How To Use the Adjusting Arrows in Model-Based Analysis

1 Contents

2 Introduction:

In model-based analysis the software searches the optimal kinetic parameters in order to get the best fit for the experimental curves. This optimization task is non-linear for the models with several reaction steps, and result depends on the initial values of parameters. The closer these initial values are to the optimal values the better will be the resulting fit after optimization.

It is not always necessary, but sometimes it is extremely useful, and time saved to adjust the simulated curves manually, before optimization, to get them closer to the source measured data. This can be done by using the adjusting arrow buttons.

For example, it is possible manually:

- to move the simulated curves to the left or to the right,
- to bring the simulated curves closer to each other or far from each other,
- to correct the shape of the simulated curves,
- to correct the contribution of the current step.

3 Additional Arrow Buttons and Version Information

Complete set of 10 adjusting arrow buttons including 6 new buttons is available since Kinetics Neo version 2.4. In the earlier versions only 4 arrow buttons (EARLIER, LATER, INCREASE, DECREASE) are present.

In *Model Based Analysis* there are 8 standard arrow buttons for the manual adjusting of selected step. These buttons are always visible.

The number of adjusting arrows can be increased to 10 by selecting the checkbox in *Settings - Show two additional arrows for adjusting step by Activation Energy in Model-based Analysis*.

In this case the full set of 10 adjusting arrow buttons including2 additional arrow buttons with red border will be shown.

4 Adjustment Arrows Buttons and Their Actions

1.  Move current reaction step to the EARLIER time
2.  DECREASE Activation Energy and move the step EARLIER
3.  INCREASE contribution of the current step
4.  DECREASE contribution of the current step
5.  INCREASE Activation Energy and move the step LATER
6.  Move current reaction step to the LATER time
7.  SPREAD current reaction step
8.  COMPRESS current reaction step
9.  SHARPEN current reaction step
10.  FLATTEN current reaction step

5 General Figure and Curve Description Used In This Guide

In all figures of this document:

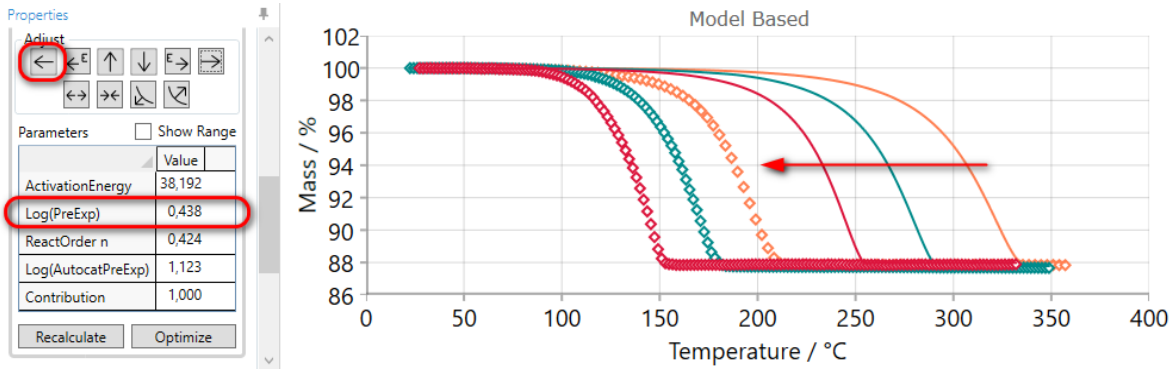
- the marker points are the experimental data,
- the solid lines are the simulations for the selected reaction step.

6 Using of the Adjusting Arrow Buttons

The experiment is done three times for different heating rates and presented as three experimental curves in the X-temperature view.

6.1 Move the Step EARLIER by INCREASING Pre-Exponential Factor (Heating)

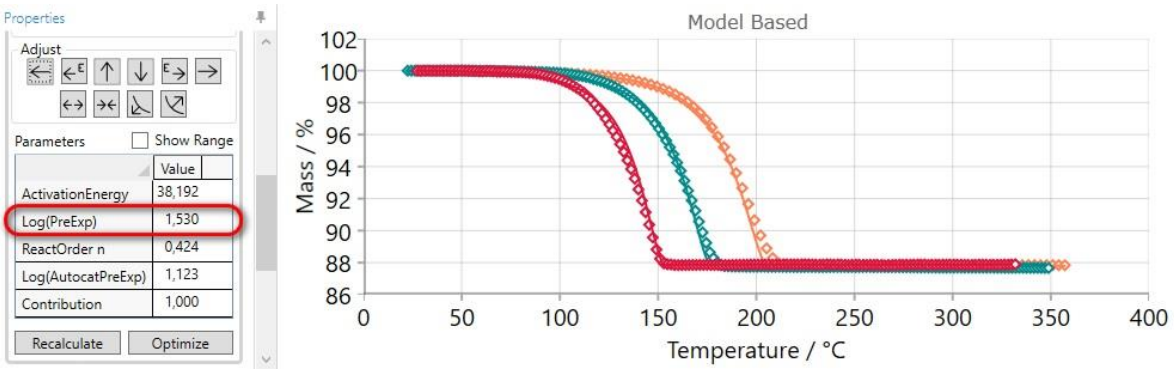
Here the simulated solid curves for selected step show the mass change much later than the mass change in the experimental data. In this case the simulated step can be moved to the earlier time (less temperature) by the using of the ERALIER arrow.



