Regression Mix for GC2GE Users

A transfer guide

DDBST - Dortmund Data Bank Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Tel.: +49 441 361819 0

support@ddbst.com

www.ddbst.com

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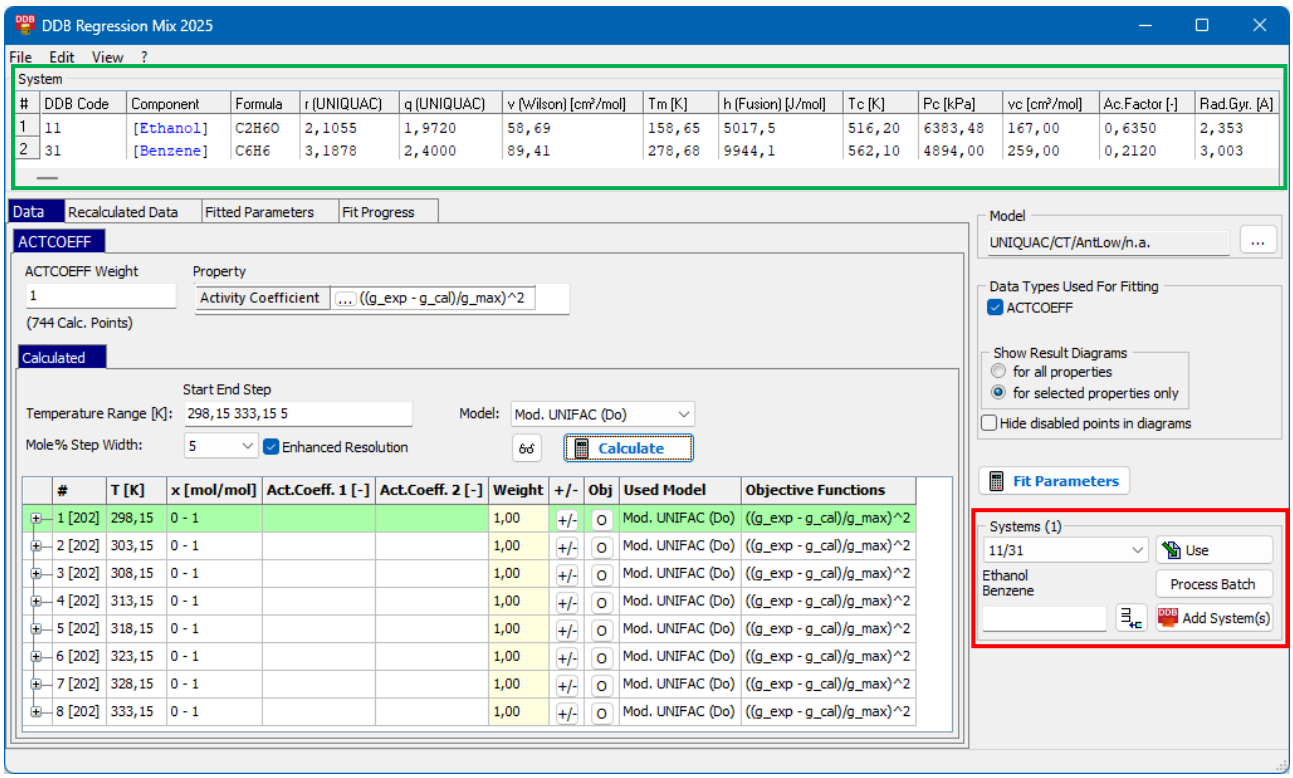
1 Introduction

Since the 2025 release of the DDB software, the GC2GE functions were moved to the *Regression Mix* application. For a smooth transition, this short introduction will explain how to access the same functions for GC2GE users.

In contrast to GC2GE, *Regression Mix* cannot only fit parameters for g^E models but also for equation of state (EOS) mixing rules and for external models of process simulators.

