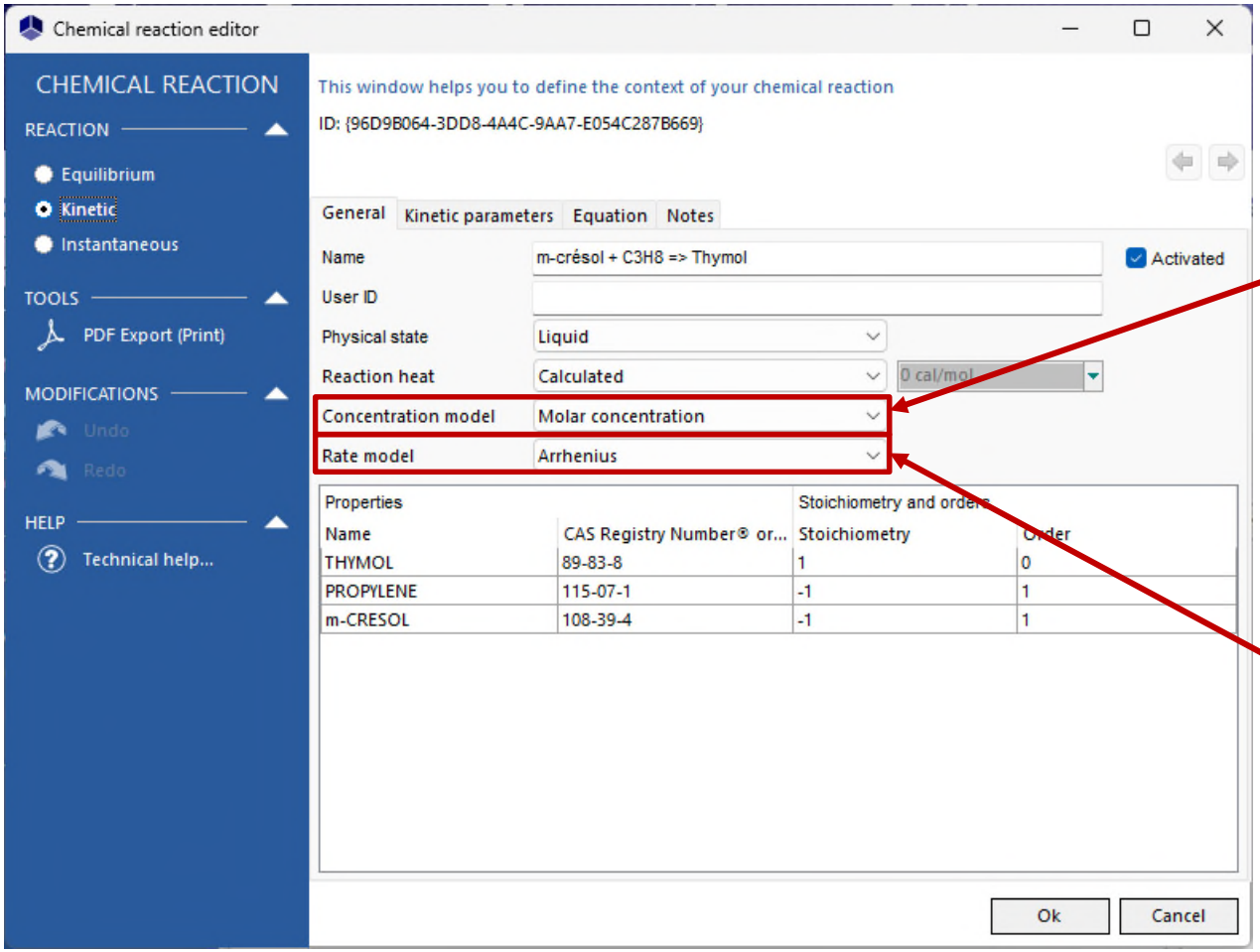
Step 3: configuration of the reaction model

Once you have selected the reaction type, specify the parameters of the reaction model:



5 - Select a concentration model:

- *Molar concentration*
- *Molar fraction*
- *Activity or fugacity*
- *Partial pressure*
- *Molality*