After clicking on the EARLIER arrow button the pre-exponential factor increases and the step on simulated curves is moved to the left in direction of earlier time or less temperature (for heating).

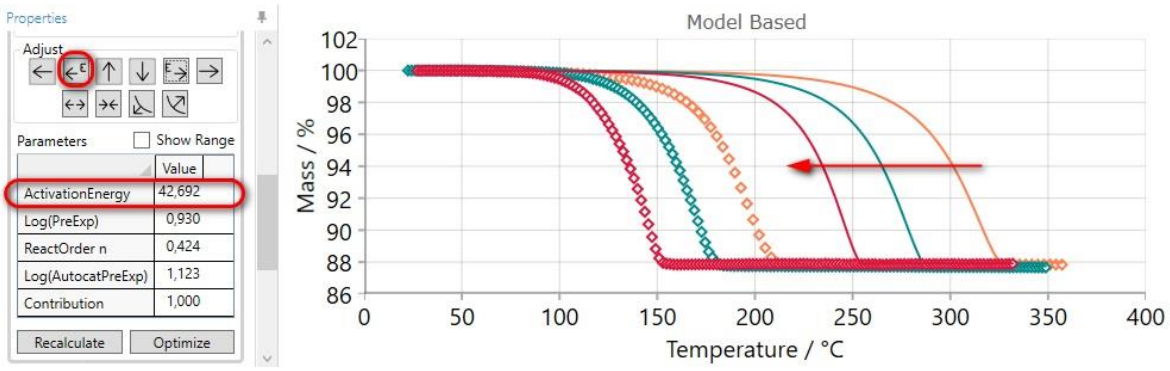
It may be necessary to click on the arrow button several times to "*move*" the simulated curves near enough to the measurements.

After manual adjustment please click on "*Optimization*" button. After that the result will be:



6.2 Move the Step EARLIER by DECREASING Activation Energy (Heating)

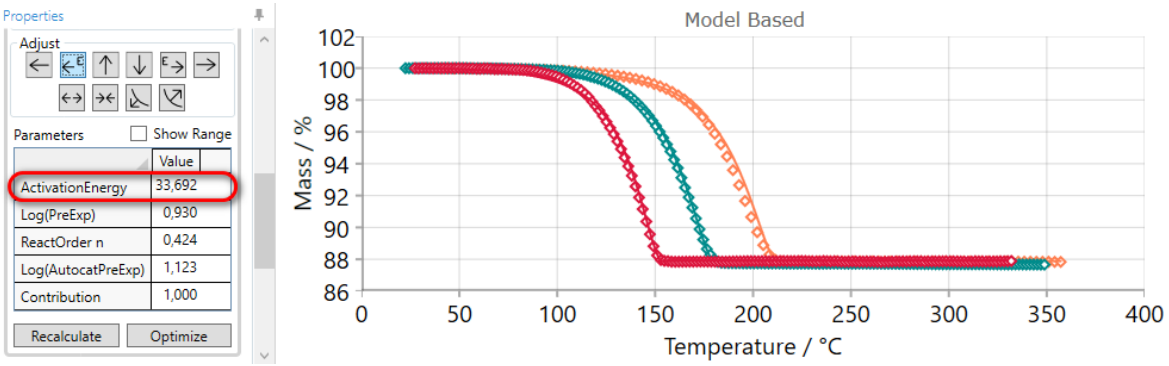
If the simulated curves for selected step are too late, then they can be moved to the earlier time by the using of DECREASE ACTIVATION EVERGY arrow. It is similar like in §6.1, but here the activation energy and not the pre-exponential factor will be decreased.



After clicking on the (DECREASE ACTIVATION EVERGY) arrow button the value of activation energy decreases and that moves the simulated curves to the earlier time or less temperature (for heating).

It may be necessary to click on the arrow button several times to “move” the simulated curves near enough to the measurements.

