

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
 - Mole fraction of methylcyclopentane
 - LLE (L1) L1 L2 (T, P)
 - LLE (L2) L1 L2 (T, P)
 - Activity coefficient of methylcyclopentane
 - (L) L G (X1/L, T)
 - Add data (Optional)
- Experimental data (display only)

Available Data Sets

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

Ready

Component 1 UNIFAC
Component 2 UNIFAC
User comments
Experimental
Mole fraction
LLE (L1)
LLE (L2)
Activity coef
(L) L G
LLE data su

UNIFAC
Original
NIST-KT
NRTL
Redlich-Kister
UNIQUAC
Van Laar
Wilson
Clear All
AC gas phase model



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...)

- 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

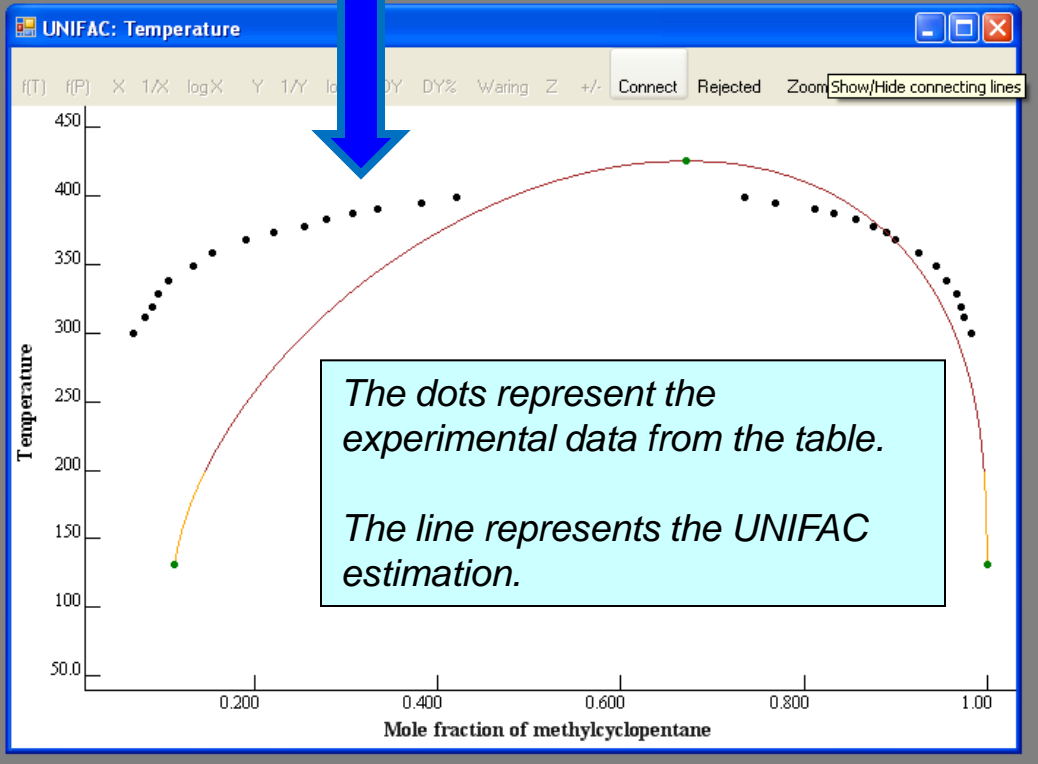
UNIFAC/IG (Read-only): Mole fraction of methylcyclopentane (T[K], P[kPa])

| # | 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 | 0.7344 | | |
| 16 | 2003 min san 0 | 2 | | 300.27 | 101.3 | 0.0673 | | |
| 17 | 2003 min san 0 | 2 | | 311.55 | 101.3 | 0.0806 | | |
| 18 | 2003 min san 0 | 2 | | 319.28 | 101.3 | 0.088 | 0.0109 | |

Plot OK Help

Double Click LLE Diagram to see results of the initial fit. A Data Table opens.

Click PLOT to yield...



To initiate a model fit...

The screenshot shows the ThermoData Engine interface for a mixture of methylcyclopentane and N-formylmorpholine. The 'Mixture' menu is open, showing various models, with 'UNIQUAC' selected. The 'Model Fitting Control Center' window is active, displaying a table of properties to be fitted. A red box highlights the table, and a red arrow points to it with the note: 'Note: All properties are included in the fit.' The 'Fit' button at the bottom of the window is also highlighted with a blue box and a blue arrow pointing to it from a text box that says: '2. Click Fit to start the initial fitting process.'