6 - Indicate the rate model

- Arrhenius
- Langmuir
- User “compiled”
- Used “interpreted”

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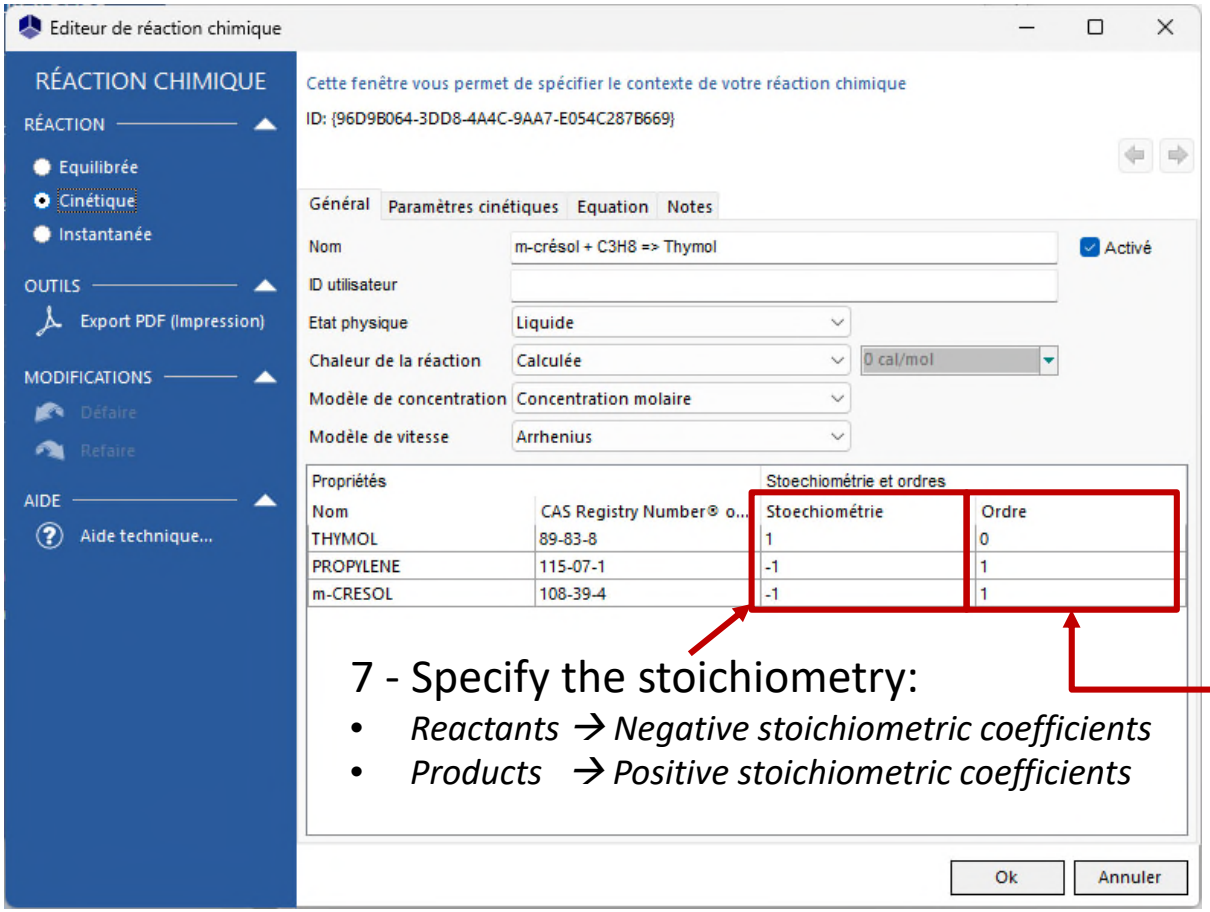
Step 3: configuration of the reaction model

Once you have selected the reaction type, specify the parameters of the reaction model:



7 - Specify the stoichiometry:

- *Reactants → Negative stoichiometric coefficients*
- *Products → Positive stoichiometric coefficients*

