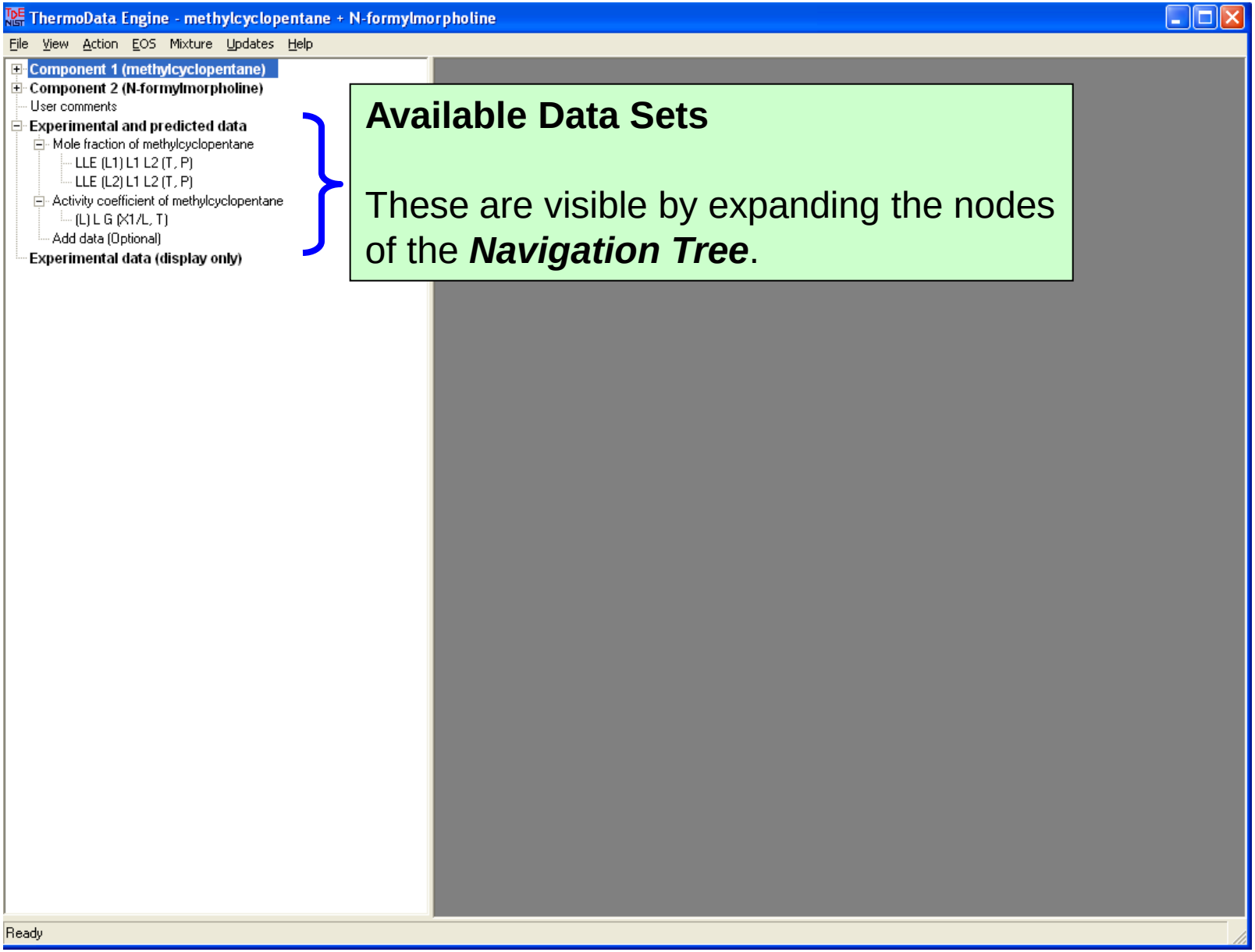
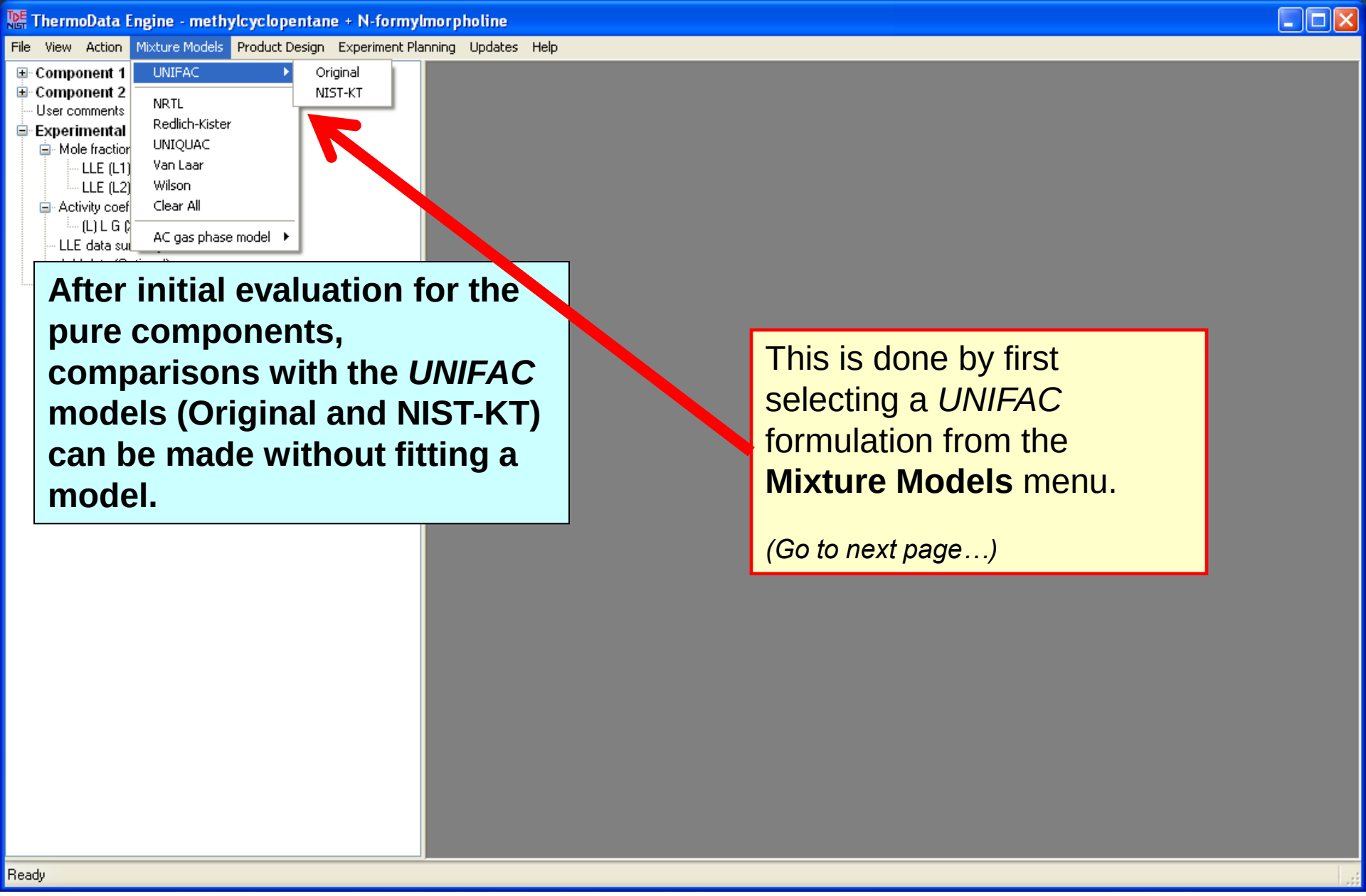