1. Select a model from the *Mixture Menu*. Here, **UNIQUAC** was selected.

| Property | Weight Factor | Data Points | Relative Weight | Starting Error | Current Error | Adequacy |
|--|---------------|-------------|-----------------|----------------|---------------|----------|
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 2.11e-008 | 0.0221 | 0.0221 | 0.00148 |
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 3.05e-007 | 0.320 | 0.320 | 0.0213 |
| <input checked="" type="checkbox"/> Activity coefficient of methylc... | 1 | 7 | 0.00143 | 1.31e+003 | 1.31e+003 | 187 |

2. Click **Fit** to start the initial fitting process.

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:
 UNIQUAC
 UNIFAC

Model Fitting Control Center: UNIQUAC

| Property | Weight Factor | Data Points | Relative Weight | Starting Error | Current Error | Adequacy |
|--|---------------|-------------|-----------------|----------------|---------------|----------|
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 2.11e-008 | 0.00434 | 0.00434 | 0.000289 |
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 3.05e-007 | 0.00429 | 0.00429 | 0.000286 |
| <input checked="" type="checkbox"/> Activity coefficient of methylc... | 1 | 7 | 0.00304 | 1.20 | 1.20 | 0.171 |

After fitting, new results appear in the Navigation Tree under **Multi-Property Equations**

UNIQUAC: Temperature

f(T) f(P) X 1/X log X Y 1/Y log Y DY DY% Warning Z +/- Connect Rejected

Temperature

Mole fraction of methylcyclopentane

Fitting Result: Converged
 Recommendation:

A poor fit.

Double Click **LLE Diagram** to see results of the initial fit. (A Data Table opens, then click **Plot**) to yield.

Last action took 0 min

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

- 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

Model Fitting Control Center: UNIQUAC

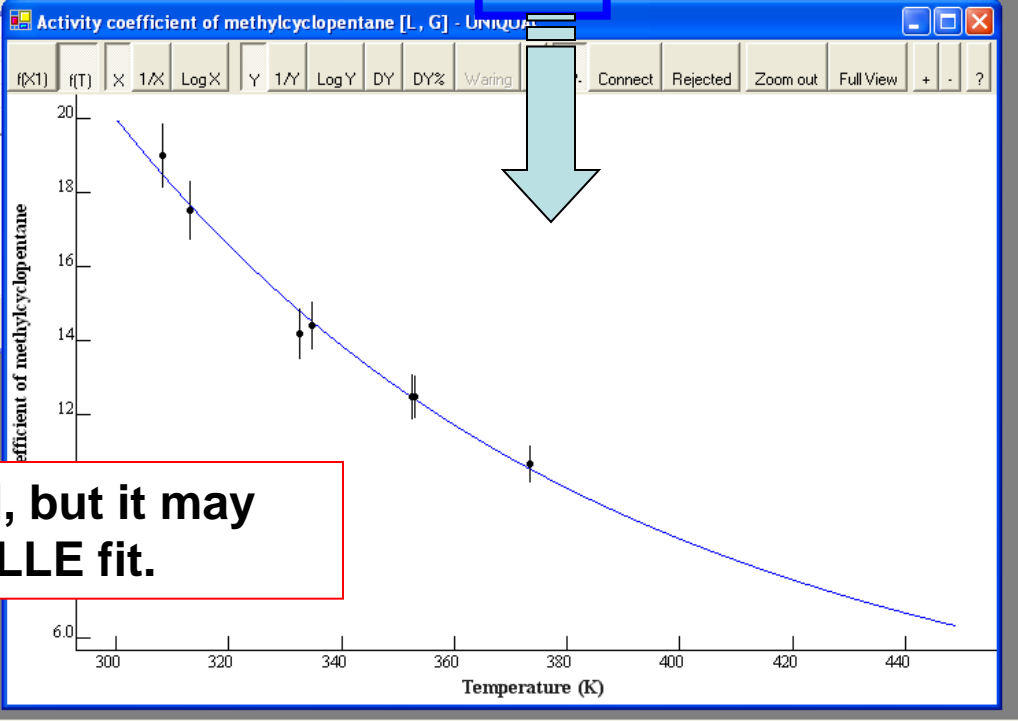
| Property | Weight Factor | Data Points | Relative Weight | Starting Error | Current Error | Adequacy |
|--|---------------|-------------|-----------------|----------------|---------------|----------|
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 2.11e-008 | 0.00434 | 0.00434 | 0.000289 |
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 3.05e-007 | 0.00429 | 0.00429 | 0.000286 |
| <input checked="" type="checkbox"/> Activity coefficient of methylc... | 1 | 7 | 0.00304 | 1.20 | 1.20 | 0.171 |

