

Getting started with Simulis Reactions®

Use Case 1: Features overview

Software & Services In Process Simulation

We guide You to efficiency






ProSim

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:

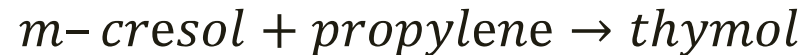
- Instantaneous reactions
- Equilibrium reactions
- Reactions controlled by the kinetic

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

Description of the reaction model

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



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

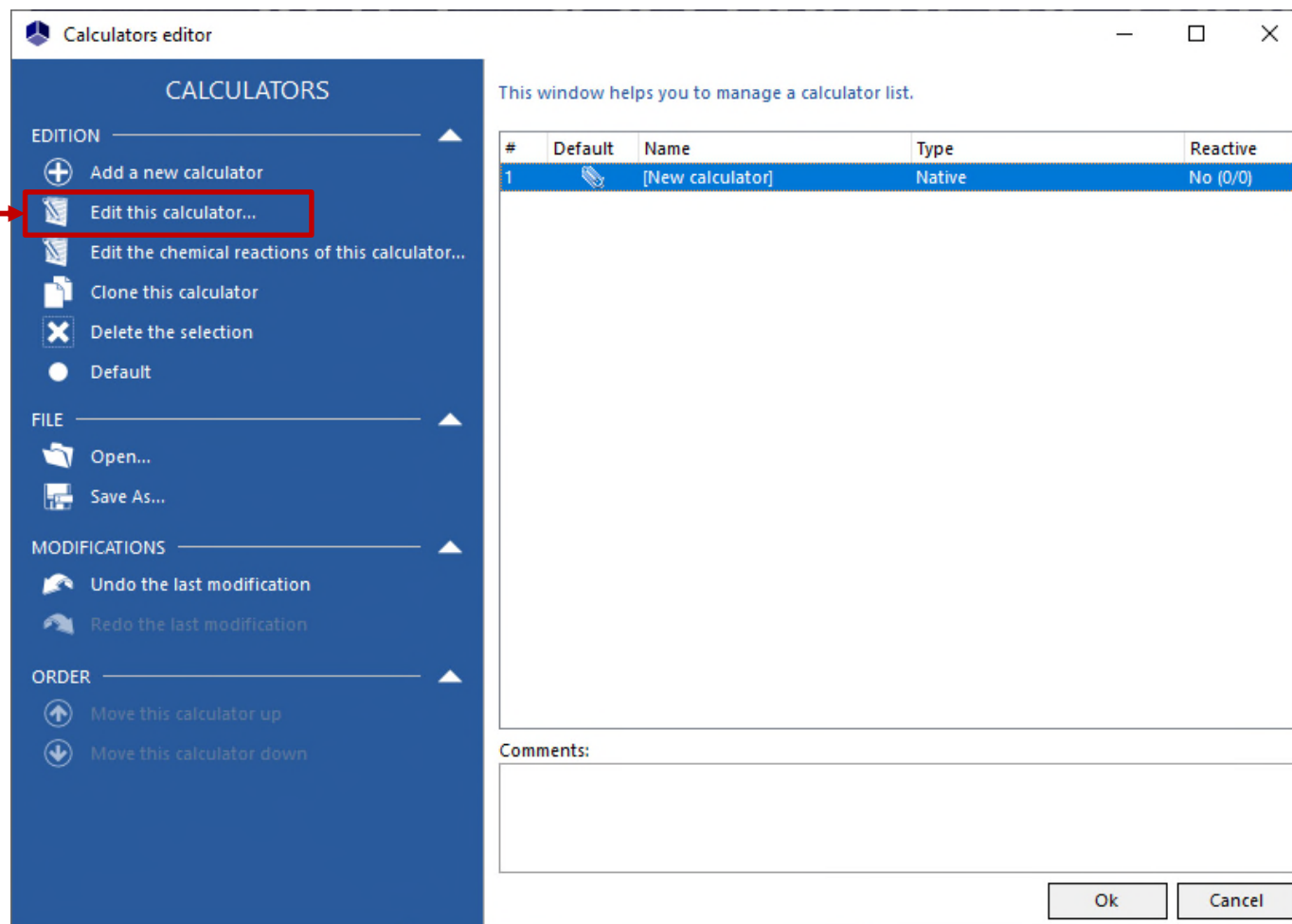
$$r = k^0 \times e^{(-E_a/RT)} \times C_{\text{propylene}} \times C_{m\text{-cresol}}$$

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)

Step 1: selection of the compounds

From the “Calculators editor” window, select “Edit this calculator”



Step 1: selection of the compounds

Thermodynamic calculator editor

FILE

Open...

