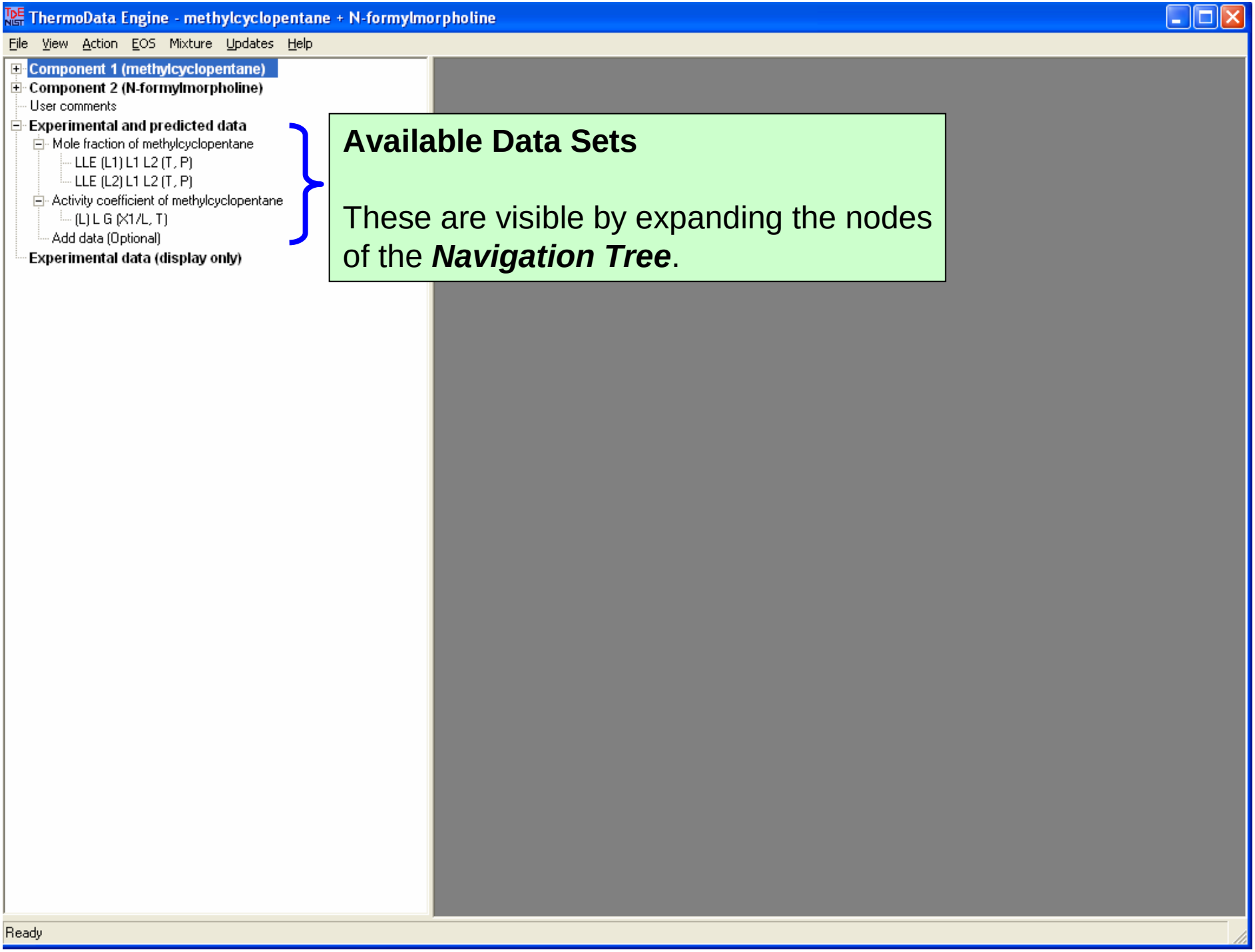
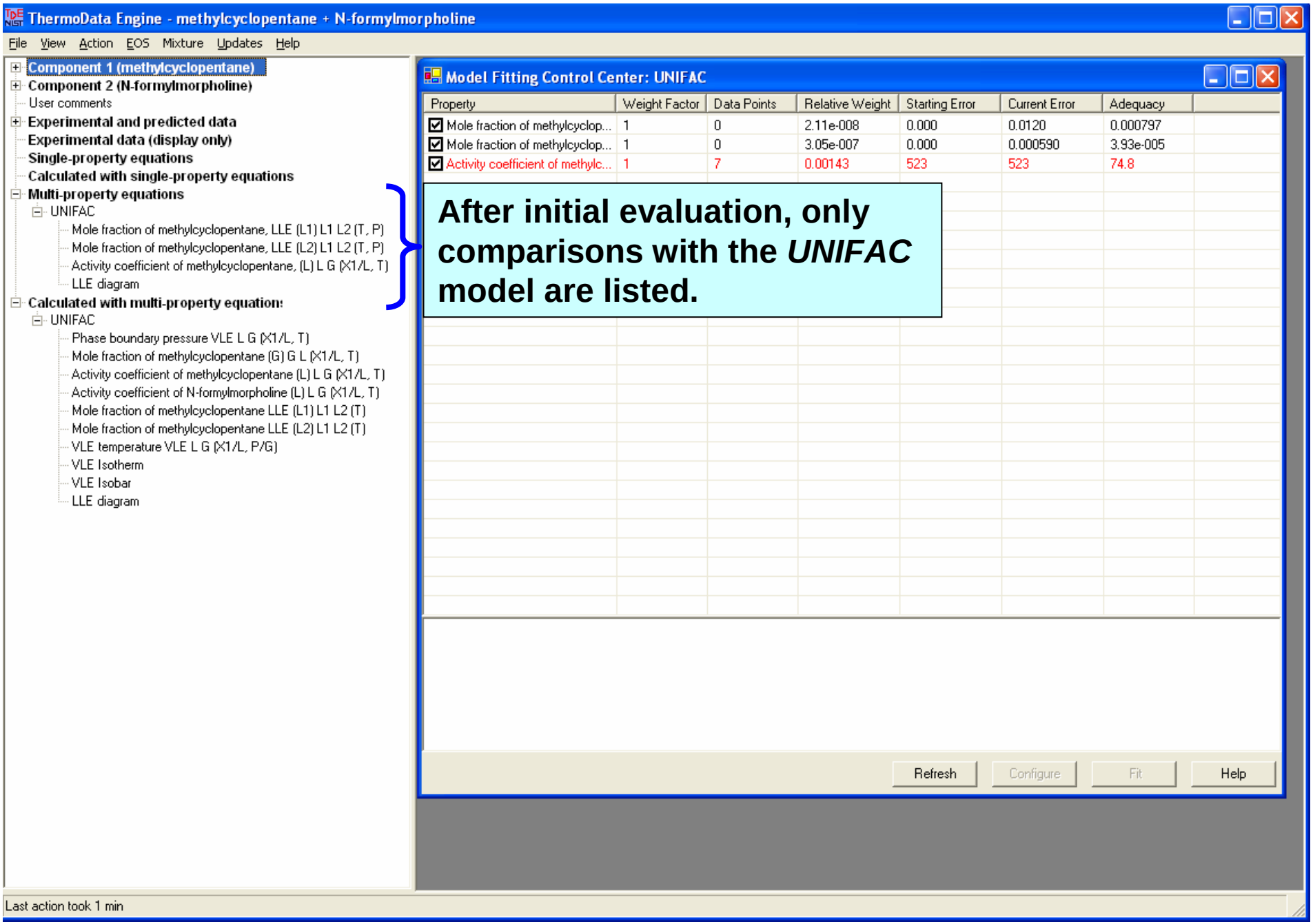
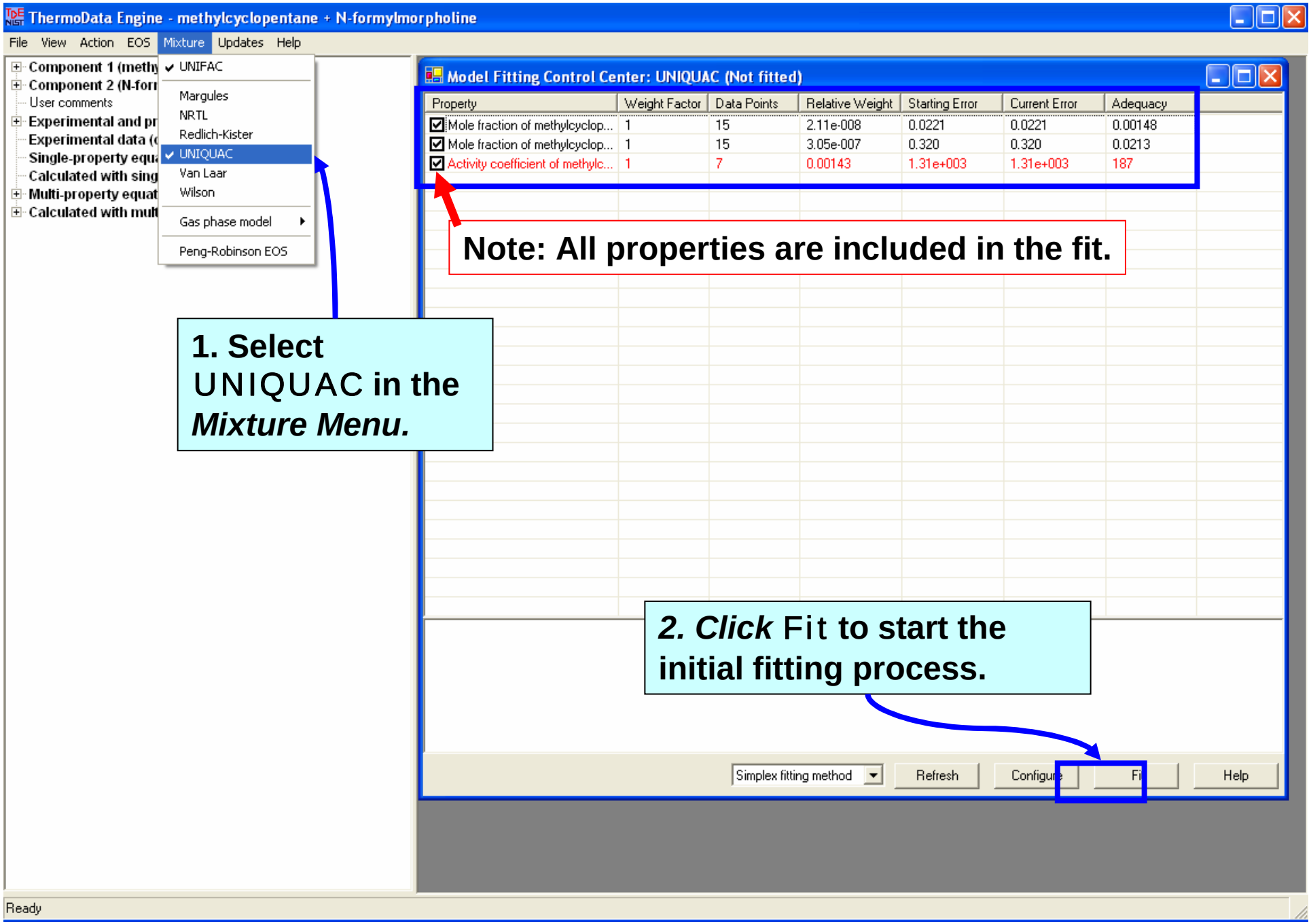
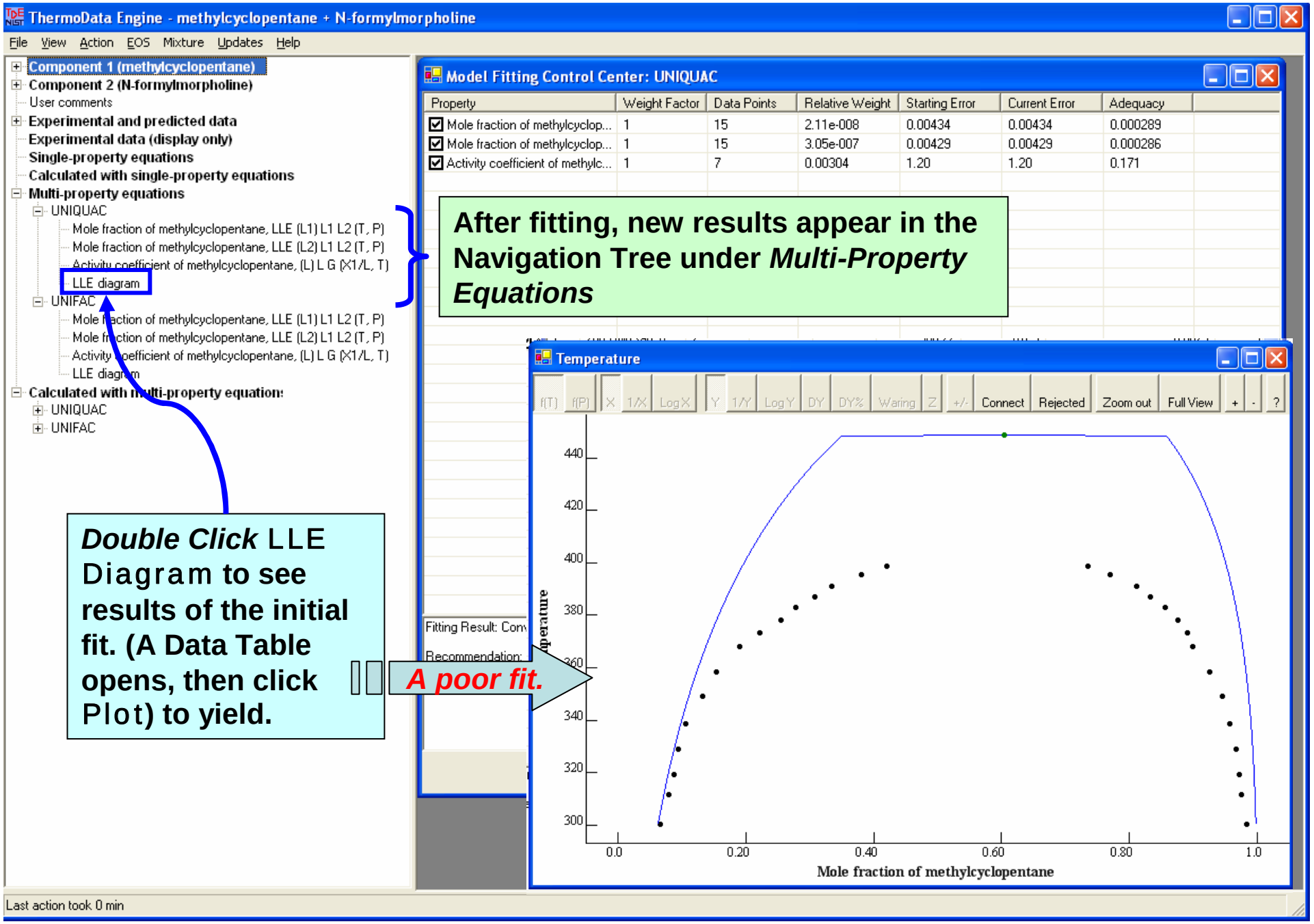


Available Data Sets

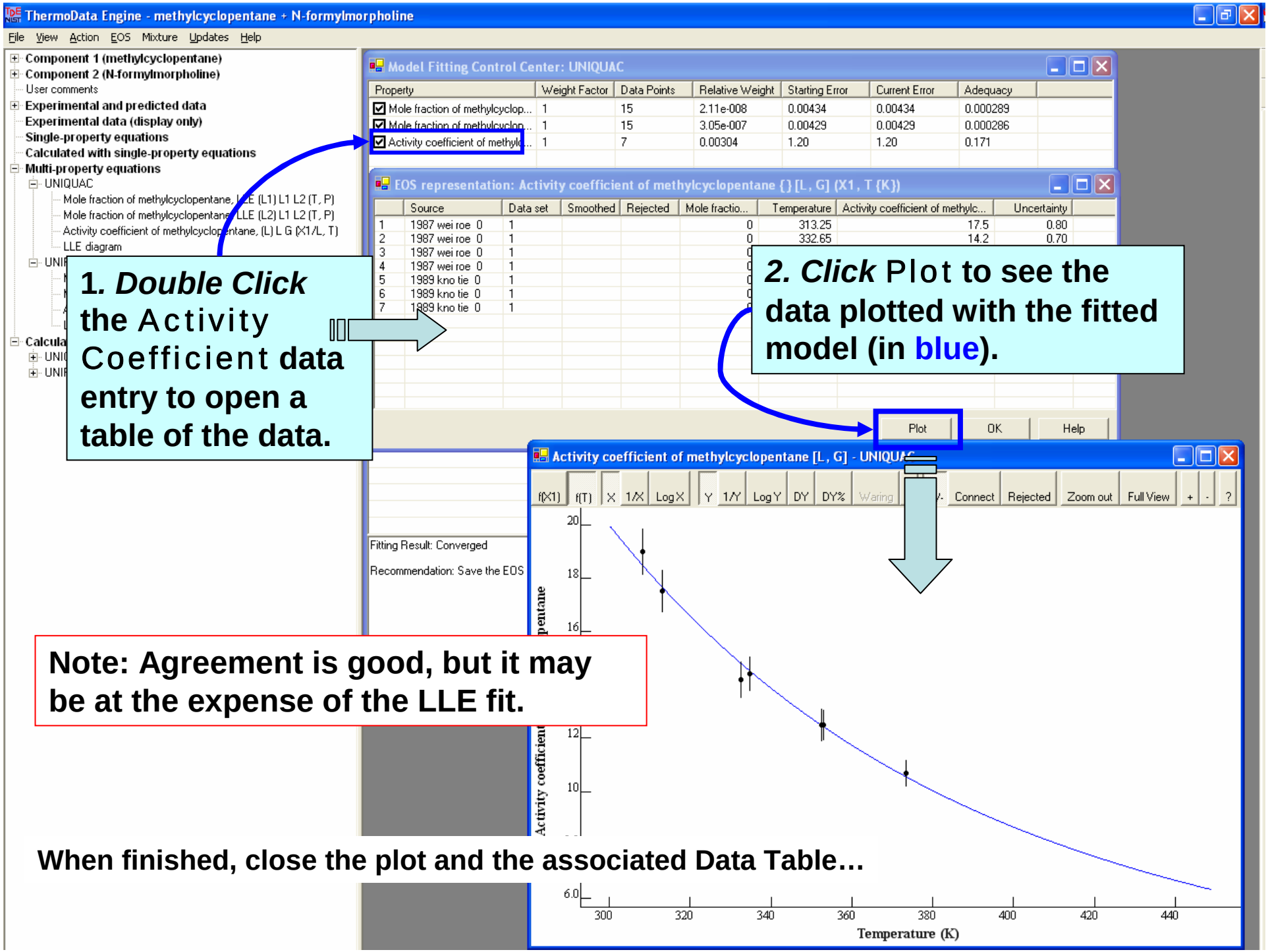
These are visible by expanding the nodes of the ***Navigation Tree***.


ThermoData Engine - methylcyclopentane + N-formylmorpholine
File View Action EOS Mixture Updates Help
Component 1 (methylcyclopentane)
Component 2 (N-formylmorpholine)
User comments
Experimental and predicted data
Experimental data (display only)
Single-property equations
Calculated with single-property equations