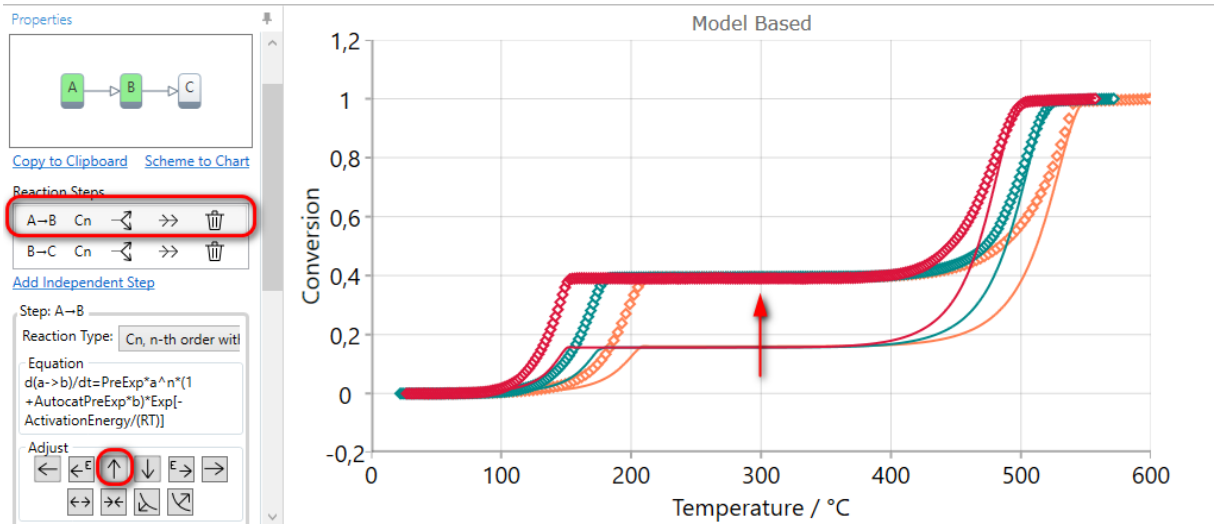
After manual adjustment please click on “Optimization” button. After that the result will be:



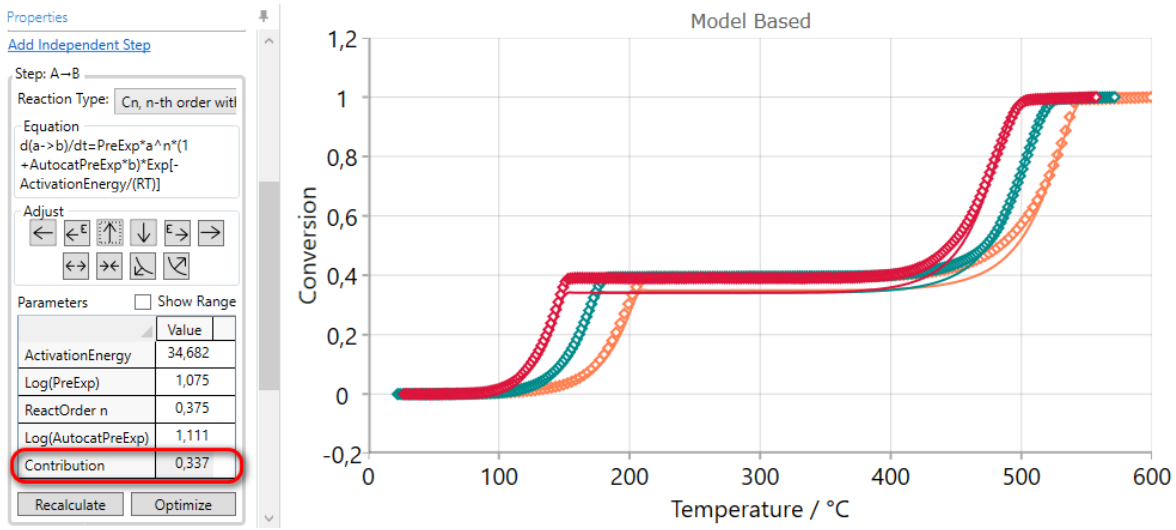
6.3 INCREASE Contribution of the Current Step

If the simulation for selected step finishes at too low conversion value in *Conversion* view, then the contribution of the current step can be increased by the using of INCREASE CONTRUBUTION arrow.

Here the final conversion for the first step is too low, therefore the first step should be selected.