8 - Specify the partial orders, by default:

- *Reactants → Absolute value of the stoichiometric coefficient*
- *Products → 0*

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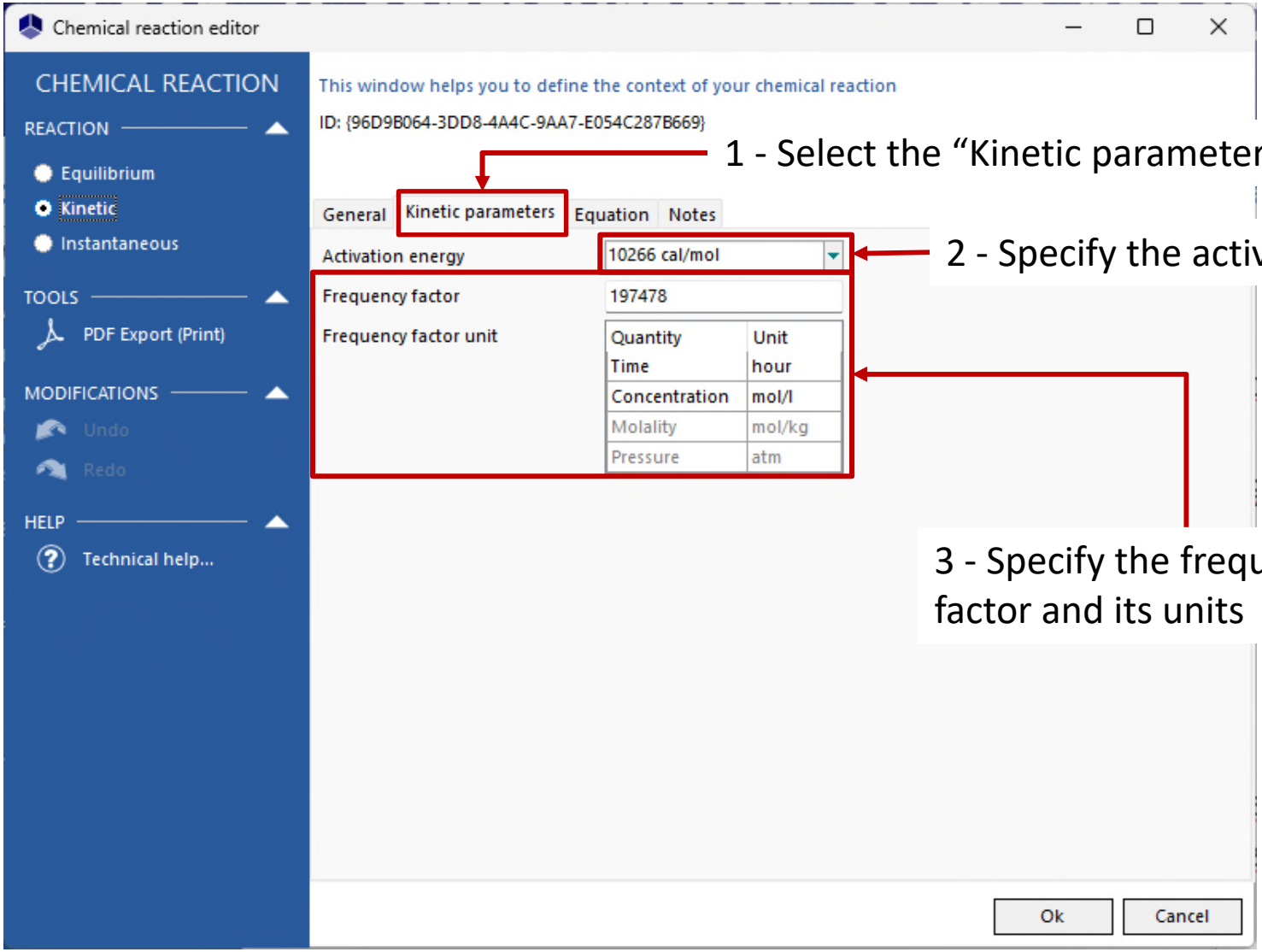
Step 3: configuration of the reaction model