Multi-property equations
UNIFAC
Mole fraction of methylcyclopentane, LLE (L1) L1 L2 (T, P)
Mole fraction of methylcyclopentane, LLE (L2) L1 L2 (T, P)
Activity coefficient of methylcyclopentane, (L) L G (X1/L, T)
LLE diagram
Calculated with multi-property equation:
UNIFAC
Phase boundary pressure VLE L G (X1/L, T)
Mole fraction of methylcyclopentane (G) G L (X1/L, T)
Activity coefficient of methylcyclopentane (L) L G (X1/L, T)
Activity coefficient of N-formylmorpholine (L) L G (X1/L, T)
Mole fraction of methylcyclopentane LLE (L1) L1 L2 (T)
Mole fraction of methylcyclopentane LLE (L2) L1 L2 (T)
VLE temperature VLE L G (X1/L, P/G)
VLE Isotherm
VLE Isobar
LLE diagram
Model Fitting Control Center: UNIFAC
Property
Weight Factor
Data Points
Relative Weight
Starting Error
Current Error
Adequacy
Mole fraction of methylcyclop... 1 0 2.11e-008 0.000 0.0120 0.000797
Mole fraction of methylcyclop... 1 0 3.05e-007 0.000 0.000590 3.93e-005
Activity coefficient of methylc... 1 7 0.00143 523 523 74.8
After initial evaluation, only comparisons with the UNIFAC model are listed.
Refresh
Configure
Fit
Help
Last action took 1 min


ThermoData Engine - methylcyclopentane + N-formylmorpholine
File View Action EOS Mixture Updates Help
UNIFAC
Margules
NRTL
Redlich-Kister
UNIQUAC
Van Laar
Wilson
Gas phase model
Peng-Robinson EOS
Component 1 (methy
Component 2 (N-for
User comments
Experimental and pr
Experimental data (
Single-property equa
Calculated with sing
Multi-property equat
Calculated with mult
Model Fitting Control Center: UNIQUAC (Not fitted)
Property
Weight Factor
Data Points
Relative Weight
Starting Error
Current Error
Adequacy
Mole fraction of methylcyclop... 1 15 2.11e-008 0.0221 0.0221 0.00148
Mole fraction of methylcyclop... 1 15 3.05e-007 0.320 0.320 0.0213
Activity coefficient of methylc... 1 7 0.00143 1.31e+003 1.31e+003 187
Note: All properties are included in the fit.