Available Data Sets

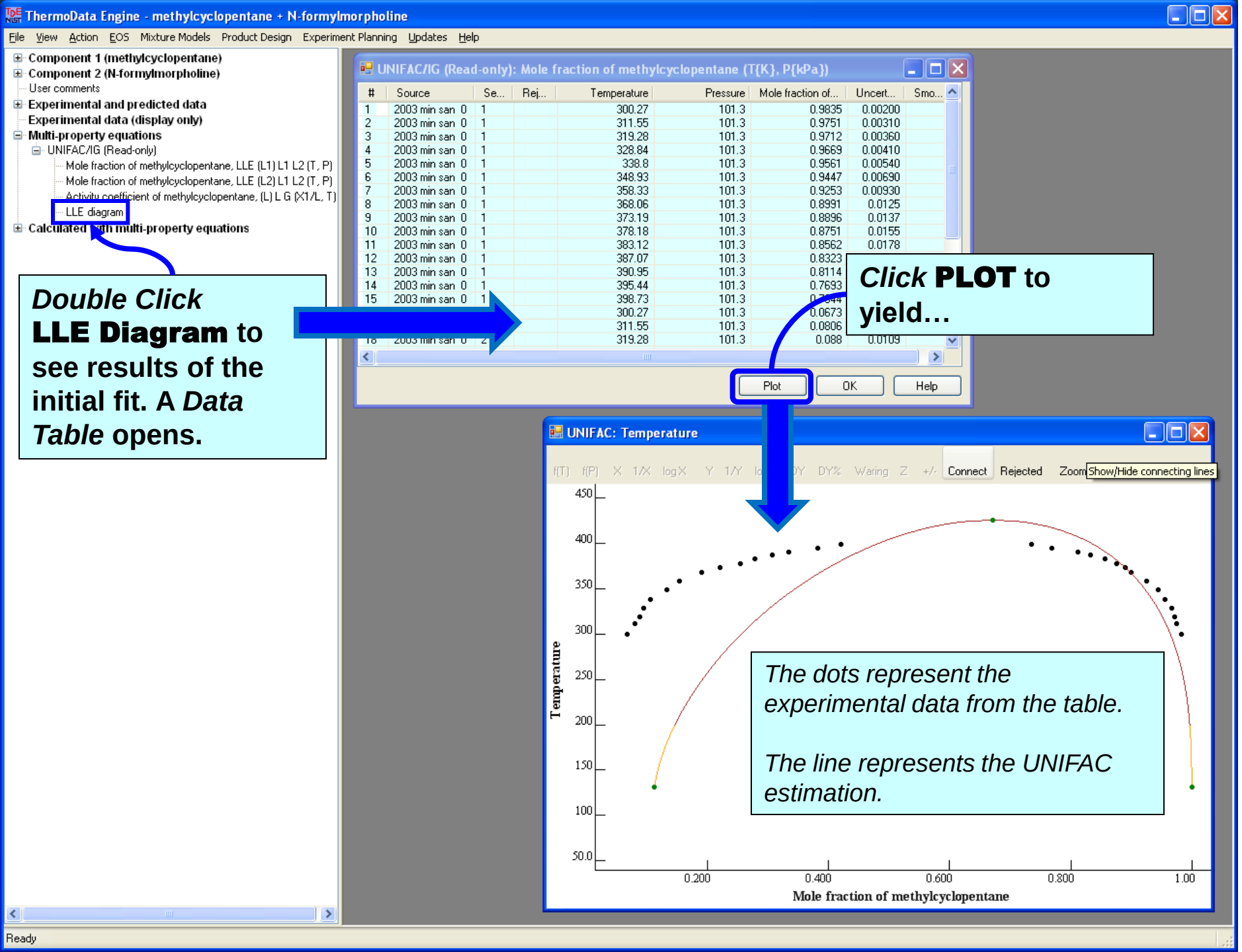
These are visible by expanding the nodes of the ***Navigation Tree***.