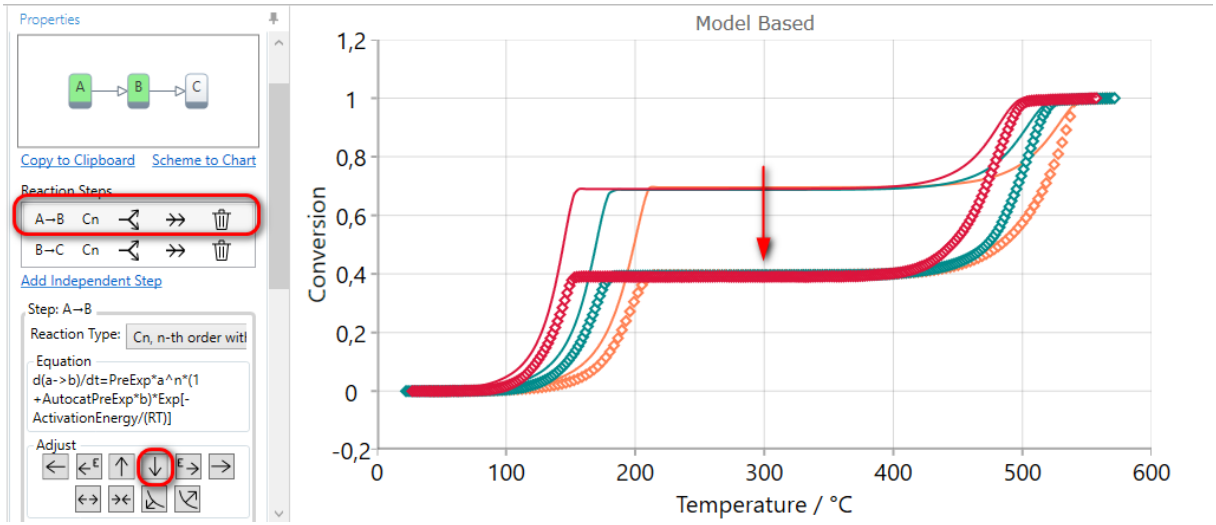
Using of INCREASE CONTRUBUTION arrow for the selected step increases the value of the contribution and then the simulated curves have the higher value of final conversion for this step. The contribution values of other reaction steps are automatically reduced in order to have the sum of all contributions equal to one.



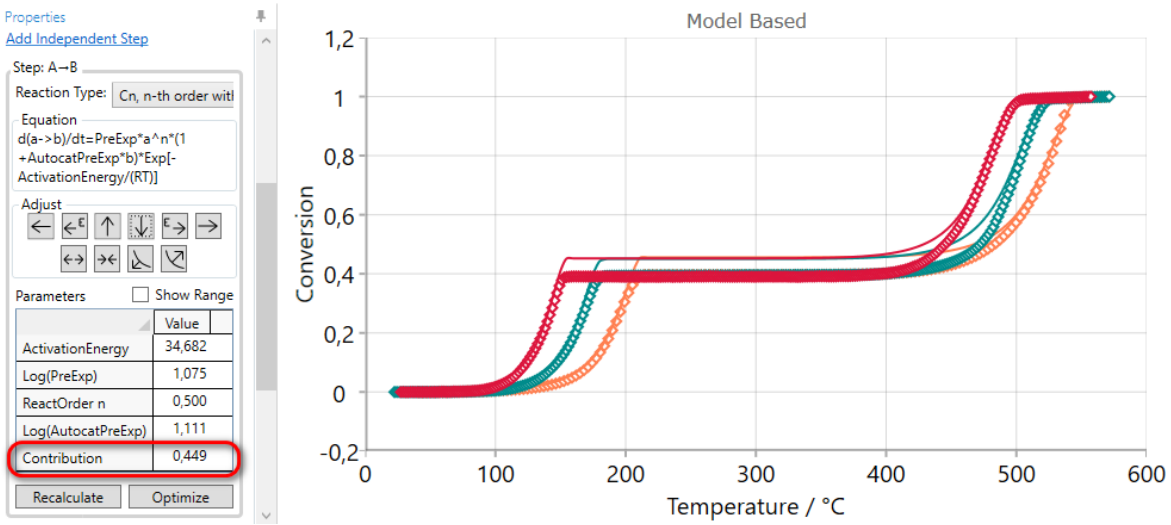
6.4 DECREASE Contribution of the Current Step

If the simulation for selected step finishes at too high conversion value in *Conversion* view, then the contribution of the current step can be decreased by the using of DECREASE CONTRUBUTION arrow.

Here the final conversion for the first step is too high, therefore the first step should be selected.

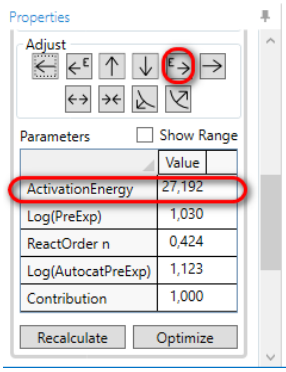


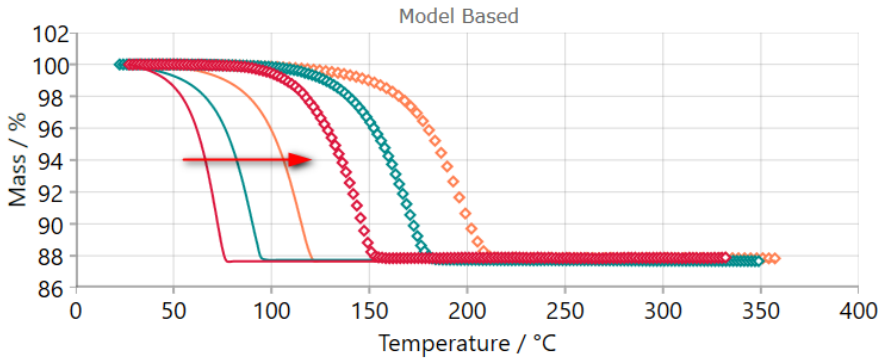
Using of DECREASE CONTRUBUTION arrow for the selected step decreases the value of the contribution and then the simulated curves have the lower value of final conversion for this step. The contribution values of other reaction steps are automatically increased in order to have the sum of all contributions equal to one.



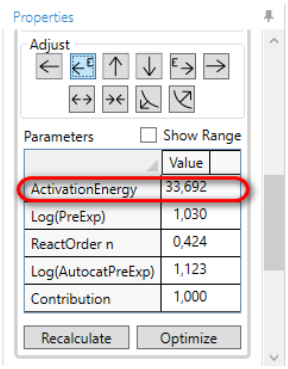
6.5  Move Reaction Step LATER by INCREASING Activation Energy

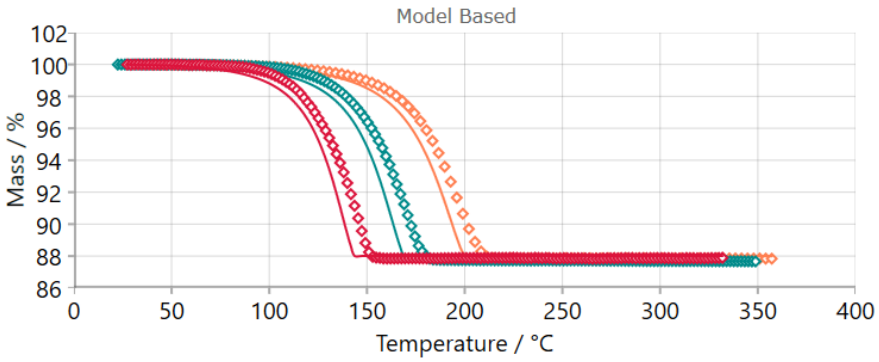
If the simulated curves for selected step are too earlier, then they can be moved to the later time by the using of INCREASE ACTIVATION EVERGY arrow.





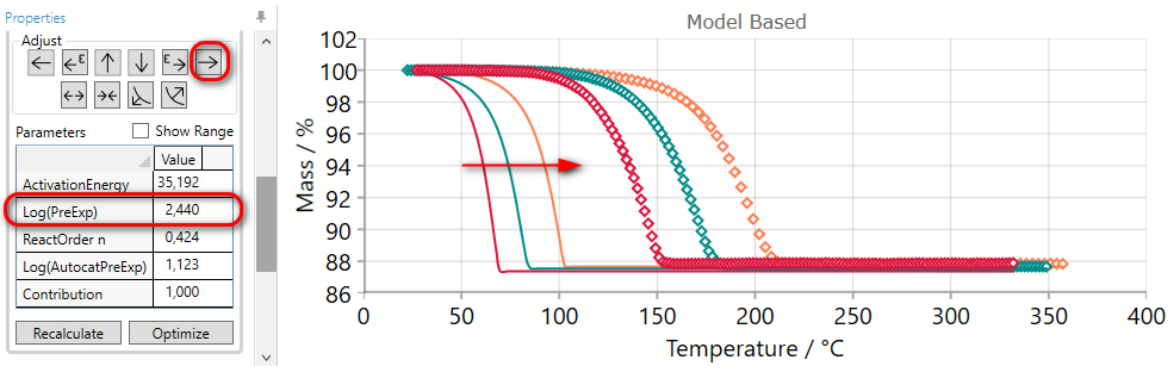
Using of INCREASE ACTIVATION EVERGY arrow increases the value of activation energy and moves simulated curves to the later time



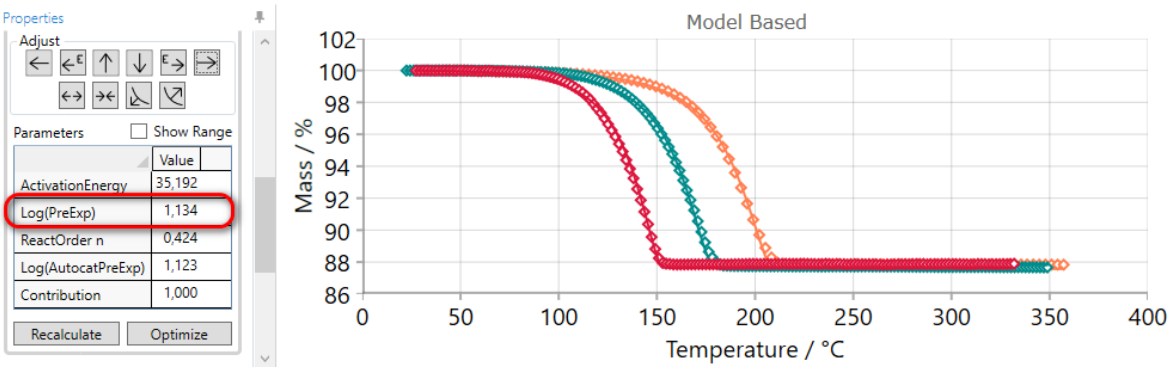


6.6  Move Reaction Step LATER by DECREASING Pre-Exponentian Factor

If the simulated curves for selected step are too early, then they can be moved to the later time by the using of LATER arrow.

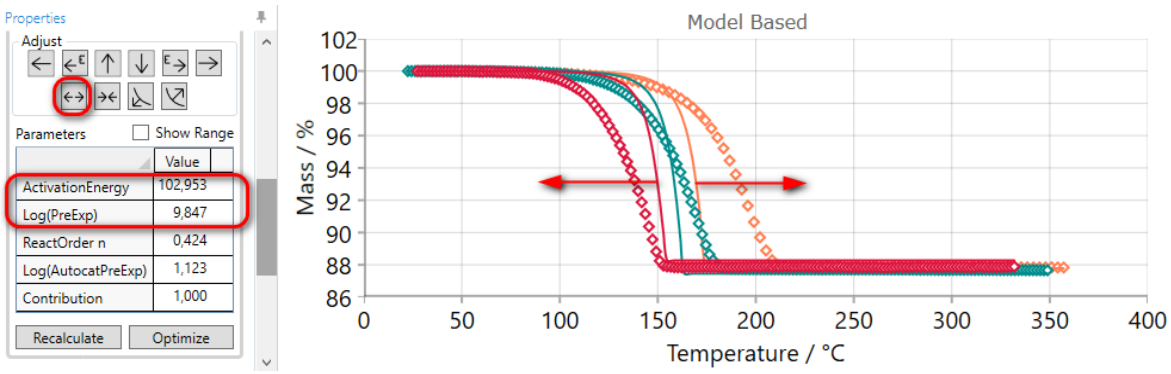


Using of LATER arrow decreases pre-exponential factor and moves simulated curves to the later time

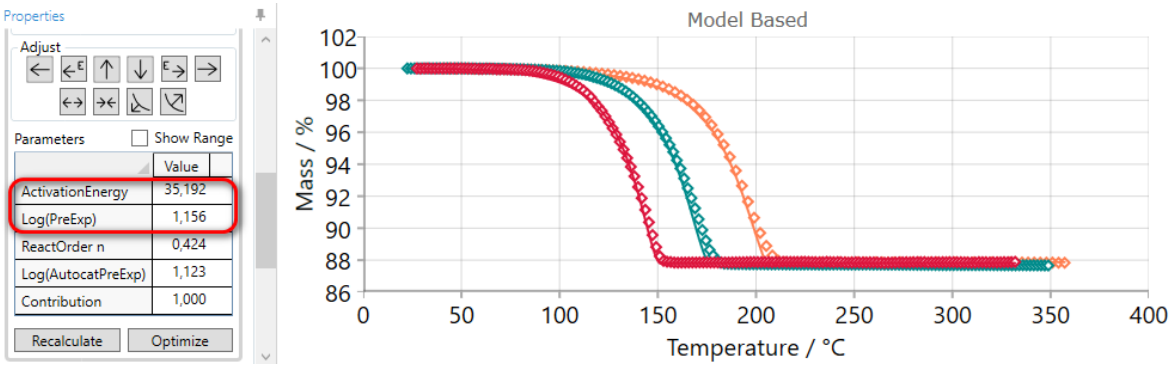


6.7 SPREAD Reaction Step

If the simulated curves for selected step are placed too close to each other, then they can be spread by the using of SPREAD arrow.