1. Select UNIQUAC in the Mixture Menu.
2. Click Fit to start the initial fitting process.
Simplex fitting method
Refresh
Configure
Fit
Help
Ready



When finished, close the plot and the associated Data Table…

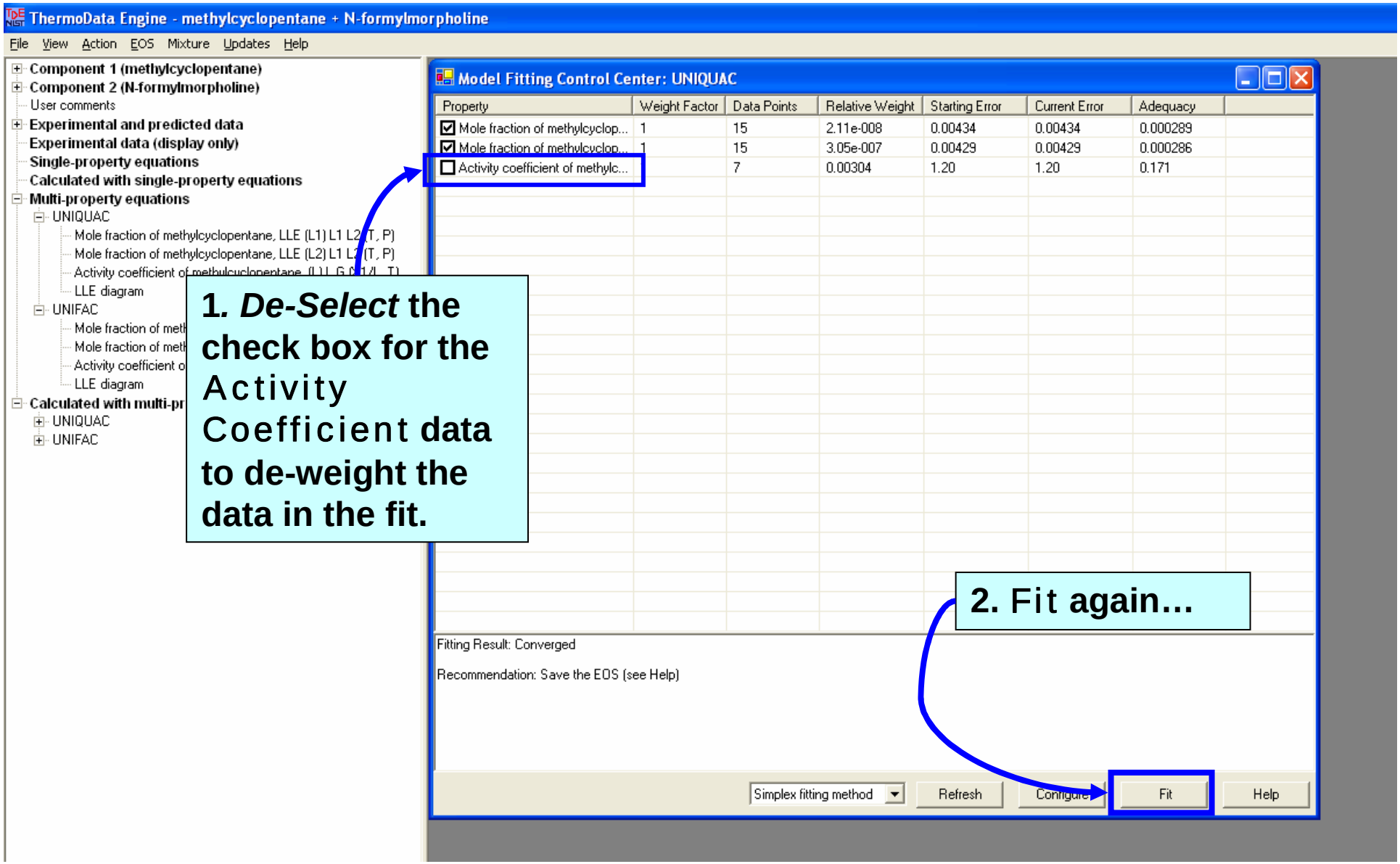


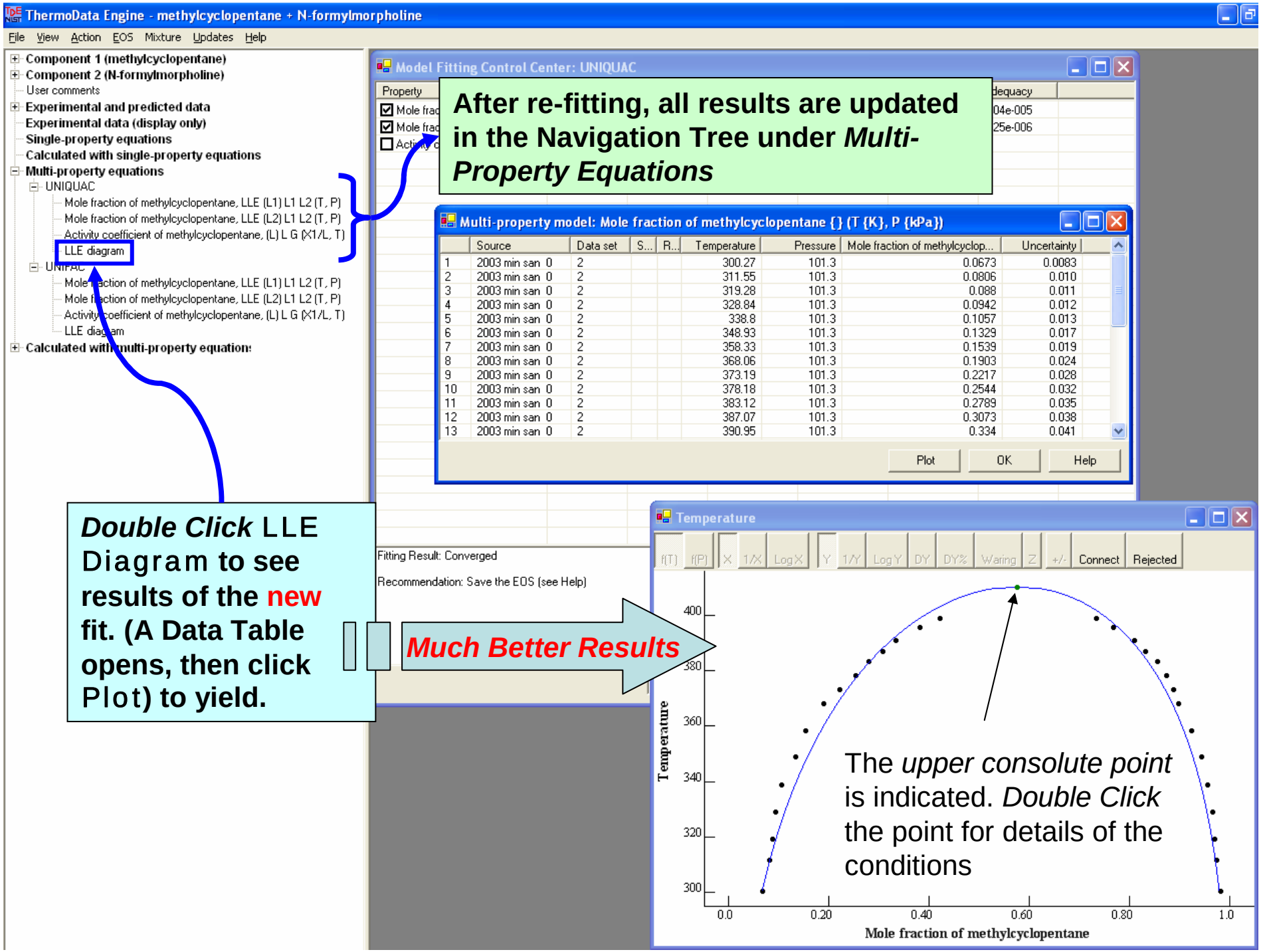
1. *Double Click* the Activity Coefficient data entry to open a table of the data.