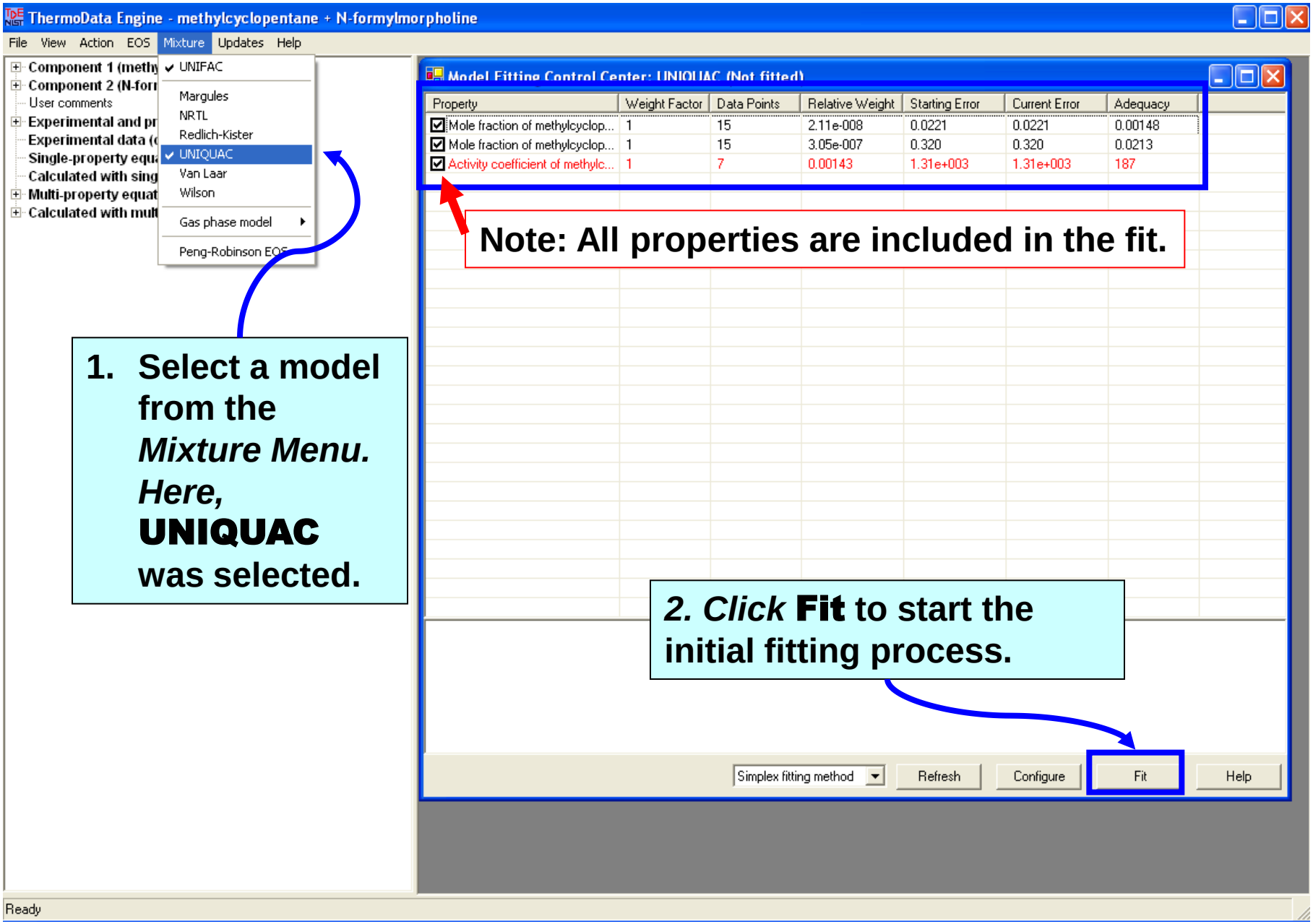
After initial evaluation for the pure components, comparisons with the *UNIFAC* models (Original and NIST-KT) can be made without fitting a model.