2 Component Selection



The function in the bottom right corner (red box) of the main dialog allows the specification of the binary systems, either by the “Add Systems(s)” button (DDB Components) or by typing the known DDB component numbers of the wanted systems in the edit box left of it. This system can be confirmed by pressing the “Enter” button or by the button between the both options. If more than two components were specified at the same time, all binary cross combination will be added. All systems will be shown in the “Systems” combo box, which shows also the total number of binary systems in brackets in the header. If more than one system was added, the desired system can be selected here and activated by the “Use” button.

The details of the components of the activated systems can be seen at the top (green box). All necessary pure component information for the fit is shown here:

- UNIQUAC: Molecular surface and volume
- Wilson: Liquid volume at approx. 298 K
- EOS: Critical temperature
- EOS: Critical pressure
- EOS: Acentric factor

If any of these values are not defined, the corresponding model cannot be used.

The values are stored in the basic component file and can be modified by DDB Components.

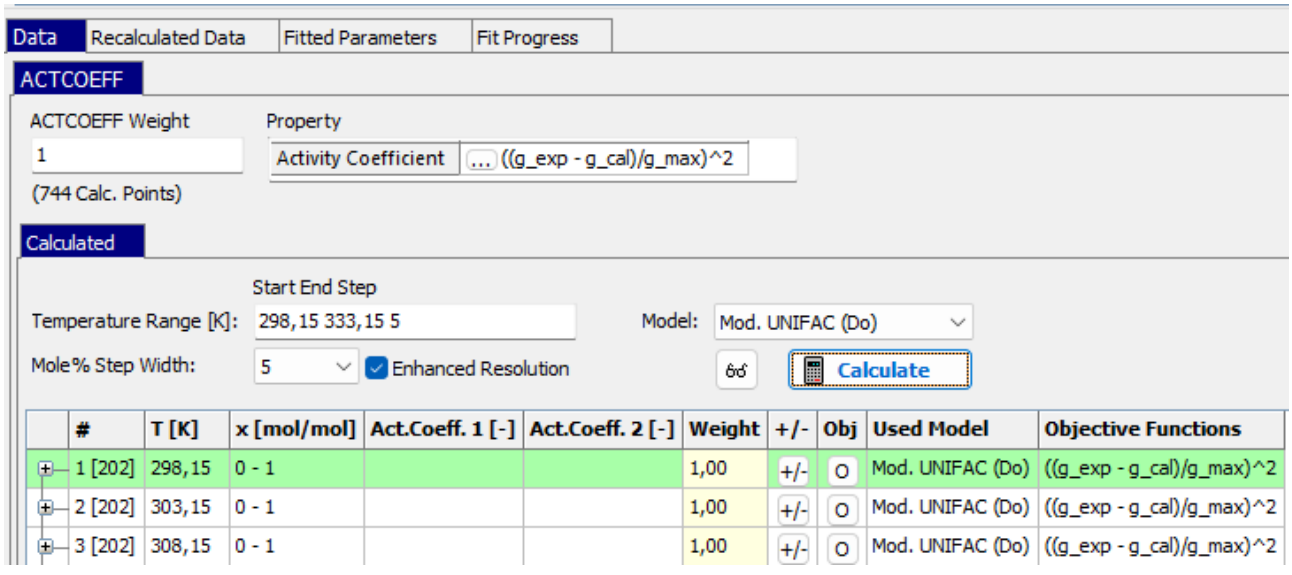
3 Calculating Activity Coefficients

Several models are available for the calculation of activity coefficients:

- UNIFAC
- UNIFAC 2.0
- Mod. UNIFAC (Dortmund)
- Mod. UNIFAC 2.0
- NIST-modified UNIFAC
- modified UNIFAC (Lyngby)
- COSMO-RS (Ol)
- COSMO-SAC
- COSMO-SAC 2010
- COSMO-SAC 2013
- PSRK
- PSRK 2.0
- VTPR

For the models UNIFAC, mod. UNIFAC (Dortmund), PSRK and VTPR the UNIFAC Consortium maintains an extended list of groups and parameters, which are available for the consortium members only.

The calculation can be specified in the “Data” page. The calculation rule for the error can be chosen on the top of menu under the “Property” option.



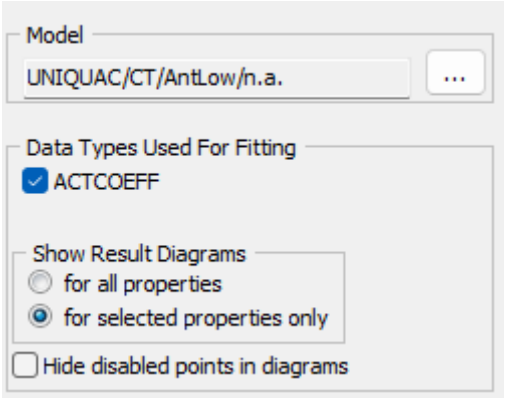
Use the “Temperature Range” edit field to specify the start and end temperature and the step width.

Use the drop-down menu to specify the step width for the concentration range. If the “Enhanced Resolution” option is set, the step width above 90% and below 10% is divided by a factor of 10 (e.g. from 5% to 0.5%) and the step width above 99% and below 1% is divided by a factor of 100 (e.g. from 5% to 0.05%).

The button with the glasses opens a dialog with information of the availability of group assignments and interaction parameters for the different group contribution models for the active binary system. Green lines indicate that this model can be used to calculate activity coefficients – group assignment and interaction parameters are available. Red lines indicate either a missing group assignment or missing interaction parameters. The *Details* page allows the user to identify the problem.

The calculation is started by the “Calculate” button. If the temperature range or concentration range settings are changed, then the “Calculate” button has to be used again to recalculate the activity coefficients. If the system or the model is changed, then the recalculation will be performed automatically. A recalculation will always replace previously calculated data.

4 Fitting



As mentioned before, several internal and external models can be used for parameter fitting. The "Model" area contains a short summary of the activated model. Use the ellipsis button next to the summary to review or change the model settings. For further descriptions have a look at the *Regression Mix* documentation.

The fit is started with the "Fit Parameters" button for the activated binary system. This will open the "Start Parameters" dialog.

4.1 Starting Values

Start Parameters

Start Parameters - NRTL
Gij = exp(-alpha*Tij/RT), Tij [cal/mol] = aij + bij*T + cij*T^2 + dij*T*ln(T) + eij*T^3 + fij/T

Parameter	Start Value	Initial Step	Constant?	min.	max.	Limits
aij	50	12.5	Constant			Respect
aji	60	15	Constant			Respect
bij	0	0	Constant			Respect
bji	0	0	Constant			Respect
cij	0	0	Constant			Respect
cji	0	0	Constant			Respect
dij	0	0	Constant			Respect
dji	0	0	Constant			Respect
eij	0		Constant			Respect
eji	0		Constant			Respect
fij	0		Constant			Respect
fji	0		Constant			Respect
alpha	0.3	0	Constant	0.01	1	Respect

Optimizer LM + SNM Fit Lev. Steps 80
Use Expert Modus

OK

Depending on the selected model and data, default start parameters are suggested.

The parameter equation and the chosen model are shown at the top of the window. All Parameters, which are not flagged constant, are fitted. For these parameters, limits can be specified with the three last columns.

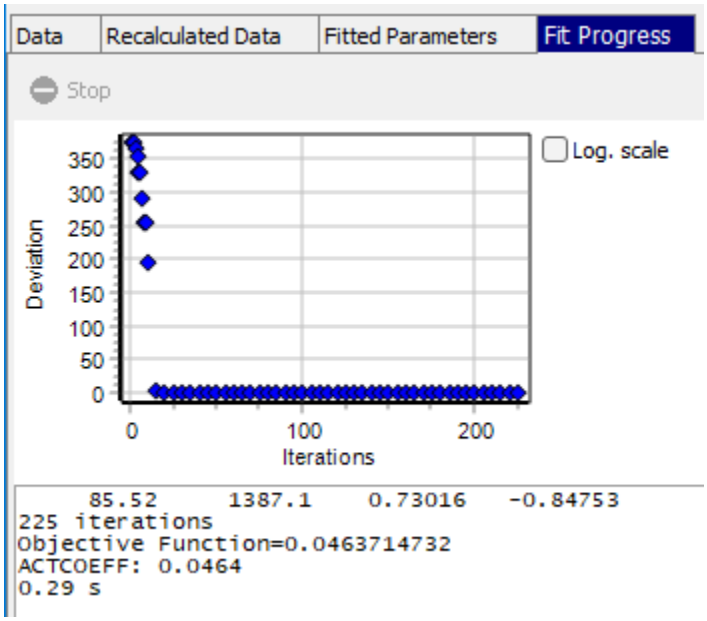
At the bottom, the Simplex-Nelder-Mead or Levenberg-Marquardt method or a combination of both methods can be chosen as optimizer method. In the case of Levenberg Marquardt a maximum number of steps can be defined with the “Fit Lev. Steps” box.

A right click opens the context menu. This allows loading parameter sets for the chosen internal model from the DDB Parameter Organizer.

With a click on the “OK” button the parameter fit will start.

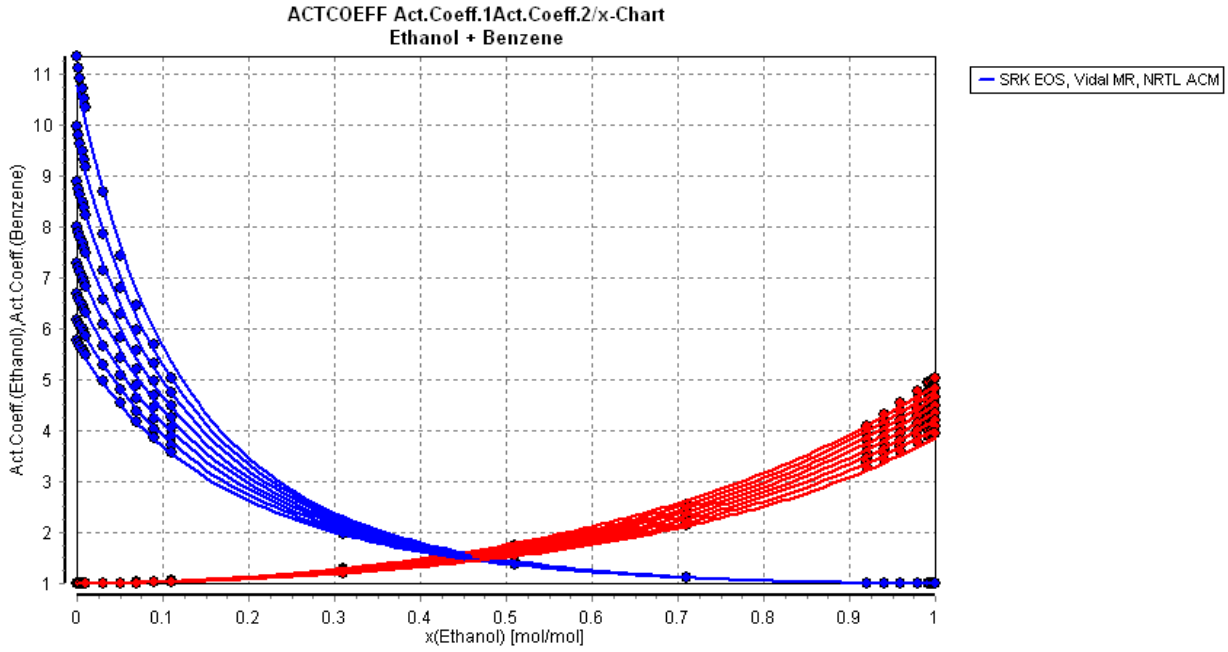
4.2 Objective Function

During the regression, a separate tab sheet (“Fit Progress”) with a diagram and a multi-line text field is shown. That control is used to present some more detailed information about the iteration progression and the values of the objective function. The diagram shows the size of the objective function against the iteration steps. Different colors represent different optimizer.



The first line shows the current parameters, the number of calls to the objective function is shown in the second line and the next line contains the number of iteration steps. The following line shows the total error calculated with the current parameters and then the contributions of the single properties are following. At the end of the fitting, the time elapsed will be given at the bottom.

These values are *scaled* and a combination of several contributions and will not represent concrete values assignable to specific properties. At the end of every fit, a diagram with the source points and the results of the fitted model is created.



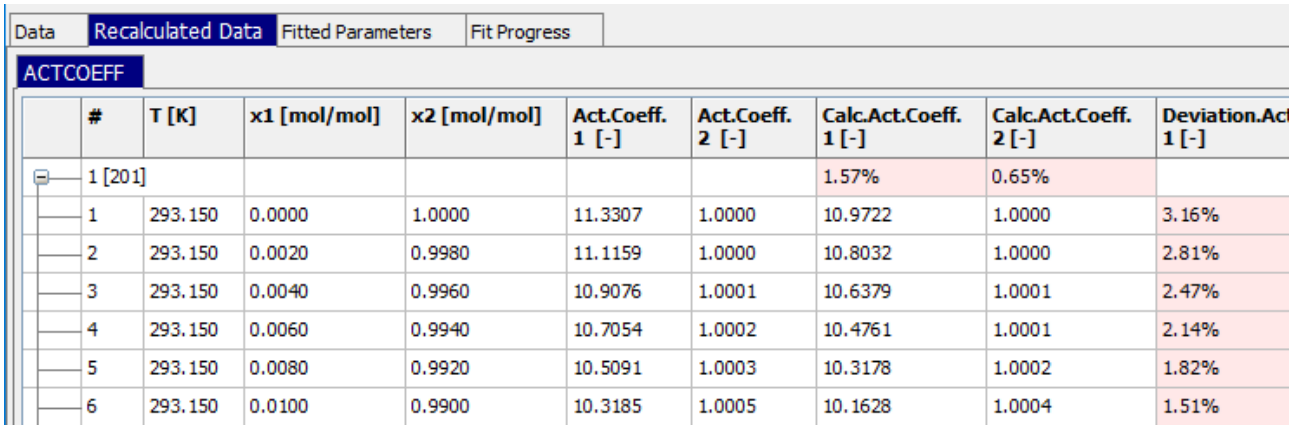
4.3 Batch Fitting

The program can also fit parameters for multiple binary systems. This is done by the “Process Batch” button. The program will work through the system list. For every system, it will recalculate the activity coefficients using the given settings and will show the “Start Parameters” dialog. After every fit, the results are given in a diagram. The resulting parameter sets are all saved under the “Fitted Parameters” page.

5 Results

5.1 Recalculated Values

The recalculated values are shown alongside the source values in the “Recalculated Data” page.



Data | Recalculated Data | Fitted Parameters | Fit Progress

ACTCOEFF

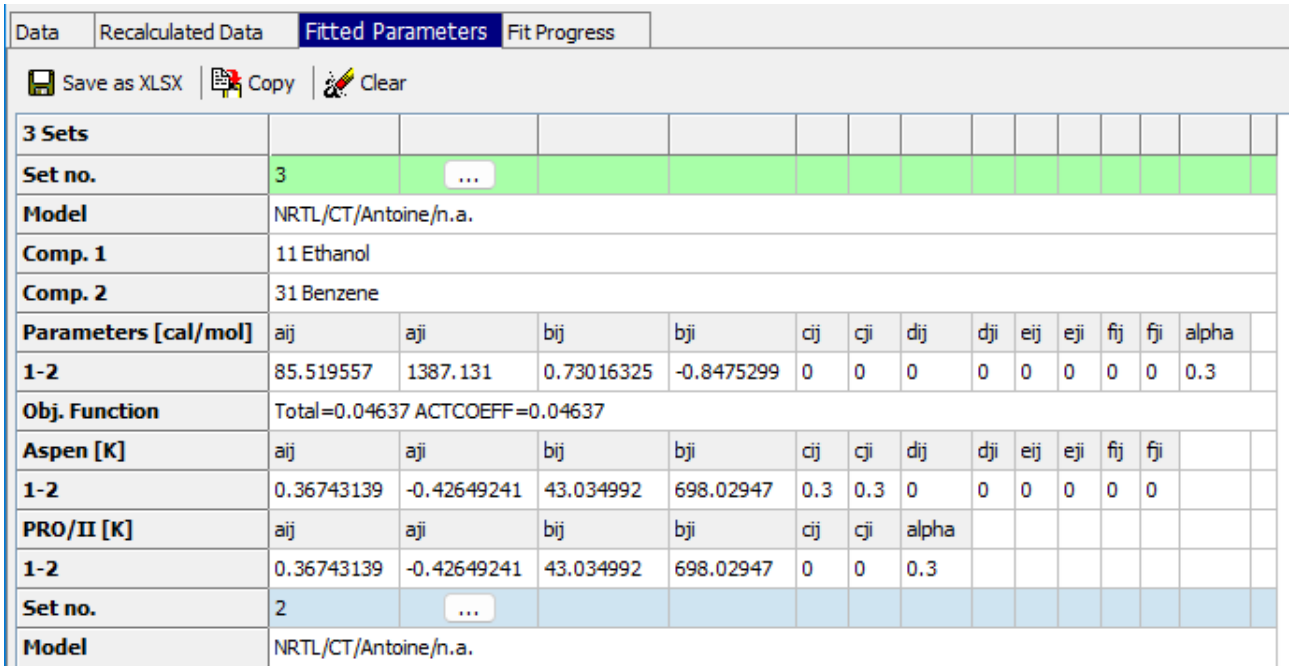
#	T [K]	x1 [mol/mol]	x2 [mol/mol]	Act.Coeff. 1 [-]	Act.Coeff. 2 [-]	Calc.Act.Coeff. 1 [-]	Calc.Act.Coeff. 2 [-]	Deviation.Act 1 [-]
1 [201]						1.57%	0.65%	
1	293.150	0.0000	1.0000	11.3307	1.0000	10.9722	1.0000	3.16%
2	293.150	0.0020	0.9980	11.1159	1.0000	10.8032	1.0000	2.81%
3	293.150	0.0040	0.9960	10.9076	1.0001	10.6379	1.0001	2.47%
4	293.150	0.0060	0.9940	10.7054	1.0002	10.4761	1.0001	2.14%
5	293.150	0.0080	0.9920	10.5091	1.0003	10.3178	1.0002	1.82%
6	293.150	0.0100	0.9900	10.3185	1.0005	10.1628	1.0004	1.51%

This table also shows the relative deviations.

This context menu of the table allows to copy the content to the windows clipboard and to create a diagram with the results.

5.2 Parameters

The obtained parameters are displayed in the “Fitted Parameters” page. This table is used to collect all fit results.



Data | Recalculated Data | Fitted Parameters | Fit Progress

Save as XLSX | Copy | Clear

3 Sets													
Set no.	3	...											
Model	NRTL/CT/Antoine/n.a.												
Comp. 1	11 Ethanol												
Comp. 2	31 Benzene												
Parameters [cal/mol]	aij	aji	bij	bji	cij	cji	dij	dji	eij	eji	fij	fji	alpha
1-2	85.519557	1387.131	0.73016325	-0.8475299	0	0	0	0	0	0	0	0	0.3
Obj. Function	Total=0.04637 ACTCOEFF=0.04637												
Aspen [K]	aij	aji	bij	bji	cij	cji	dij	dji	eij	eji	fij	fji	
1-2	0.36743139	-0.42649241	43.034992	698.02947	0.3	0.3	0	0	0	0	0	0	
PRO/II [K]	aij	aji	bij	bji	cij	cji	alpha						
1-2	0.36743139	-0.42649241	43.034992	698.02947	0	0	0.3						
Set no.	2	...											
Model	NRTL/CT/Antoine/n.a.												

The green background color shows the last used parameter set. The ellipsis button allows several actions for the given parameter set. The set can be used to replot or refit or can be removed. It is also possible to save them in the ParameterDDB or as INP or PPDX. If an external model was used, it is also possible to save the parameter set directly in the simulator project file.