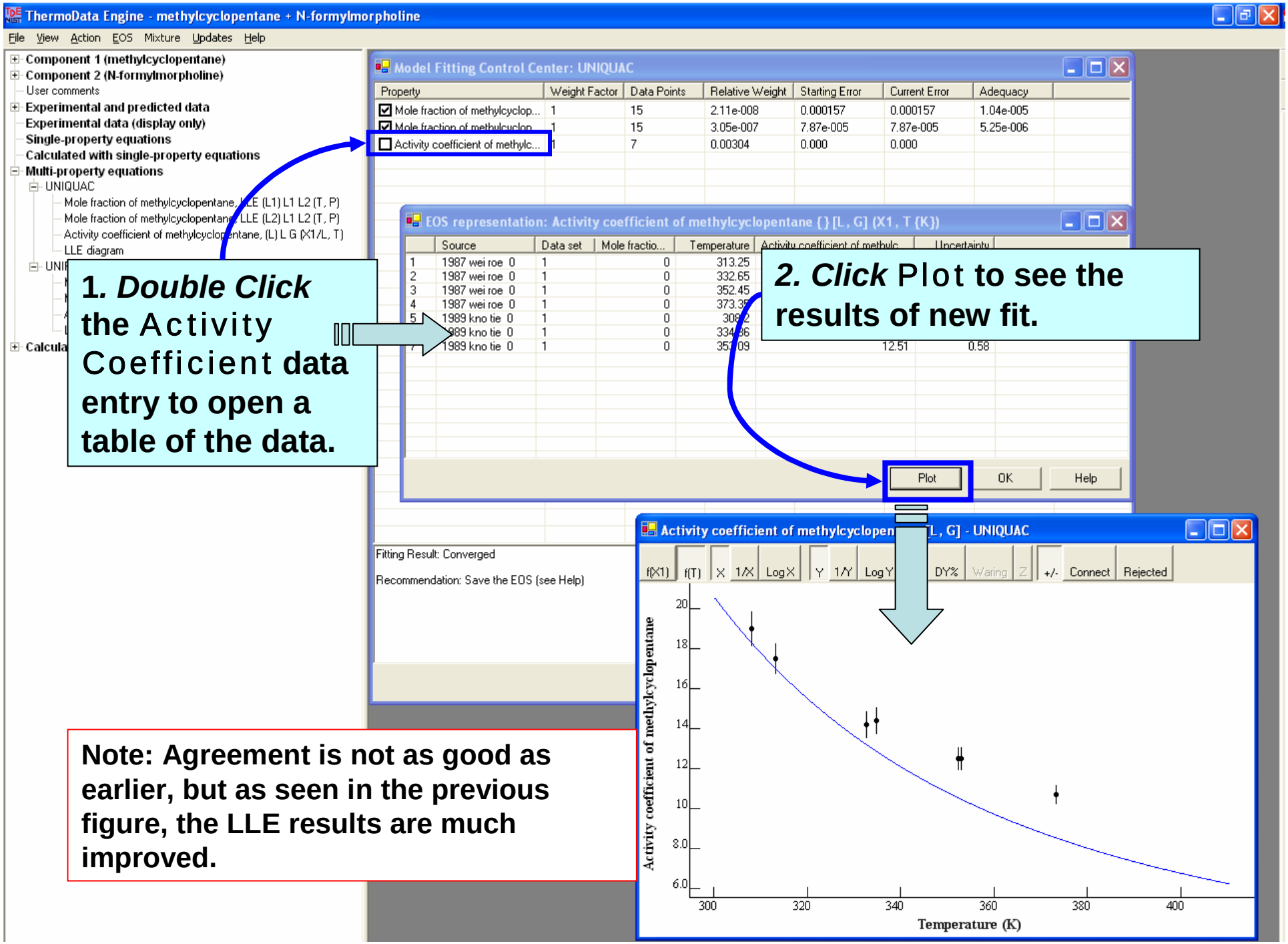
2. *Click* Plot to see the data plotted with the fitted model (in blue).