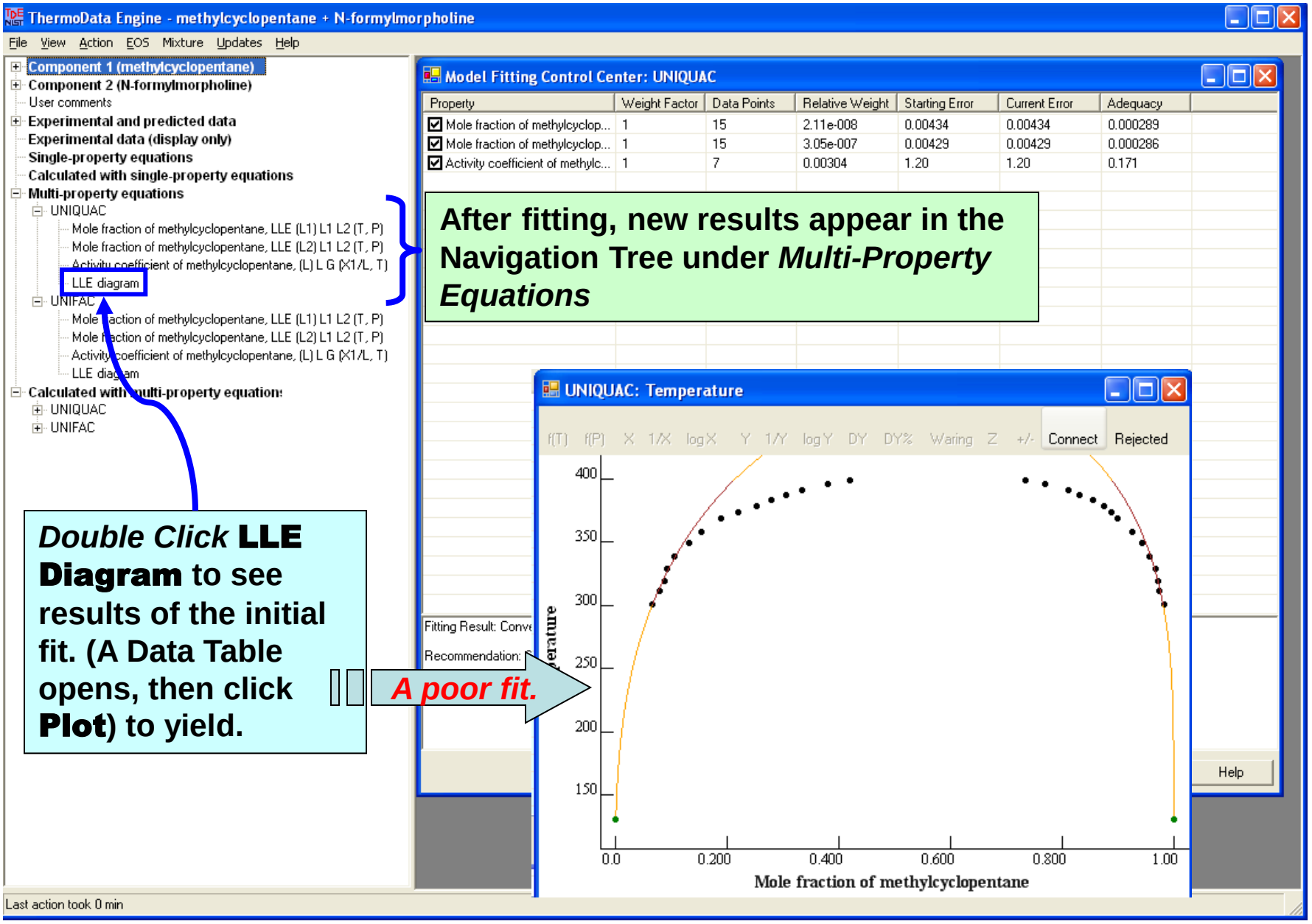
This is done by first selecting a *UNIFAC* formulation from the **Mixture Models** menu.

(Go to next page…)

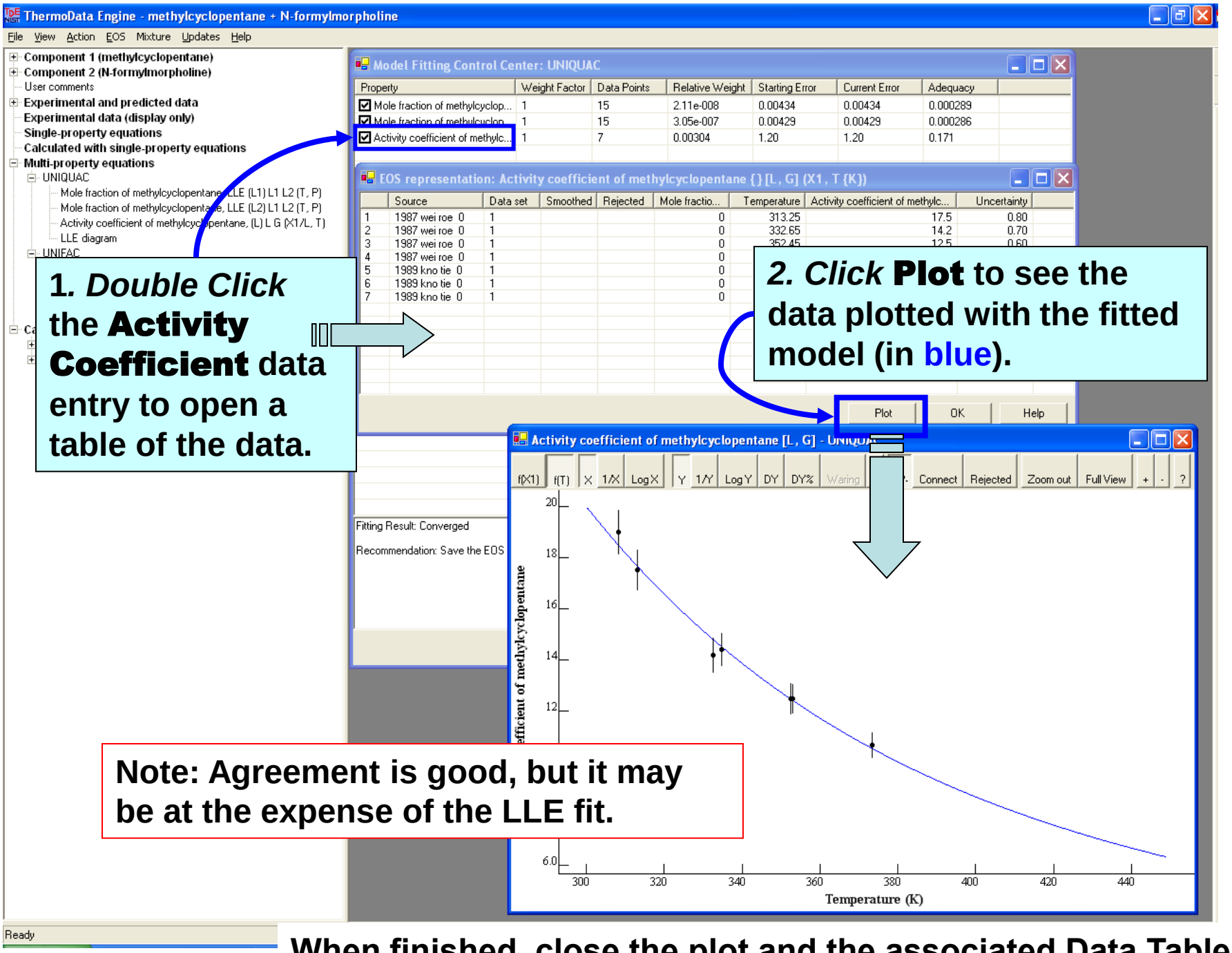

ThermoData Engine - methylcyclopentane + N-formylmorpholine
File View Action EOS Mixture Models Product Design Experiment Planning Updates Help
Component 1 (methylcyclopentane)
Component 2 (N-formylmorpholine)
User comments
Experimental and predicted data
Experimental data (display only)
Multi-property equations
UNIFAC/IG (Read-only)
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 equations
Double Click LLE Diagram to see results of the initial fit. A Data Table opens.
UNIFAC/IG (Read-only): Mole fraction of methylcyclopentane (T{K}, P{kPa})
Source Se... Rej... Temperature Pressure Mole fraction of... Uncert... Smo...
1 2003 min san 0 1 300.27 101.3 0.9835 0.00200
2 2003 min san 0 1 311.55 101.3 0.9751 0.00310
3 2003 min san 0 1 319.28 101.3 0.9712 0.00360
4 2003 min san 0 1 328.84 101.3 0.9669 0.00410
5 2003 min san 0 1 338.8 101.3 0.9561 0.00540
6 2003 min san 0 1 348.93 101.3 0.9447 0.00690
7 2003 min san 0 1 358.33 101.3 0.9253 0.00930
8 2003 min san 0 1 368.06 101.3 0.8991 0.0125
9 2003 min san 0 1 373.19 101.3 0.8896 0.0137
10 2003 min san 0 1 378.18 101.3 0.8751 0.0155
11 2003 min san 0 1 383.12 101.3 0.8562 0.0178
12 2003 min san 0 1 387.07 101.3 0.8323
13 2003 min san 0 1 390.95 101.3 0.8114
14 2003 min san 0 1 395.44 101.3 0.7693
15 2003 min san 0 1 398.73 101.3
300.27 101.3 0.0673
311.55 101.3 0.0806
319.28 101.3 0.088 0.0109
Plot OK Help
Click PLOT to yield…
UNIFAC: Temperature
f(T) f(P) X 1/X logX Y 1/Y DY DY% Waring Z +/- Connect Rejected Zoom Show/Hide connecting lines
Temperature
450 400 350 300 250 200 150 100 50.0
0.200 0.400 0.600 0.800 1.00
Mole fraction of methylcyclopentane
The dots represent the experimental data from the table.
The line represents the UNIFAC estimation.
Ready