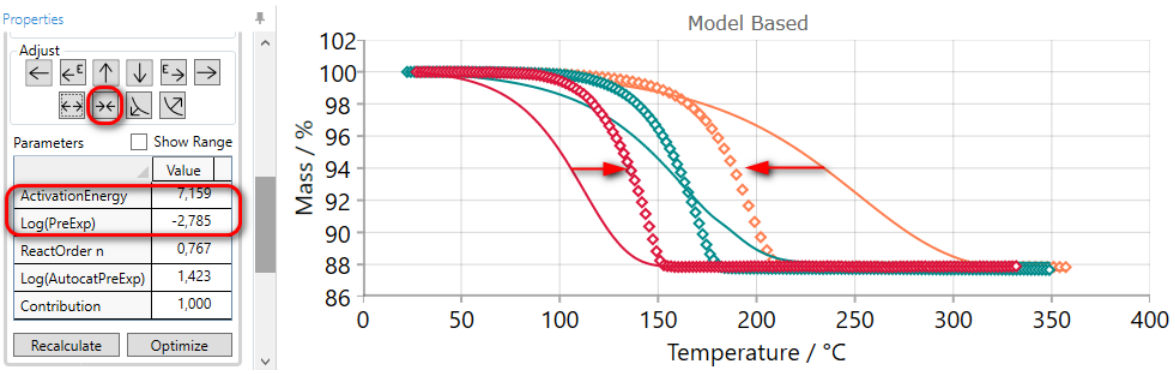


Using of SPREAD arrow decreases the value of activation energy and increases pre-exponential factor simultaneously. Thus, new simulated curves will be far from each other.

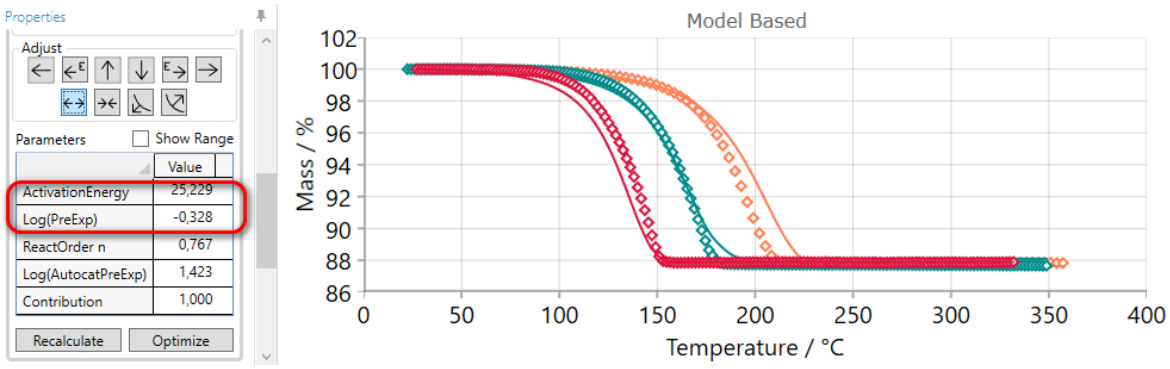


6.8  COMPRESS Reaction Step

If the simulated curves for selected step are placed too far from each other, then they can be compressed by the using of COMPRESS arrow.