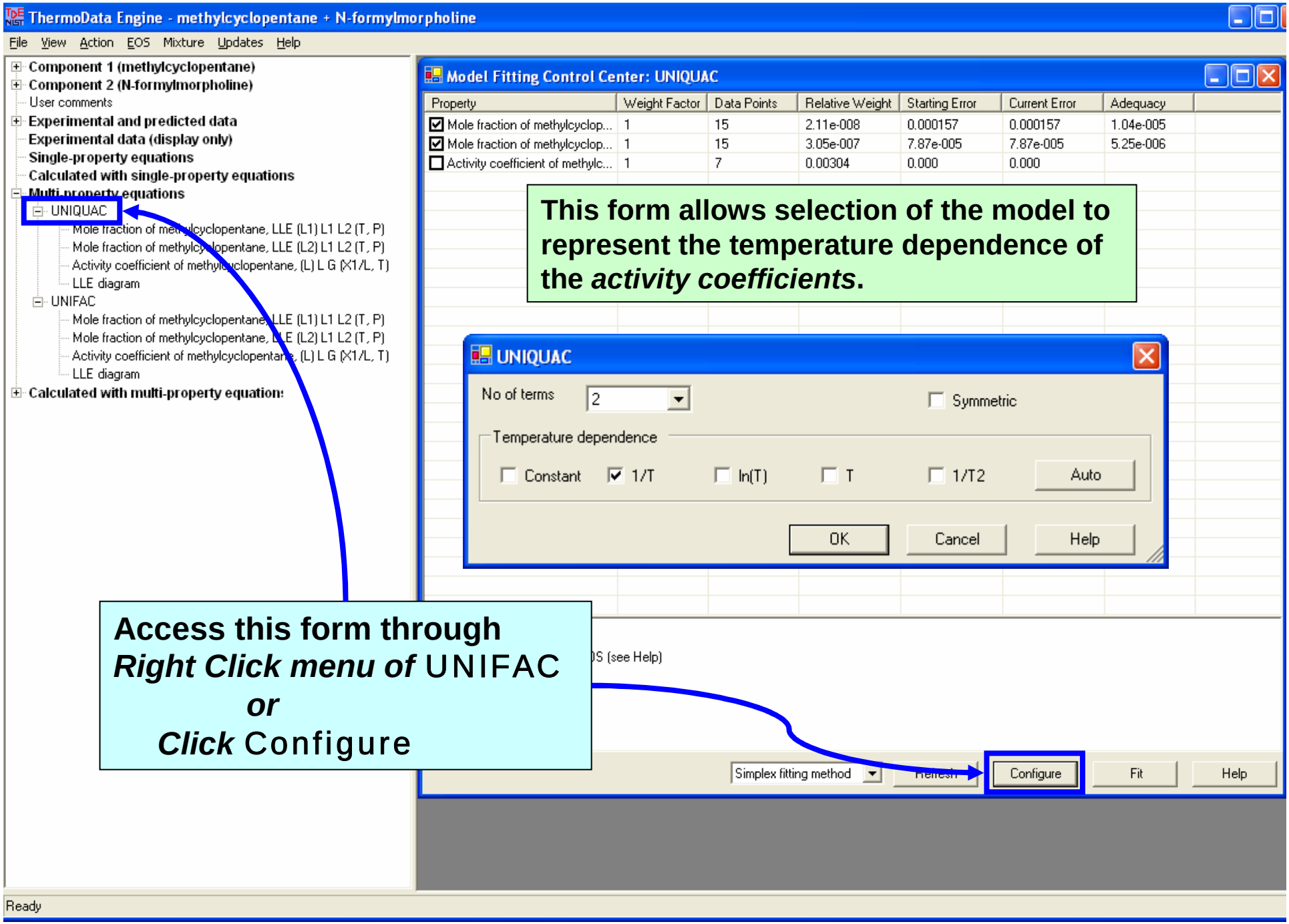
Note: Agreement is good, but it may be at the expense of the LLE fit.

When finished, close the plot and the associated Data Table…


ThermoData Engine - methylcyclopentane + N-formylmorpholine
File View Action EOS Mixture Updates Help
Component 1 (methylcyclopentane)
Component 2 (N-formylmorpholine)
User comments
Experimental and predicted data
Experimental data (display only)
Single-property equations
Calculated with single-property equations
Multi-property equations
UNIQUAC
Mole fraction of methylcyclopentane, LLE (L1) L1 L2 (T, P)
Mole fraction of methylcyclopentane, LLE (L2) L1 L2 (T, P)
LLE diagram
UNIFAC
LLE diagram
Calculated with multi-pr
UNIQUAC
UNIFAC
Model Fitting Control Center: UNIQUAC
Property
Weight Factor
Data Points
Relative Weight
Starting Error
Current Error
Adequacy
Mole fraction of methylcyclop...
1
15
2.11e-008
0.00434
0.00434
0.000289
Mole fraction of methylcyclop...
1
15
3.05e-007
0.00429
0.00429
0.000286
Activity coefficient of methylc...