To initiate a model fit…





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

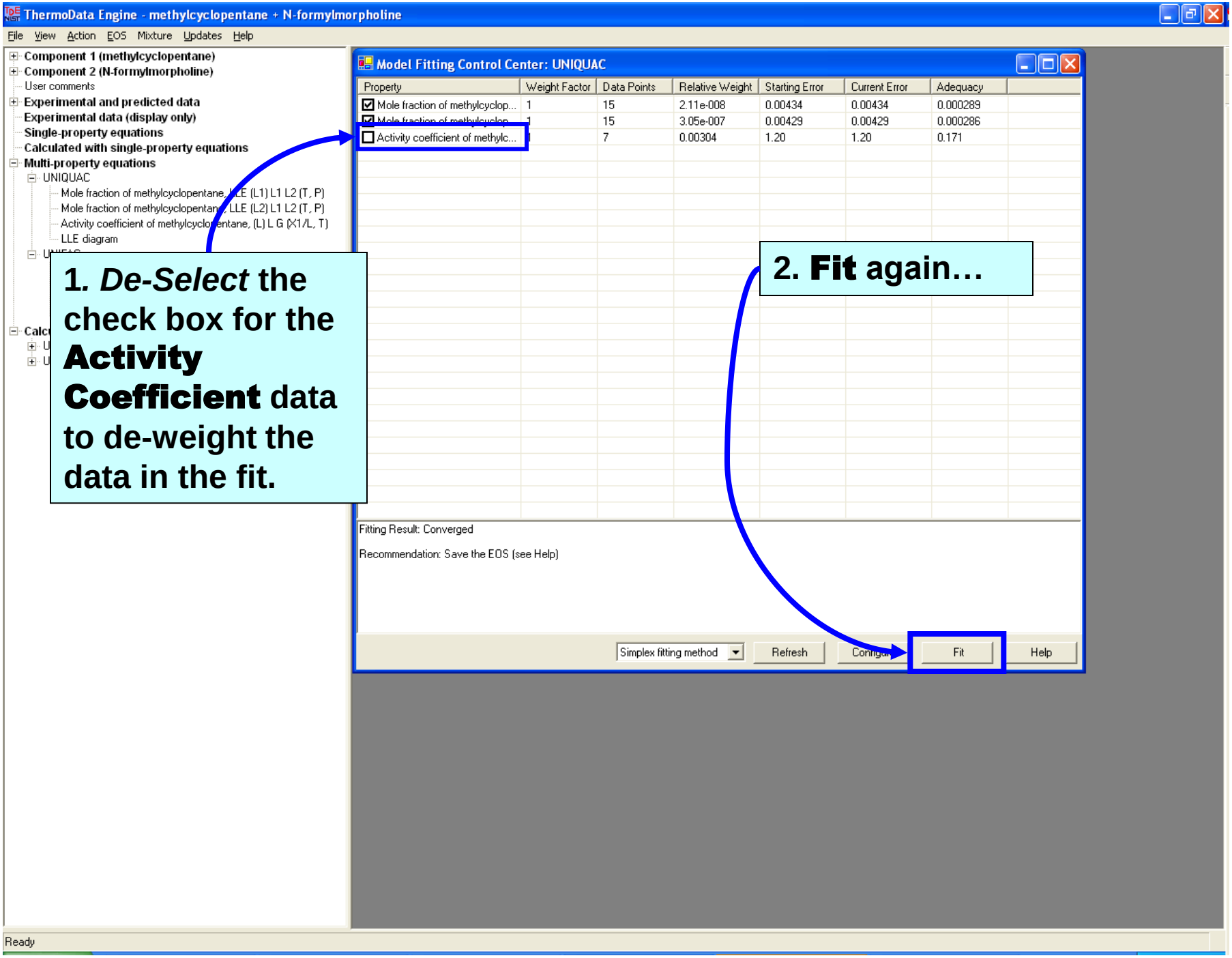


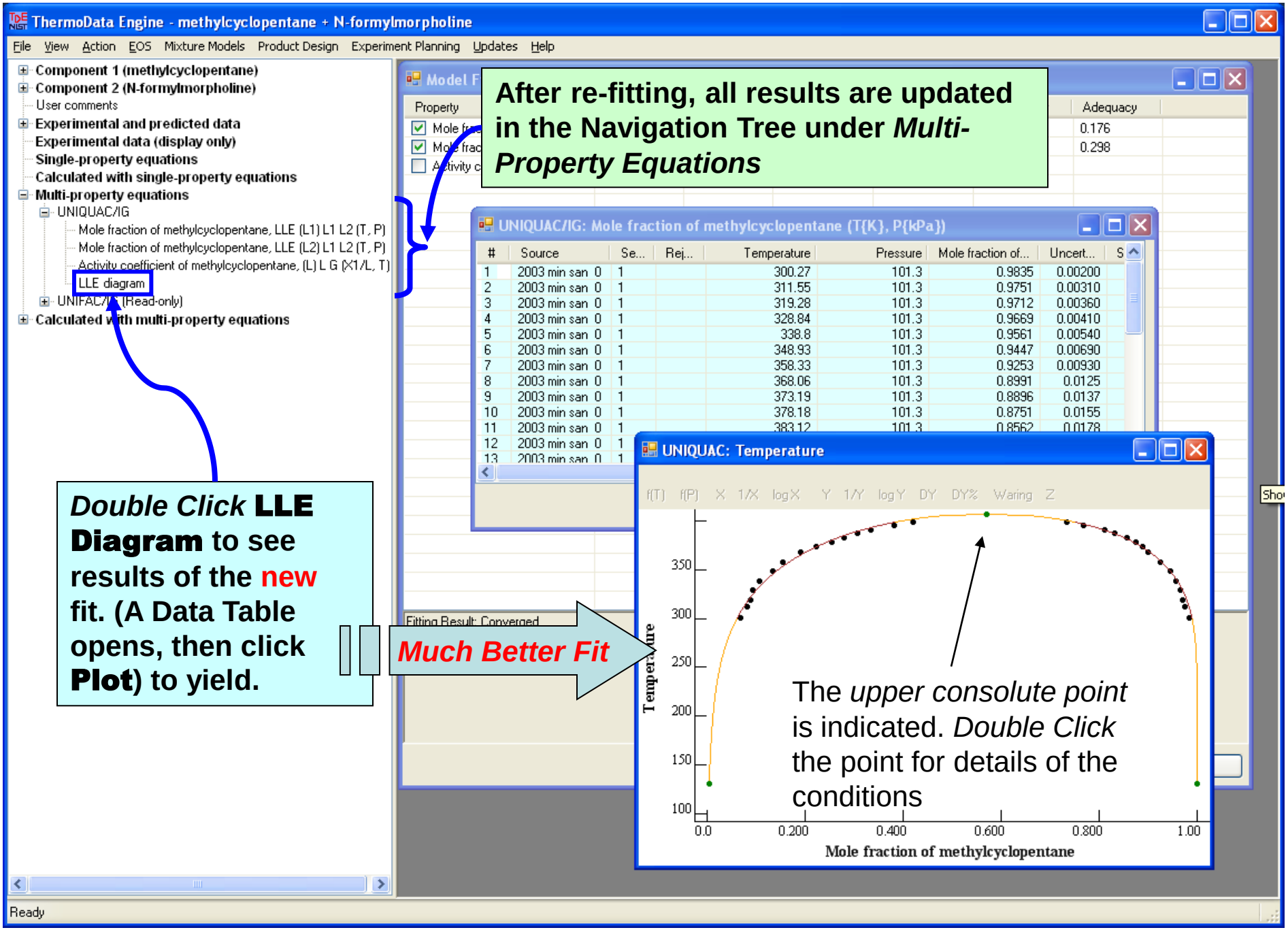
1. *Double Click* the Activity Coefficient data entry to open a table of the data.

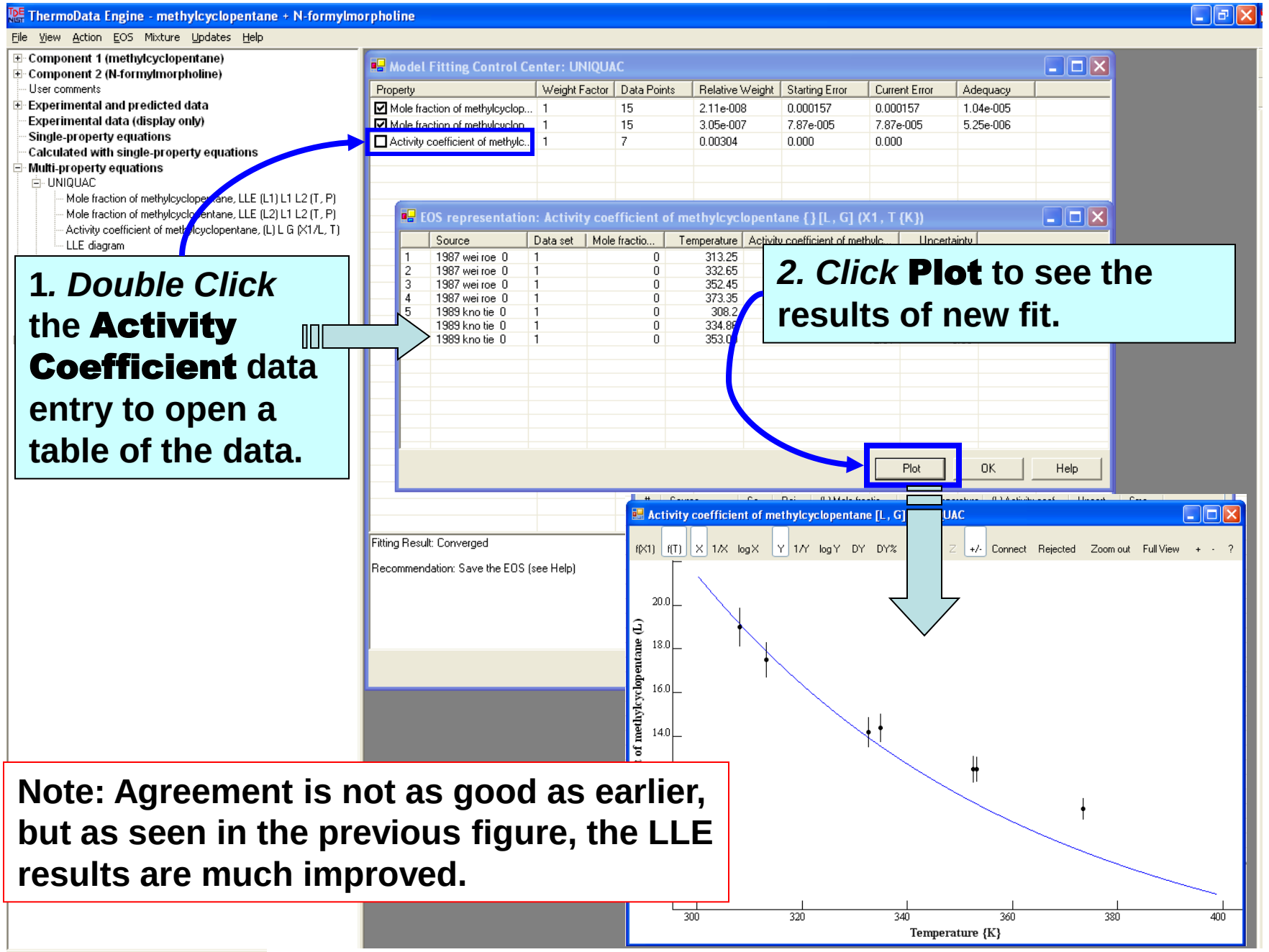
***2. Click* Plot to see the data plotted with the fitted model (in blue).**

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)
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...
1
15
2.11e-008
0.00434
0.00434
0.000289
15
3.05e-007
0.00429
0.00429
0.000286
Activity coefficient of methylc...
7
0.00304
1.20
1.20
0.171
Fitting Result: Converged
Recommendation: Save the EOS (see Help)
Simplex fitting method
Refresh
Fit
Help
1. De-Select the check box for the Activity Coefficient data to de-weight the data in the fit.
2. Fit again…
Ready


ThermoData Engine - methylcyclopentane + N-formylmorpholine
File View Action EOS Mixture Models Product Design Experiment Planning 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/IG
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/IG (Read-only)
Calculated with multi-property equations
After re-fitting, all results are updated in the Navigation Tree under Multi-Property Equations
Property
Adequacy
0.176
0.298
UNIQUAC/IG: Mole fraction of methylcyclopentane {T{K}, P{kPa}}
Source Se... Rej... Temperature Pressure Mole fraction of... Uncert...
1 2003 min san 0 1 300.27 101.3 0.9835 0.00200
2 2003 min san 0 1 311.55 101.3 0.9751 0.00310
3 2003 min san 0 1 319.28 101.3 0.9712 0.00360
4 2003 min san 0 1 328.84 101.3 0.9669 0.00410
5 2003 min san 0 1 338.8 101.3 0.9561 0.00540
6 2003 min san 0 1 348.93 101.3 0.9447 0.00690
7 2003 min san 0 1 358.33 101.3 0.9253 0.00930
8 2003 min san 0 1 368.06 101.3 0.8991 0.0125
9 2003 min san 0 1 373.19 101.3 0.8896 0.0137
10 2003 min san 0 1 378.18 101.3 0.8751 0.0155
11 2003 min san 0 1 383.12 101.3 0.8562 0.0178
12 2003 min san 0 1
13 2003 min san 0 1
Fitting Result: Converged
Double Click LLE Diagram to see results of the new fit. (A Data Table opens, then click Plot) to yield.
Much Better Fit
UNIQUAC: Temperature
f(T) f(P) X 1/X log X Y 1/Y log Y DY DY% Waring Z
Temperature
350
300
250
200
150
100
0.0
0.200
0.400
0.600
0.800
1.00
Mole fraction of methylcyclopentane
The upper consolute point is indicated. Double Click the point for details of the conditions
Ready