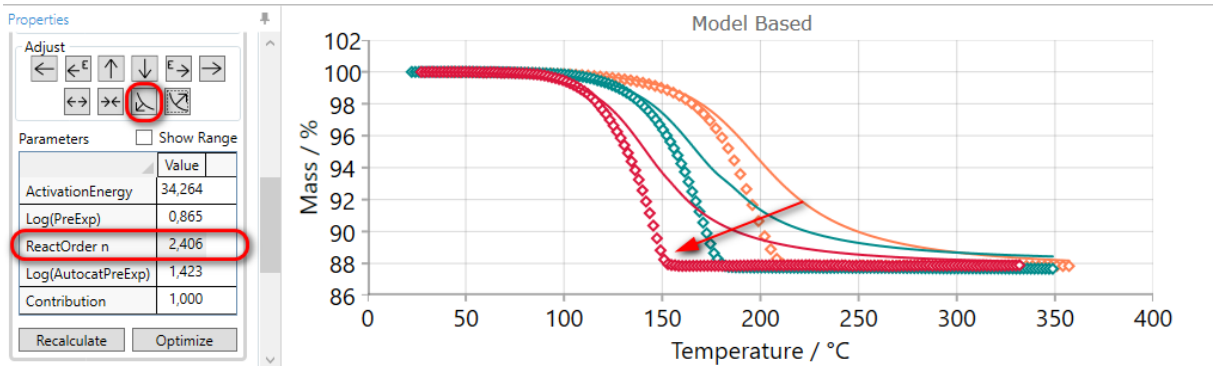


Using of COMPRESS arrow increases the value of activation energy and decreases pre-exponential factor simultaneously. Thus, new simulated curves will be close to each other.



6.9  SHARPEN Reaction Step

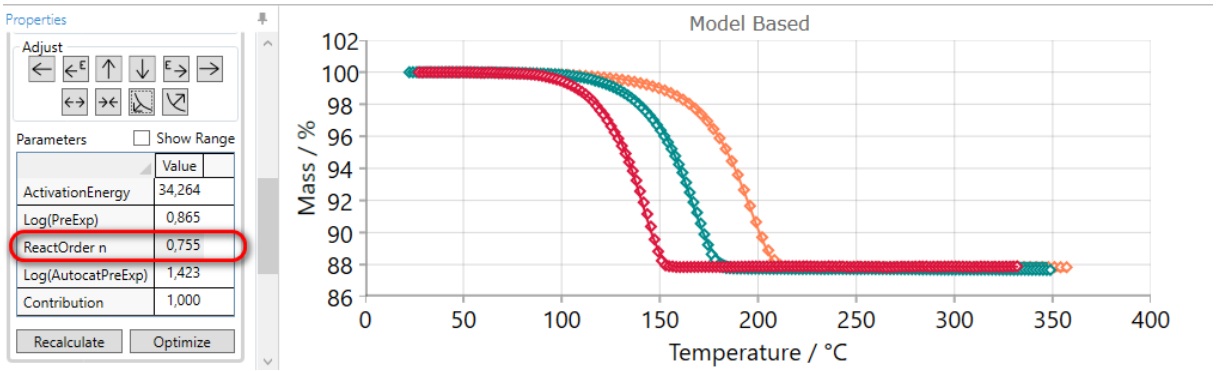
If the slope of the simulated curves for selected step is too low then they it can be increased by the using of SHARPEN arrow.



Using of SHARPEN arrow:

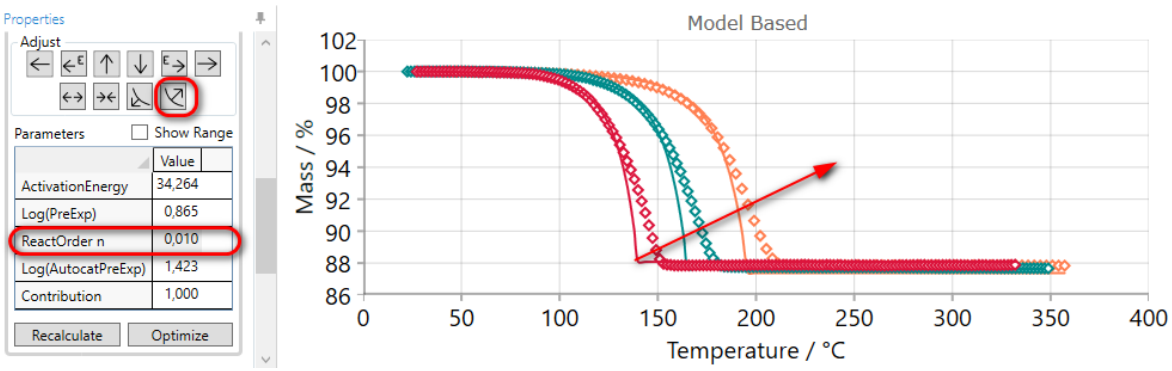
- decreases the value of reaction order,
- or increases dimension of nucleation for Avrami reactions,
- or decreases autocatalytic order for reactions where reaction order is fixed.

This adjusting arrow gives no any changes for reaction types having no reaction order or nucleation dimension as the parameter.



6.10 FLATTEN Reaction Step

If the slope of the simulated curves for selected step is too high then they it can be decreased by the using of FLATTEN arrow.



Using of FLATTEN arrow:

- increases the value of reaction order,
- or decreases dimension of nucleation for Avrami reactions,
- or increases autocatalytic order for reactions where reaction order is fixed.

This adjusting arrow gives no changes for reaction types having no reaction order or nucleation dimension as the parameter.