Once you have selected the reaction type, specify the parameters of the reaction model:



1 - Select the “Kinetic parameters” tab

2 - Specify the activation energy

3 - Specify the frequency factor and its units

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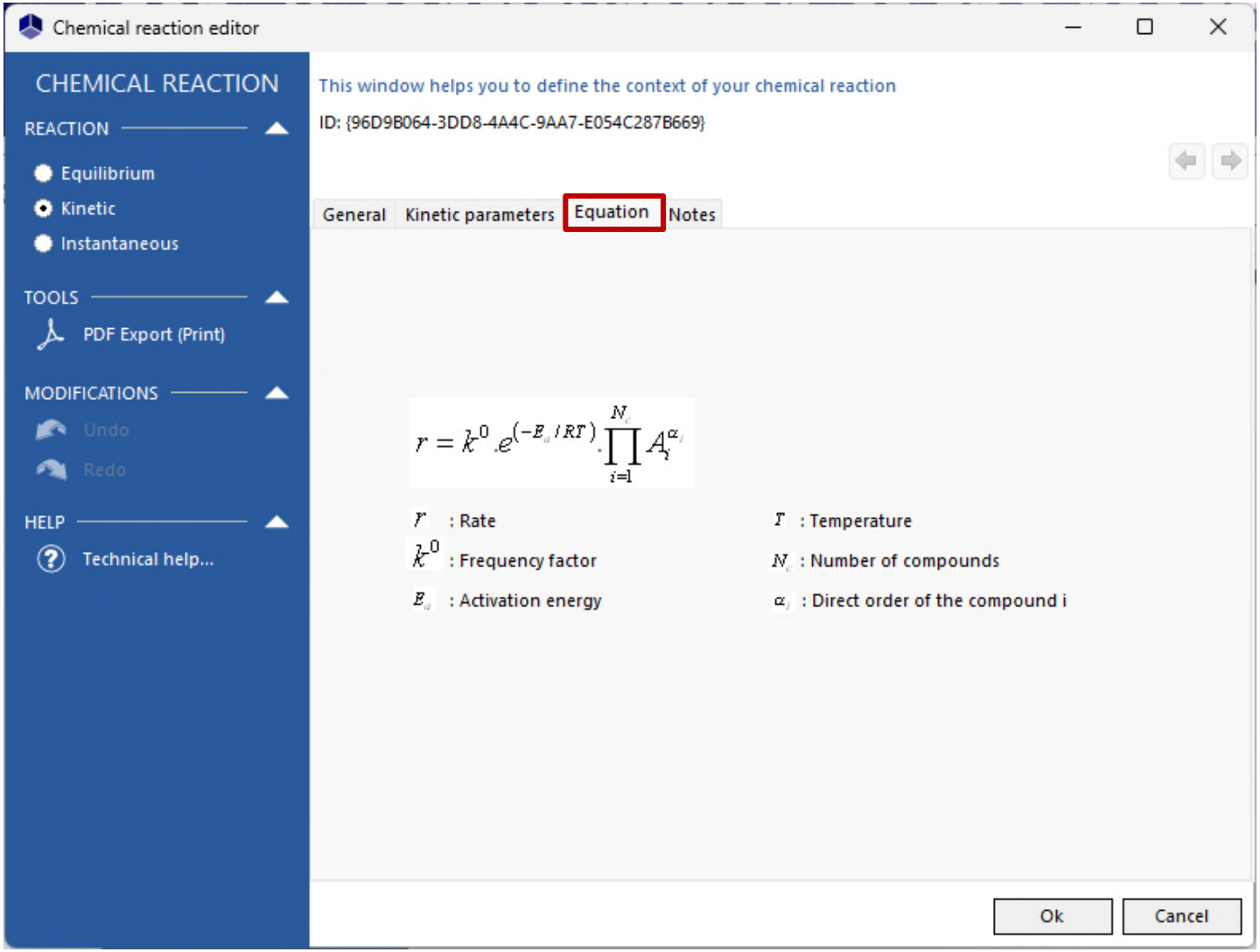
Step 3: configuration of the reaction model

Once you have selected the reaction type, the model is displayed here:



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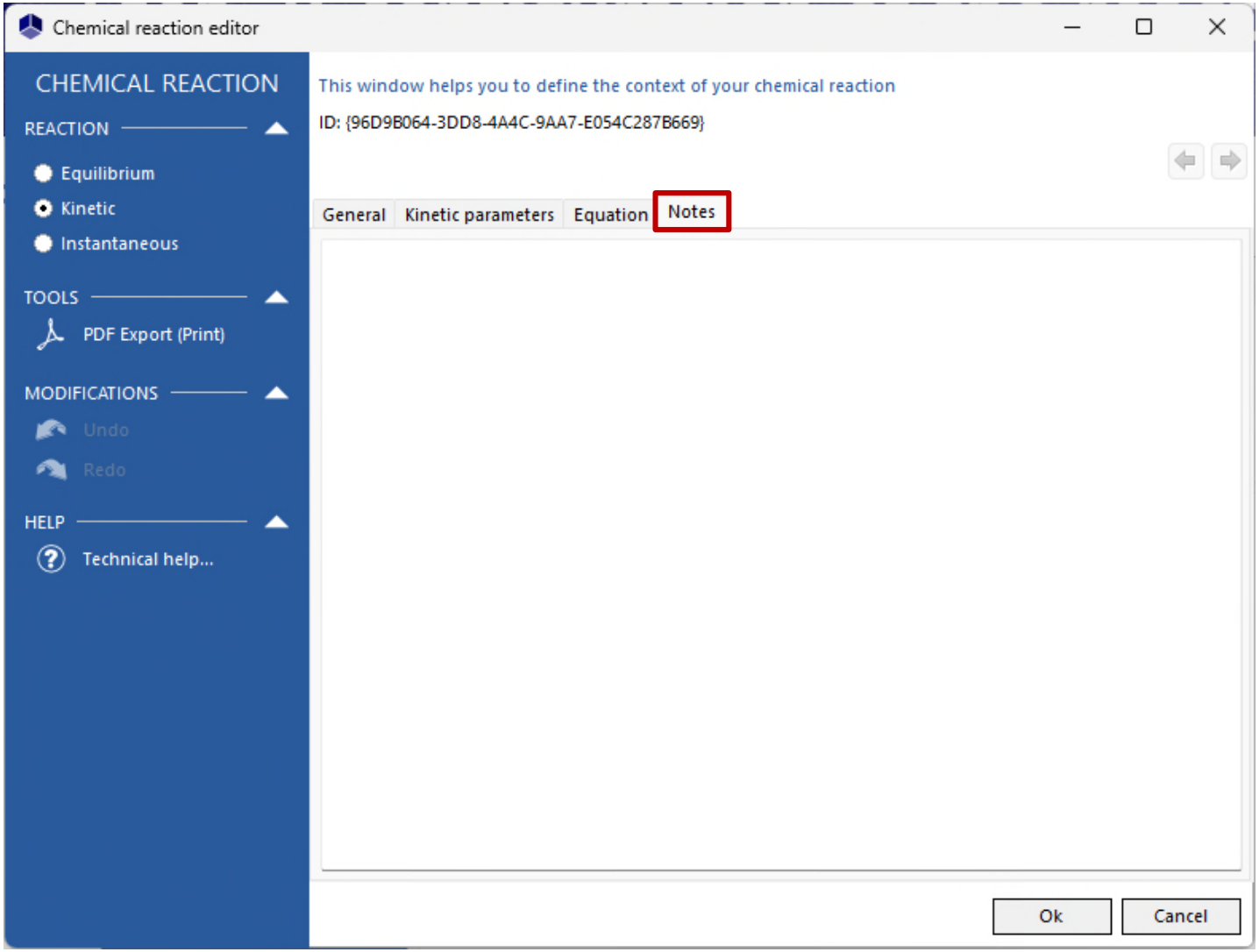
Step 3: configuration of the reaction model

Once you have selected the reaction type, you can write your notes here:



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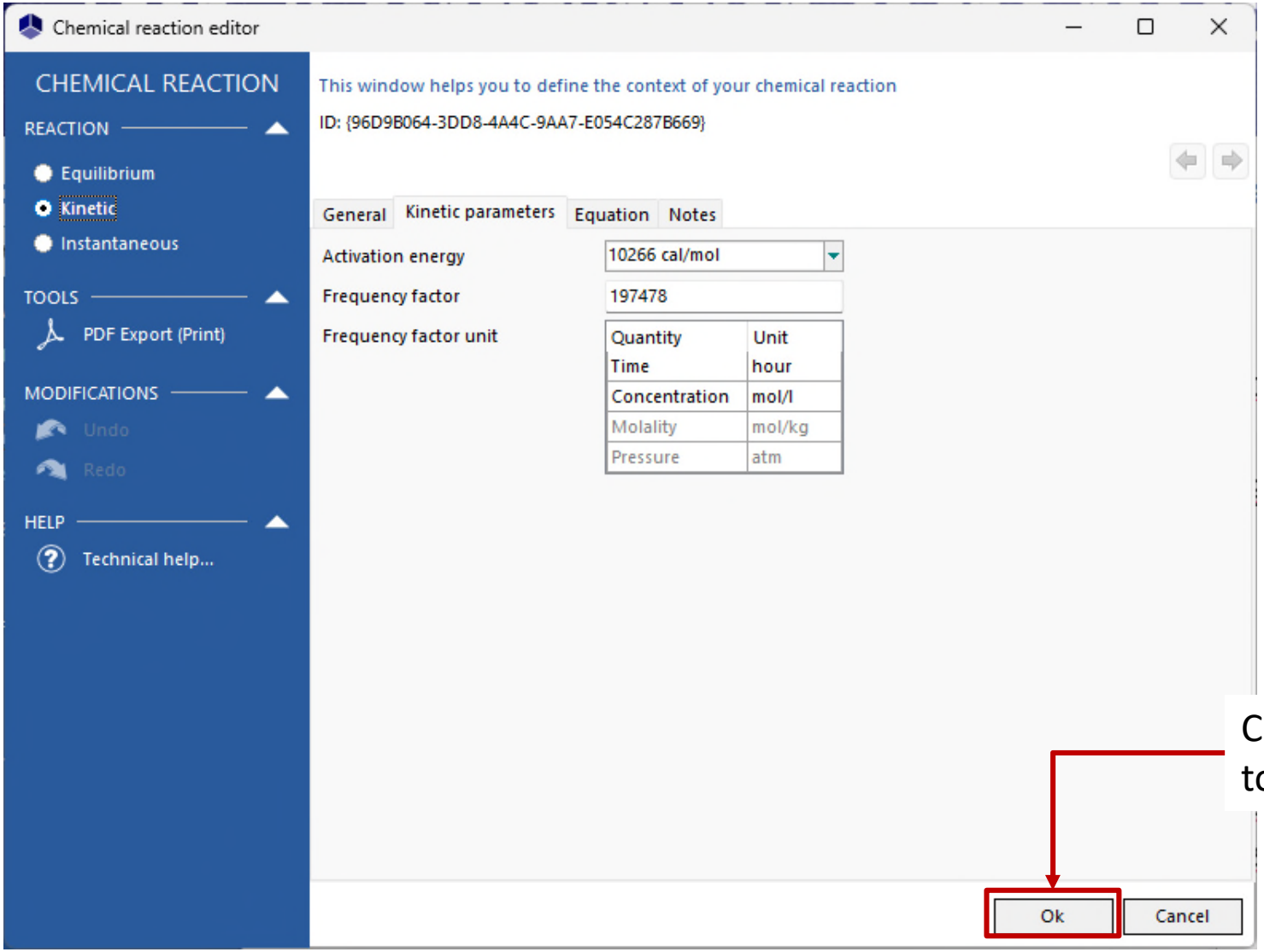
Step 3: configuration of the reaction model

Once you have entered all parameters:



Click on "*Ok*" to validate

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