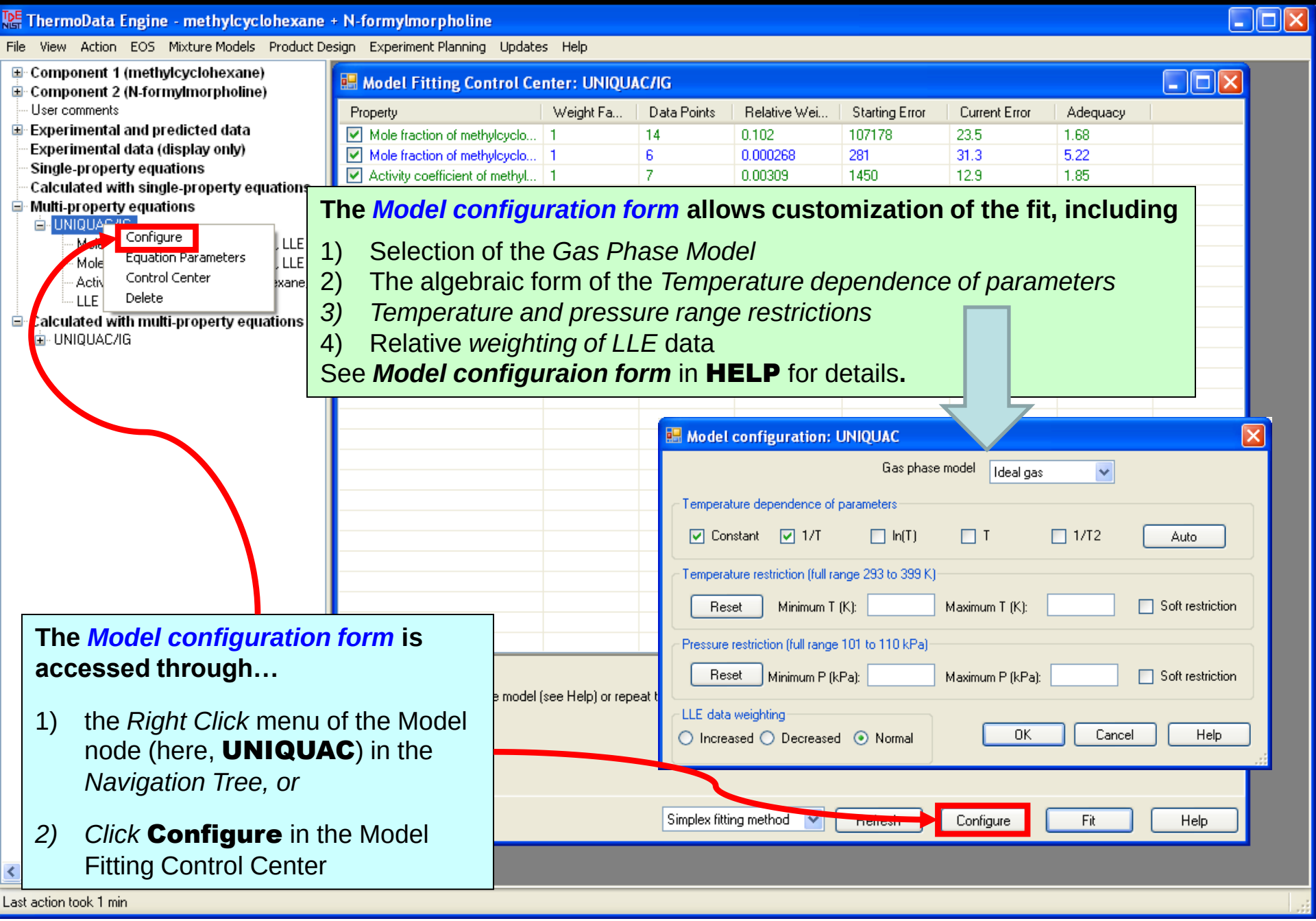


1. *Double Click* the **Activity Coefficient** data entry to open a table of the data.

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.

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


ThermoData Engine - methylcyclohexane + N-formylmorpholine
File View Action EOS Mixture Models Product Design Experiment Planning Updates Help
Component 1 (methylcyclohexane)
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/IG
Configure
Equation Parameters
Control Center
Delete
Calculated with multi-property equations
UNIQUAC/IG
Model Fitting Control Center: UNIQUAC/IG
Property
Weight Fa...
Data Points
Relative Wei...
Starting Error
Current Error
Adequacy
Mole fraction of methylcyclo... 1 14 0.102 107178 23.5 1.68
Mole fraction of methylcyclo... 1 6 0.000268 281 31.3 5.22
Activity coefficient of methyl... 1 7 0.00309 1450 12.9 1.85
The Model configuration form allows customization of the fit, including
1) Selection of the Gas Phase Model
2) The algebraic form of the Temperature dependence of parameters
3) Temperature and pressure range restrictions
4) Relative weighting of LLE data
See Model configuraion form in HELP for details.
Model configuration: UNIQUAC
Gas phase model
Ideal gas
Temperature dependence of parameters
Constant
1/T
ln(T)
T
1/T2
Auto
Temperature restriction (full range 293 to 399 K)
Reset
Minimum T (K):
Maximum T (K):
Soft restriction
Pressure restriction (full range 101 to 110 kPa)
Reset
Minimum P (kPa):
Maximum P (kPa):
Soft restriction
LLE data weighting
Increased
Decreased
Normal
OK
Cancel
Help
Simplex fitting method
Refresh
Configure
Fit
Help
The Model configuration form is accessed through…
1) the Right Click menu of the Model node (here, UNIQUAC) in the Navigation Tree, or
2) Click Configure in the Model Fitting Control Center
Last action took 1 min