Save as...

PACKAGE

SERVICES

Calculate

Export as a PSF file

Diagrams

Residue...

Export as a PVT file

Stream...

Sigma profiles

MODIFICATIONS

CONFIGURATION

Name

[New calculator]

Comments

Calculator type

Native

Show the expert mode

This window helps you to define the context of your thermodynamic calculator

COMPOUNDS MODEL PARAMETERS

#	IUPAC Name	CAS Registry Number®
1	THYMOL	89-83-8
2	PROPYLENE	115-07-1
3	m-CRESOL	108-39-4

COMPOUNDS

FILE

Open...

Save as...

Publish...

PACKAGE

EDIT

Import compounds...

Edit this compound...

Create a new compound

Remove all the compounds

Clone this compound

Update the compounds

Delete the selection

SERVICES

Create a pseudo-compound...

Temperature dependent properties...

Editor array

Compare with the original

Compare the compounds

ORDER

Move this compound up

Ok Cancel

1 - Select the following compounds:

- Thymol
- Propylene
- m-cresol

2 - Click on « Ok »

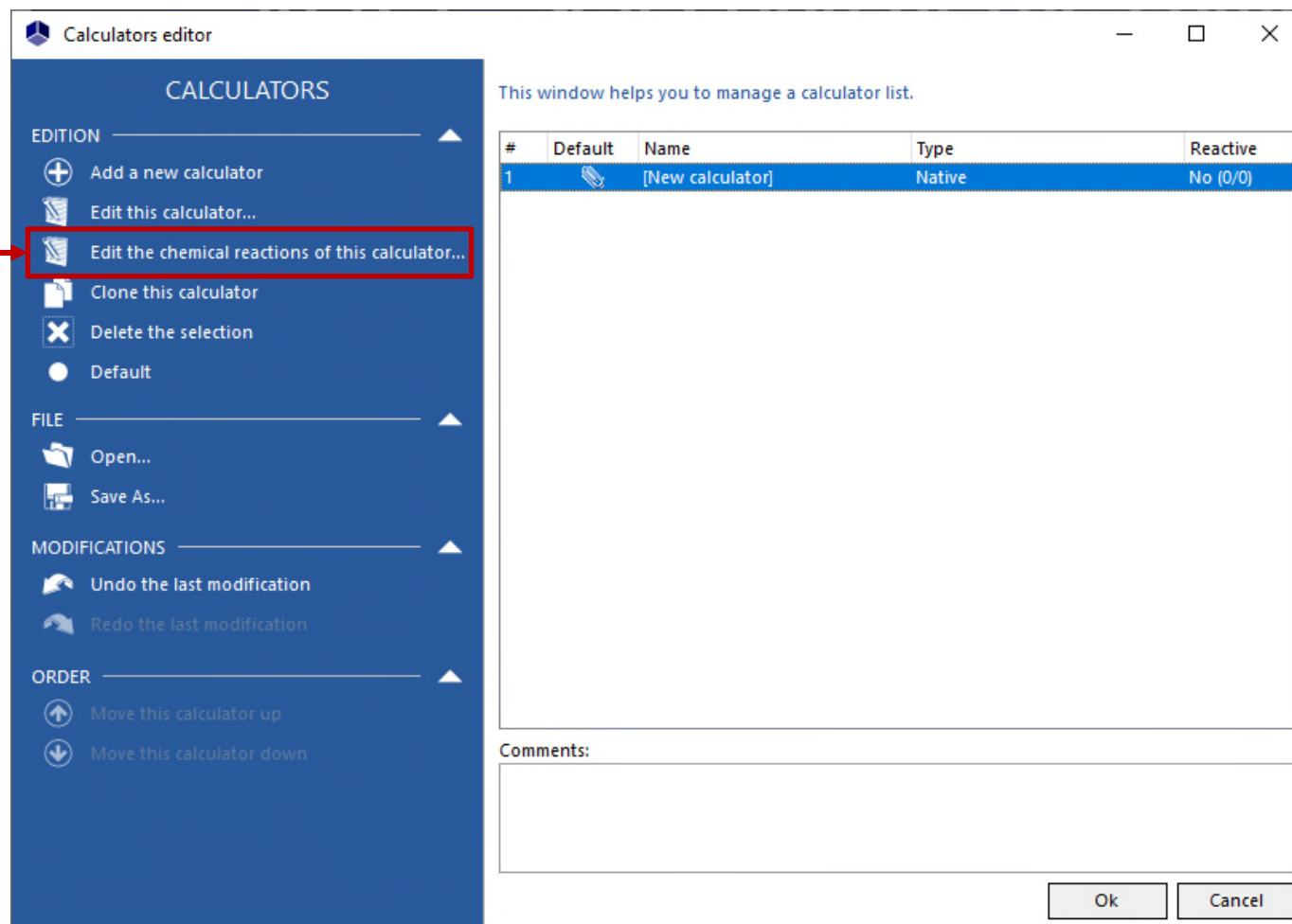
CAS Registry Numbers® are the intellectual property of the American Chemical Society; and are used by ProSim SA with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate.



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

Step 2: selection of the chemical reaction type

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



Step 2: selection of the chemical reaction type

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

It is possible to generate the literal expressions of the reactions

The screenshot shows the 'Chemical reactions editor' window. On the left is a sidebar with several sections: 'CHEMICAL REACTIONS', 'ORDER', 'MODIFICATIONS', and 'PACKAGE'. The 'CHEMICAL REACTIONS' section contains a list of actions: 'Add a reaction', 'Edit this reaction...', 'Clone this reaction', 'Delete this reaction', and 'Literal expressions...'. A red box highlights these actions, with a red arrow pointing from the first callout box. The 'ORDER' section has 'Move up the reaction' and 'Move down the reaction'. The 'MODIFICATIONS' section has 'Undo' and 'Redo'. The 'PACKAGE' section has 'Show the package manager...', 'Import a package...', and 'Build a package...'. A red arrow points from the second callout box to the 'Literal expressions...' option. The main area of the window is titled 'This window helps you to manage your chemical reaction list' and contains a table with the following data:

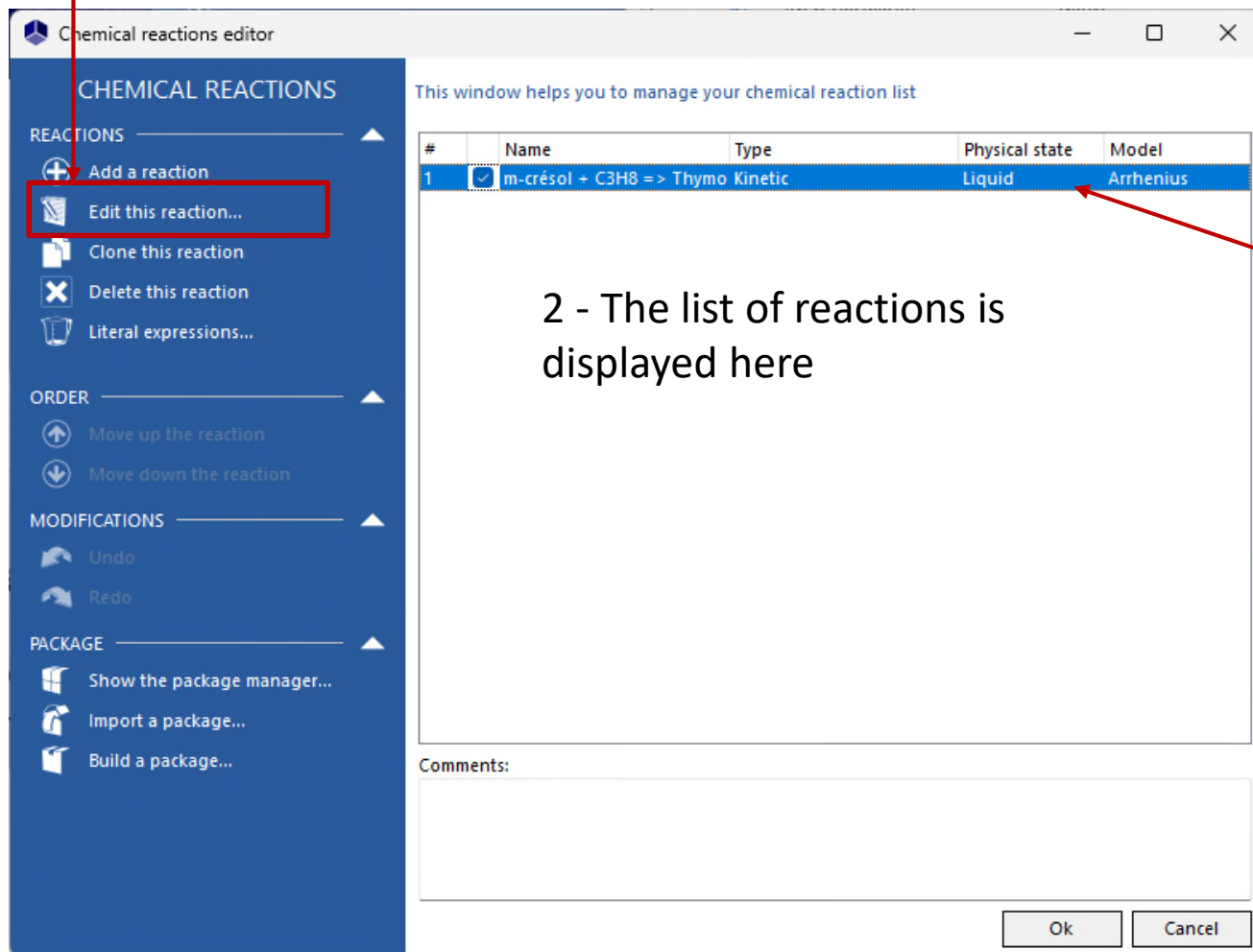
#	Name	Type	Physical state	Model
1	m-crésol + C3H8 => Thymo	Kinetic	Liquid	Arrhenius

A red box highlights the checkbox in the first column of the table, with a red arrow pointing from the third callout box. Below the table is a 'Comments:' text area and 'Ok' and 'Cancel' buttons.

It is possible to activate or deactivate each reaction

Step 2: selection of the chemical reaction type

1 - Click on "Add a reaction"



2 - The list of reactions is displayed here

3 - Double click on the new reaction to configure it

Step 2: selection of the chemical reaction type

3 types of reactions are available:

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

Tabs used to define the parameters of the reaction model

Chemical reaction editor

CHIMICAL REACTION

REACTION

☐ Equilibrium
☒ **Kinetic**
☐ Instantaneous

TOOLS

PDF Export (Print)

MODIFICATIONS

Undo
Redo

HELP

Technical help...

This window helps you to define the context of your chemical reaction
ID: {96D9B064-3DD8-4A4C-9AA7-E054C287B669}

General Kinetic parameters Equation Notes

Name: m-crésol + C3H8 => Thymol ☒ Activated

User ID:

Physical state: Liquid

Reaction heat: Calculated 0 cal/mol

Concentration model: Molar concentration

Rate model: Arrhenius

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
THYMOL	89-83-8	1	0
PROPYLENE	115-07-1	-1	1
m-CRESOL	108-39-4	-1	1

Ok Cancel

1 - Select the chemical reaction type: "Kinetic"

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

Step 3: configuration of the reaction model

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

Chemical reaction editor

CHEMICAL REACTION

REACTION ▲

Equilibrium

Kinetic

Instantaneous

TOOLS ▲

PDF Export (Print)

MODIFICATIONS ▲

Undo

Redo

HELP ▲

Technical help...

This window helps you to define the context of your chemical reaction

ID: {96D9B064-3DD8-4A4C-9AA7-E054C287B669}

1 - Select the "General" tab

General Kinetic parameters Equation Notes

Name m-crésol + C3H8 => Thymol

2 - Indicate a name (optional)

User ID

Physical state Liquid

3 - Indicate the reactive phase (vapor or liquid)

Reaction heat Calculated 0 cal/mol

Concentration model Molar concentration

Rate model Arrhenius

Properties		Stoichiometry and orders	
Name	CAS Registry Number® or...	Stoichiometry	Order
THYMOL	89-83-8	1	0
PROPYLENE	115-07-1	-1	1
m-CRESOL	108-39-4	-1	1

Ok Cancel

Step 3: configuration of the reaction model

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

The screenshot shows the 'Chemical reaction editor' window. The left sidebar has sections for 'CHEMICAL REACTION' (with 'Kinetic' selected), 'TOOLS' (with 'PDF Export (Print)'), 'MODIFICATIONS' (with 'Undo' and 'Redo'), and 'HELP' (with 'Technical help...'). The main area has tabs for 'General', 'Kinetic parameters', 'Equation', and 'Notes'. The 'Kinetic parameters' tab is active, showing fields for 'Name' (m-crésol + C3H8 => Thymol), 'User ID', 'Physical state' (Liquid), 'Reaction heat' (Calculated), 'Concentration model' (Molar concentration), and 'Rate model' (Arrhenius). The 'Reaction heat' field is highlighted with a red box, and a red arrow points from the text '4 - Indicate that the "reaction heat" is calculated from the ΔH_f^0 ' to it. A grey callout box points to the 'Reaction heat' field with the text: 'The heat of reaction can be:

- Specified
 - Negative if exothermic
 - Positive if endothermic
- Calculated from the ΔH_f^0

'. The 'Activated' checkbox is checked. At the bottom are 'Ok' and 'Cancel' buttons.

Chemical reaction editor

CHEMICAL REACTION

REACTION ▲

Equilibrium

Kinetic

Instantaneous

TOOLS ▲

PDF Export (Print)

MODIFICATIONS ▲

Undo

Redo

HELP ▲

Technical help...

This window helps you to define the context of your chemical reaction

ID: {96D9B064-3DD8-4A4C-9AA7-E054C287B669}

General Kinetic parameters Equation Notes

Name m-crésol + C3H8 => Thymol Activated

User ID

Physical state Liquid

Reaction heat Calculated 0 cal/mol

Concentration model Molar concentration

Rate model Arrhenius

Properties

Name	Order
THYMO	0
PROPY	1
m-CRE	1

Ok Cancel

4 - Indicate that the "reaction heat" is calculated from the ΔH_f^0

The heat of reaction can be:

- Specified
 - Negative if exothermic
 - Positive if endothermic
- Calculated from the ΔH_f^0

Step 3: configuration of the reaction model

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

The screenshot shows the 'Chemical reaction editor' window. The 'REACTION' tab is selected, and the 'Kinetic' option is chosen under 'TOOLS'. The 'Concentration model' is set to 'Molar concentration' and the 'Rate model' is set to 'Arrhenius'. The 'Properties' table lists the reactants and products with their stoichiometry and order.

Chemical reaction editor

CHIMICAL REACTION

REACTION ▲

- Equilibrium
- Kinetic**
- Instantaneous

TOOLS ▲

- PDF Export (Print)

MODIFICATIONS ▲

- Undo
- Redo

HELP ▲

- Technical help...

This window helps you to define the context of your chemical reaction

ID: {96D9B064-3DD8-4A4C-9AA7-E054C287B669}

General Kinetic parameters Equation Notes

Name: m-crésol + C3H8 => Thymol Activated

User ID:

Physical state: Liquid

Reaction heat: Calculated 0 cal/mol

Concentration model: Molar concentration

Rate model: Arrhenius

Properties		Stoichiometry and order	
Name	CAS Registry Number® or...	Stoichiometry	Order
THYMOL	89-83-8	1	0
PROPYLENE	115-07-1	-1	1
m-CRESOL	108-39-4	-1	1

Ok Cancel

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"

Step 3: configuration of the reaction model

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

Editeur de réaction chimique

RÉACTION CHIMIQUE

RÉACTION

- Equilibrée
- **Cinétique**
- Instantanée

OUTILS

Export PDF (Impression)

MODIFICATIONS

Défaire

Refaire

AIDE

Aide technique...

Cette fenêtre vous permet de spécifier le contexte de votre réaction chimique

ID: {96D9B064-3DD8-4A4C-9AA7-E054C287B669}

Général Paramètres cinétiques Equation Notes

Nom m-crésol + C3H8 => Thymol ☒ Activé

ID utilisateur

Etat physique Liquide

Chaleur de la réaction Calculée 0 cal/mol

Modèle de concentration Concentration molaire

Modèle de vitesse Arrhenius

Propriétés		Stoechiométrie et ordres	
Nom	CAS Registry Number® o...	Stoechiométrie	Ordre
THYMOL	89-83-8	1	0
PROPYLENE	115-07-1	-1	1
m-CRESOL	108-39-4	-1	1

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

Ok Annuler

Step 3: configuration of the reaction model

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

Chemical reaction editor

CHIMICAL REACTION

REACTION

- Equilibrium
- Kinetic**
- Instantaneous

TOOLS

- PDF Export (Print)

MODIFICATIONS

- Undo
- Redo

HELP

- Technical help...