EOS representation: Activity coefficient of methylcyclopentane {} [L, G] (X1, T (K))

| | Source | Data set | Smoothed | Rejected | Mole fractio... | Temperature | Activity coefficient of methylc... | Uncertainty |
|---|----------------|----------|----------|----------|-----------------|-------------|------------------------------------|-------------|
| 1 | 1987 wei roe 0 | 1 | | | 0 | 313.25 | 17.5 | 0.80 |
| 2 | 1987 wei roe 0 | 1 | | | 0 | 332.65 | 14.2 | 0.70 |
| 3 | 1987 wei roe 0 | 1 | | | 0 | 352.45 | 12.5 | 0.60 |
| 4 | 1987 wei roe 0 | 1 | | | 0 | | | |
| 5 | 1989 kno tie 0 | 1 | | | 0 | | | |
| 6 | 1989 kno tie 0 | 1 | | | 0 | | | |
| 7 | 1989 kno tie 0 | 1 | | | 0 | | | |

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...

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

1. De-Select the check box for the **Activity Coefficient** data to de-weight the data in the fit.

Model Fitting Control Center: UNIQUAC

| Property | Weight Factor | Data Points | Relative Weight | Starting Error | Current Error | Adequacy |
|--|---------------|-------------|-----------------|----------------|---------------|----------|
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 2.11e-008 | 0.00434 | 0.00434 | 0.000289 |
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 3.05e-007 | 0.00429 | 0.00429 | 0.000286 |
| <input type="checkbox"/> 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 | Configure | **Fit** | Help

2. Fit again...

- 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

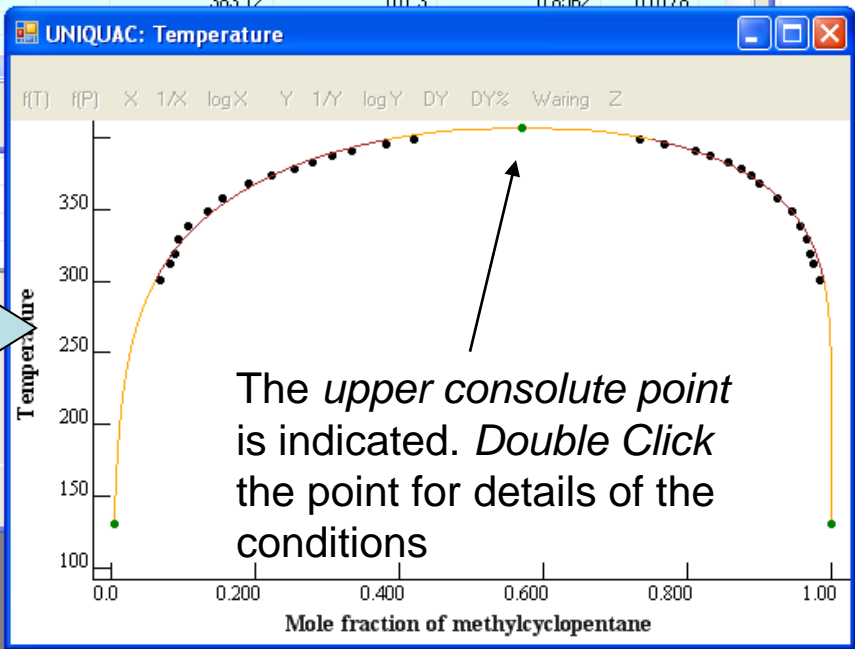
After re-fitting, all results are updated in the Navigation Tree under **Multi-Property Equations**

UNIQUAC/IG: Mole fraction of methylcyclopentane (T[K], P[kPa])

| # | Source | Se... | Rej... | Temperature | Pressure | Mole fraction of... | Uncert... | S |
|----|----------------|-------|--------|-------------|----------|---------------------|-----------|---|
| 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 | | | | | | |

Double Click **LLE Diagram** to see results of the **new fit**. (A Data Table opens, then click **Plot**) to yield.