7
0.00304
1.20
1.20
0.171
1. De-Select the check box for the Activity Coefficient data to de-weight the data in the fit.
2. Fit again…
Fitting Result: Converged
Recommendation: Save the EOS (see Help)
Simplex fitting method
Refresh
Configure
Fit
Help


ThermoData Engine - methylcyclopentane + N-formylmorpholine
File View Action EOS Mixture Updates Help
Component 1 (methylcyclopentane)
Component 2 (N-formylmorpholine)
User comments
Experimental and predicted data
Experimental data (display only)
Single-property equations
Calculated with single-property equations
Multi-property equations
UNIQUAC
Mole fraction of methylcyclopentane, LLE (L1) L1 L2 (T, P)
Mole fraction of methylcyclopentane, LLE (L2) L1 L2 (T, P)
Activity coefficient of methylcyclopentane, (L) L G (X1/L, T)
LLE diagram
UNIFAC
Mole fraction of methylcyclopentane, LLE (L1) L1 L2 (T, P)
Mole fraction of methylcyclopentane, LLE (L2) L1 L2 (T, P)
Activity coefficient of methylcyclopentane, (L) L G (X1/L, T)
LLE diagram
Calculated with multi-property equation
Model Fitting Control Center: UNIQUAC
Property
Mole frac
Mole frac
dequacy
04e-005
25e-006
After re-fitting, all results are updated in the Navigation Tree under Multi-Property Equations
Multi-property model: Mole fraction of methylcyclopentane {} (T {K}, P {kPa})
Source Data set S... R... Temperature Pressure Mole fraction of methylcyclop... Uncertainty
1 2003 min san 0 2 300.27 101.3 0.0673 0.0083
2 2003 min san 0 2 311.55 101.3 0.0806 0.010
3 2003 min san 0 2 319.28 101.3 0.088 0.011
4 2003 min san 0 2 328.84 101.3 0.0942 0.012
5 2003 min san 0 2 338.8 101.3 0.1057 0.013
6 2003 min san 0 2 348.93 101.3 0.1329 0.017
7 2003 min san 0 2 358.33 101.3 0.1539 0.019
8 2003 min san 0 2 368.06 101.3 0.1903 0.024
9 2003 min san 0 2 373.19 101.3 0.2217 0.028
10 2003 min san 0 2 378.18 101.3 0.2544 0.032
11 2003 min san 0 2 383.12 101.3 0.2789 0.035
12 2003 min san 0 2 387.07 101.3 0.3073 0.038
13 2003 min san 0 2 390.95 101.3 0.334 0.041
Plot
OK
Help
Double Click LLE Diagram to see results of the new fit. (A Data Table opens, then click Plot) to yield.
Fitting Result: Converged
Recommendation: Save the EOS (see Help)
Much Better Results
Temperature
f(T) f(P) X 1/X LogX Y 1/Y LogY DY DY% Waring Z +/- Connect Rejected
400
380
360
340
320
300
Temperature
0.0
0.20
0.40
0.60
0.80
1.0
Mole fraction of methylcyclopentane
The upper consolute point is indicated. Double Click the point for details of the conditions


ThermoData Engine - methylcyclopentane + N-formylmorpholine
File View Action EOS Mixture Updates Help
Component 1 (methylcyclopentane)
Component 2 (N-formylmorpholine)
User comments
Experimental and predicted data
Experimental data (display only)
Single-property equations
Calculated with single-property equations
Multi-property equations
UNIQUAC
Mole fraction of methylcyclopentane, LLE (L1) L1 L2 (T, P)
Mole fraction of methylcyclopentane, LLE (L2) L1 L2 (T, P)
Activity coefficient of methylcyclopentane, (L) L G (X1/L, T)
LLE diagram
Model Fitting Control Center: UNIQUAC
Property
Weight Factor
Data Points
Relative Weight
Starting Error
Current Error
Adequacy
Mole fraction of methylcyclop...
Activity coefficient of methylc...
EOS representation: Activity coefficient of methylcyclopentane {} [L, G] (X1, T {K})
Source
Data set
Mole fractio...
Temperature
Uncertainty
1987 wei roe
1989 kno tie
Plot
OK
Help
Fitting Result: Converged
Recommendation: Save the EOS (see Help)
Activity coefficient of methylcyclopen [L, G] - UNIQUAC
f(X1)
f(T)
X
1/X
Log X
Y
1/Y
Log Y
DY%
Waring
Z
+/-
Connect
Rejected
Activity coefficient of methylcyclopentane
Temperature (K)
1. Double Click the Activity Coefficient data entry to open a table of the data.
2. Click Plot to see the results of new fit.
Note: Agreement is not as good as earlier, but as seen in the previous figure, the LLE results are much improved.


ThermoData Engine - methylcyclopentane + N-formylmorpholine
File View Action EOS Mixture Updates Help
Component 1 (methylcyclopentane)
Component 2 (N-formylmorpholine)
User comments
Experimental and predicted data
Experimental data (display only)
Single-property equations
Calculated with single-property equations
Multi-property equations
UNIQUAC
Mole fraction of methylcyclopentane, LLE (L1) L1 L2 (T, P)
Mole fraction of methylcyclopentane, LLE (L2) L1 L2 (T, P)
Activity coefficient of methylcyclopentane, (L) L G (X1/L, T)
LLE diagram
UNIFAC
Mole fraction of methylcyclopentane, LLE (L1) L1 L2 (T, P)
Mole fraction of methylcyclopentane, LLE (L2) L1 L2 (T, P)
Activity coefficient of methylcyclopentane, (L) L G (X1/L, T)
LLE diagram
Calculated with multi-property equation:
Model Fitting Control Center: UNIQUAC
Property | Weight Factor | Data Points | Relative Weight | Starting Error | Current Error | Adequacy
Mole fraction of methylcyclop... | 1 | 15 | 2.11e-008 | 0.000157 | 0.000157 | 1.04e-005
Mole fraction of methylcyclop... | 1 | 15 | 3.05e-007 | 7.87e-005 | 7.87e-005 | 5.25e-006
Activity coefficient of methylc... | 1 | 7 | 0.00304 | 0.000 | 0.000
This form allows selection of the model to represent the temperature dependence of the activity coefficients.
UNIQUAC
No of terms 2
Symmetric
Temperature dependence
Constant 1/T ln(T) T 1/T2 Auto
OK Cancel Help
Access this form through
Right Click menu of UNIFAC
or
Click Configure
Simplex fitting method
Refresh
Configure
Fit
Help
Ready