This window helps you to define the context of your chemical reaction

ID: {96D9B064-3DD8-4A4C-9AA7-E054C287B669}

General **Kinetic parameters** Equation Notes

Activation energy 10266 cal/mol

Frequency factor 197478

Frequency factor unit

Quantity	Unit
Time	hour
Concentration	mol/l
Molality	mol/kg
Pressure	atm

Ok Cancel

1 - Select the "Kinetic parameters" tab

2 - Specify the activation energy

3 - Specify the frequency factor and its units

Step 3: configuration of the reaction model

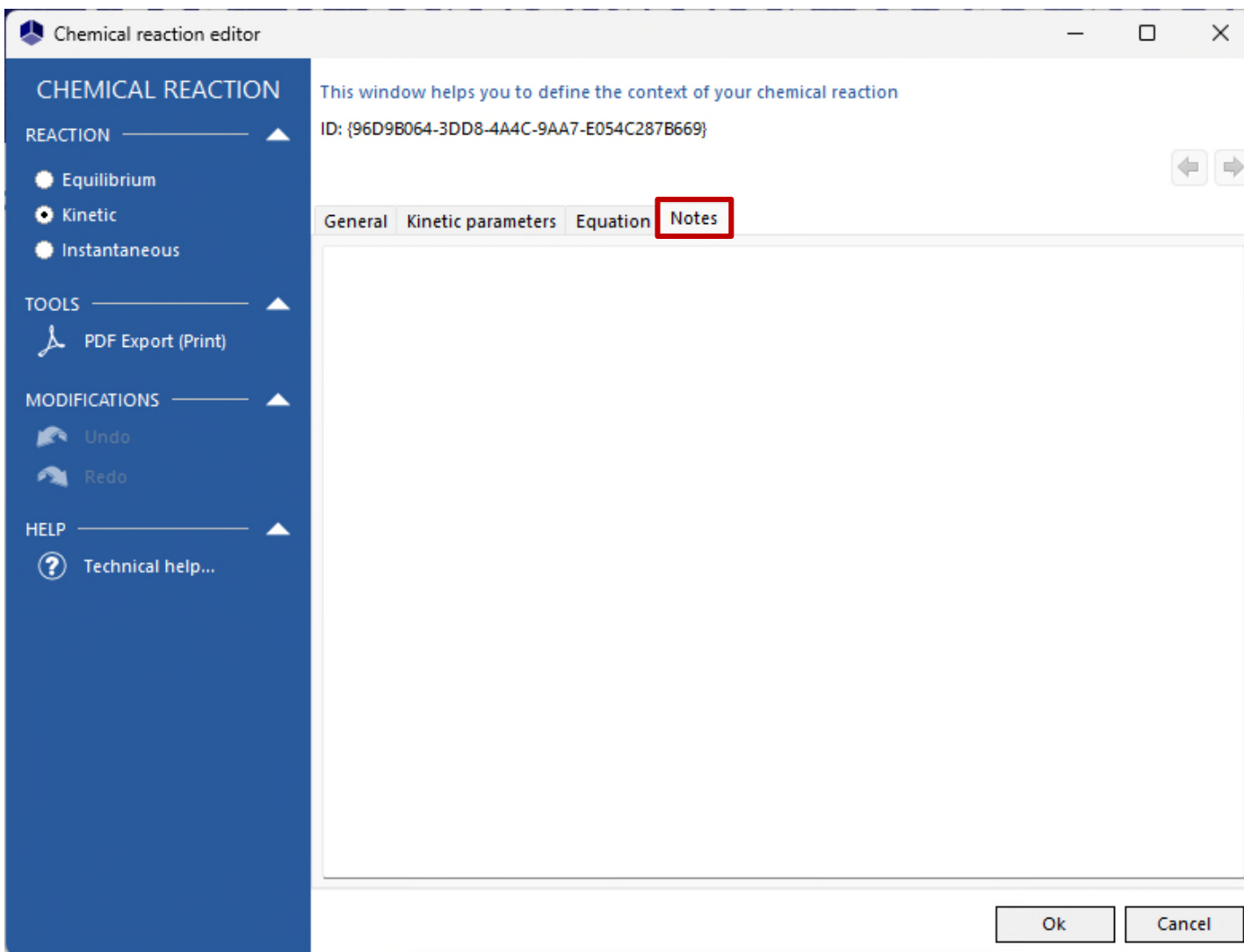
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Once you have selected the reaction type, the model is displayed here:

The screenshot shows the 'Chemical reaction editor' window. On the left is a dark blue sidebar with sections: 'CHEMICAL REACTION' (with 'Kinetic' selected), 'TOOLS' (with 'PDF Export (Print)'), 'MODIFICATIONS' (with 'Undo' and 'Redo'), and 'HELP' (with 'Technical help...'). The main area has a title bar and a subtitle 'This window helps you to define the context of your chemical reaction'. Below this is an ID field containing '{96D9B064-3DD8-4A4C-9AA7-E054C287B669}'. There are four tabs: 'General', 'Kinetic parameters', 'Equation' (highlighted with a red box), and 'Notes'. The 'Equation' tab displays the Arrhenius equation:
$$r = k^0 \cdot e^{(-E_a / RT)} \cdot \prod_{i=1}^{N_c} A_i^{\alpha_i}$$
 Below the equation, there are two columns of variable definitions:
Left column: r : Rate, k^0 : Frequency factor, E_a : Activation energy
Right column: T : Temperature, N_c : Number of compounds, α_i : Direct order of the compound i
At the bottom right are 'Ok' and 'Cancel' buttons.

Step 3: configuration of the reaction model

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



Step 3: configuration of the reaction model

Once you have entered all parameters:

The screenshot shows the 'Chemical reaction editor' window. The left sidebar contains sections for 'CHEMICAL REACTION' (with 'Kinetic' selected), 'TOOLS' (including 'PDF Export (Print)'), 'MODIFICATIONS' (including 'Undo' and 'Redo'), and 'HELP' (including 'Technical help...'). The main area has tabs for 'General', 'Kinetic parameters', 'Equation', and 'Notes'. The 'Kinetic parameters' tab is active, showing 'Activation energy' as 10266 cal/mol, 'Frequency factor' as 197478, and a table for 'Frequency factor unit'.

Quantity	Unit
Time	hour
Concentration	mol/l
Molality	mol/kg
Pressure	atm

At the bottom right, the 'Ok' button is highlighted with a red box and a red arrow pointing to it from a text box.

Click on "Ok"
to validate



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