Fitting Result: Converged
Much Better Fit



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 |
|--|---------------|-------------|-----------------|----------------|---------------|-----------|
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 2.11e-008 | 0.000157 | 0.000157 | 1.04e-005 |
| <input checked="" type="checkbox"/> Mole fraction of methylcyclop... | 1 | 15 | 3.05e-007 | 7.87e-005 | 7.87e-005 | 5.25e-006 |
| <input type="checkbox"/> Activity coefficient of methylc... | 1 | 7 | 0.00304 | 0.000 | 0.000 | |

EOS representation: Activity coefficient of methylcyclopentane [] [L, G] (X1, T [K])

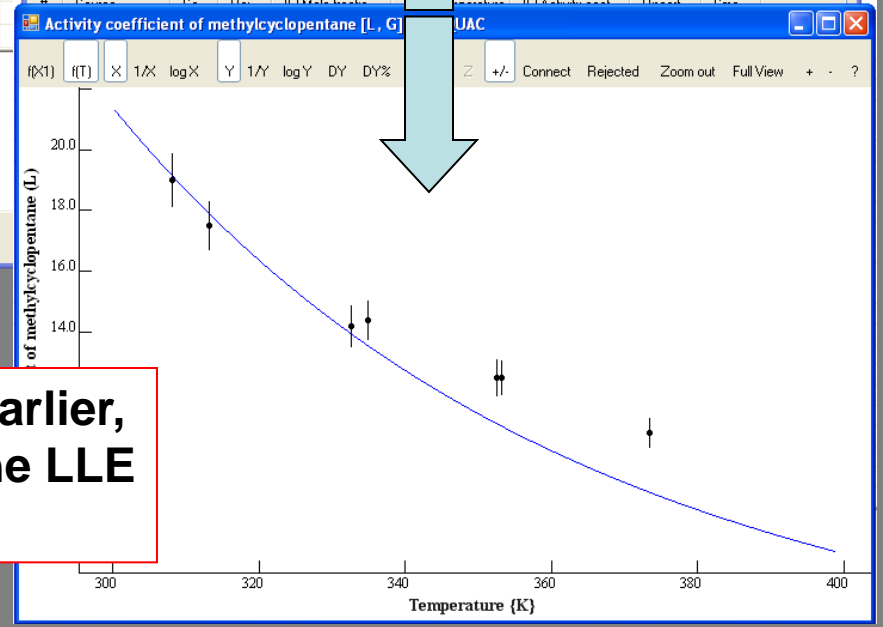
| | Source | Data set | Mole fractio... | Temperature | Activity coefficient of methyhc... | Uncertainty |
|---|----------------|----------|-----------------|-------------|------------------------------------|-------------|
| 1 | 1987 wei roe 0 | 1 | 0 | 313.25 | | |
| 2 | 1987 wei roe 0 | 1 | 0 | 332.65 | | |
| 3 | 1987 wei roe 0 | 1 | 0 | 352.45 | | |
| 4 | 1987 wei roe 0 | 1 | 0 | 373.35 | | |
| 5 | 1989 kno tie 0 | 1 | 0 | 308.2 | | |
| | 1989 kno tie 0 | 1 | 0 | 334.8 | | |
| | 1989 kno tie 0 | 1 | 0 | 353.0 | | |

Buttons: Plot, OK, Help

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...

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
 Mark
 Mole
 Activ
 LLE
 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 |
|---|--------------|-------------|-----------------|----------------|---------------|----------|
| <input checked="" type="checkbox"/> Mole fraction of methylcyclo... | 1 | 14 | 0.102 | 107178 | 23.5 | 1.68 |
| <input checked="" type="checkbox"/> Mole fraction of methylcyclo... | 1 | 6 | 0.000268 | 281 | 31.3 | 5.22 |
| <input checked="" type="checkbox"/> 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.

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

Model configuration: UNIQUAC

Gas phase model: Ideal gas

Temperature dependence of parameters:
 Constant 1/T ln(T) T 1/T2

Temperature restriction (full range 293 to 399 K):
 Minimum T (K): Maximum T (K): Soft restriction

Pressure restriction (full range 101 to 110 kPa):
 Minimum P (kPa): Maximum P (kPa): Soft restriction

LLE data weighting:
 Increased Decreased Normal

Simplex fitting method: