



Fluid Package Selection





Example: For a mixture consisting of 25% methanol and 75% methyl acetate with flowrate of 1 kmole/hr. determine the followings once with NRTL package and once with PSRV package:

- The bubbling pressure of the mixture at 45C
- The methanol fraction in gaseous mixture at above condition
-

1.As first step we define the components

Source Databank: HYSYS

Select: **Pure Components** Filter: **All Families**

Search for: Search by: **Formula**

Simulation Name	Full Name / Synonym	Formula
Methane	C1	CH4
Ethane	C2	C2H6
Propane	C3	C3H8
i-Butane	i-C4	C4H10
n-Butane	n-C4	C4H10
i-Pentane	i-C5	C5H12
n-Pentane	n-C5	C5H12
n-Hexane	C6	C6H14
n-Heptane	C7	C7H16
n-Octane	C8	C8H18
n-Nonane	C9	C9H20
n-Decane	C10	C10H22

Status: **OK**

2.Select NRTL as the fluid package and for vapor model select Ideal

Set Up Binary Coeffs StabTest Phase Order Tabular Notes

Package Type: HYSYS Component List Selection: **Component List - 1 [HYSYS Databanks]** View

Property Package Selection:

- Kabadi-Danner
- Lee-Kesler-Plocker
- MBWR
- NBS Steam
- NRTL**
- Peng-Robinson
- PR-Twu
- PRSV
- Sour PR
- Sour SRK
- Sour Water
- SRK
- SRK-Twu
- SulSim (Sulfur Recovery)
- Twu-Sim-Tassone
- UNIQUAC
- Wilson
- Zudkevitch-Joffe

Activity Model Specifications:

Vapour Model: **Ideal**

Density Method: **Ideal**

UNIFAC Estimation Temp: **RK**

Use Poynting Correction: **Virial**

PR

SRK

No Parameters required for the selected Property Package.

Property Pkg: **OK** Edit Properties



In Binary Coeffs tab you can see the binary parameters between methanol and M-acetate.

Activity Model Interaction Parameters

Coeff Matrix To View: Aij Bij Alphaj / Cij

	Methanol	M-Acetate
Methanol	---	290.353
M-Acetate	443.893	---

Coeff Estimation

UNIFAC VLE
 UNIFAC LLE
 Immiscible

Individual Pair
Unknowns Only
ALL Binaries
Reset Params.

R = 1.98721 cal/gmol K

Property Pkg

3. Enter simulation environment, enter 1 kmole/hr. as the flowrate, 45C as the operating temperature, and finally set the gas fraction to zero since we want to calculate the bubbling pressure.

Flowsheet Case (Main) - Solver Active

Material Stream: Mixture

Worksheet Attachments Dynamics

Worksheet	Stream Name	Mixture
Conditions	Vapour / Phase Fraction	0.0000
Properties	Temperature [C]	45.00
Composition	Pressure [kPa]	<empty>
Oil & Gas Feed	Molar Flow [kgmole/h]	1.000
Petroleum Assay	Mass Flow [kg/h]	<empty>
K Value	Std Ideal Liq Vol Flow [m3/h]	<empty>
User Variables	Molar Enthalpy [kJ/kgmole]	<empty>
Notes	Molar Entropy [kJ/kgmole-C]	<empty>
Cost Parameters	Heat Flow [kJ/h]	<empty>
Normalized Yields	Liq Vol Flow @Std Cond [m3/h]	<empty>
Emissions	Fluid Package	Basis-1
	Utility Type	

Unknown Compositions

Delete Define from Stream... View Assay

Model Palette

Views Streams Flowsheets

All Dynamics & Control External Model Heat Transfer Manipulator Piping & Hydraulics Pressure Changer Reactor Separator

4. Enter the composition: 0.25 for methanol and 0.75 for methyl acetate.



Material Stream: Mixture

Worksheet Attachments Dynamics

Worksheet

- Conditions
- Properties
- Composition
- Oil & Gas Feed
- Petroleum Assay
- K Value
- User Variables
- Notes
- Cost Parameters
- Normalized Yields
- Emissions

	Mole Fractions	Liquid Phase
Methanol	0.2500	0.2500
M-Acetate	0.7500	0.7500

Total

Edit... View Properties... Basis...

OK

Delete Define from Stream... View Assay ← →

5. Based on the result, the bubbling pressure is 72.71 kPa.

Material Stream: Mixture

Worksheet Attachments Dynamics

Worksheet

- Conditions
- Properties
- Composition
- Oil & Gas Feed
- Petroleum Assay
- K Value
- User Variables
- Notes
- Cost Parameters
- Normalized Yields
- Emissions

Stream Name	Mixture	Liquid Phase
Vapour / Phase Fraction	0.0000	1.0000
Temperature [C]	45.00	45.00
Pressure [kPa]	72.71	72.71
Molar Flow [kgmole/h]	1.000	1.000
Mass Flow [kg/h]	63.57	63.57
Std Ideal Liq Vol Flow [m3/h]	6.922e-002	6.922e-002
Molar Enthalpy [kJ/kgmole]	-3.884e+005	-3.884e+005
Molar Entropy [kJ/kgmole-C]	124.2	124.2
Heat Flow [kJ/h]	-3.884e+005	-3.884e+005
Liq Vol Flow @Std Cond [m3/h]	6.905e-002	6.905e-002
Fluid Package	Basis-1	
Utility Type		

OK

Delete Define from Stream... View Assay ← →



5. To answer the second part, click on the K-value and the following window shows up:

The screenshot shows a software window titled "Material Stream: Mixture" with a "Worksheet" tab selected. On the left is a navigation pane with options like "Conditions", "Properties", "Composition", "Oil & Gas Feed", "Petroleum Assay", "K Value", "User Variables", "Notes", "Cost Parameters", "Normalized Yields", and "Emissions". The main area displays a table with the following data:

	Mixed	Light
Methanol	1.112	1.112
M-Acetate	0.9627	0.9627

An "OK" button is visible at the bottom of the window.

To calculate the methanol fraction in gas phase, thermodynamic equation is applied:

$Y_i = K_i \times X_i$
$Y_{\text{methanol}} = K_{\text{methanol}} \times X_{\text{methanol}}$
$Y_{\text{methanol}} = 1.112 \times 0.25 = 0.278$



6. At this stage, we start the procedure again for PRSV package. Go to Properties/Fluid package and select PRSV.

Property Package Selection

Options

Property	Method
Enthalpy	Peng-Robinson Equation
Density Method	Costald
Surface Tension Method	HYSYS Method

PRSV Component Parameters

Component	Kappa
Methanol	0.3938
M-Acetate	0.0197

7. Based on the result, the bubbling pressure is 61.36 kPa.

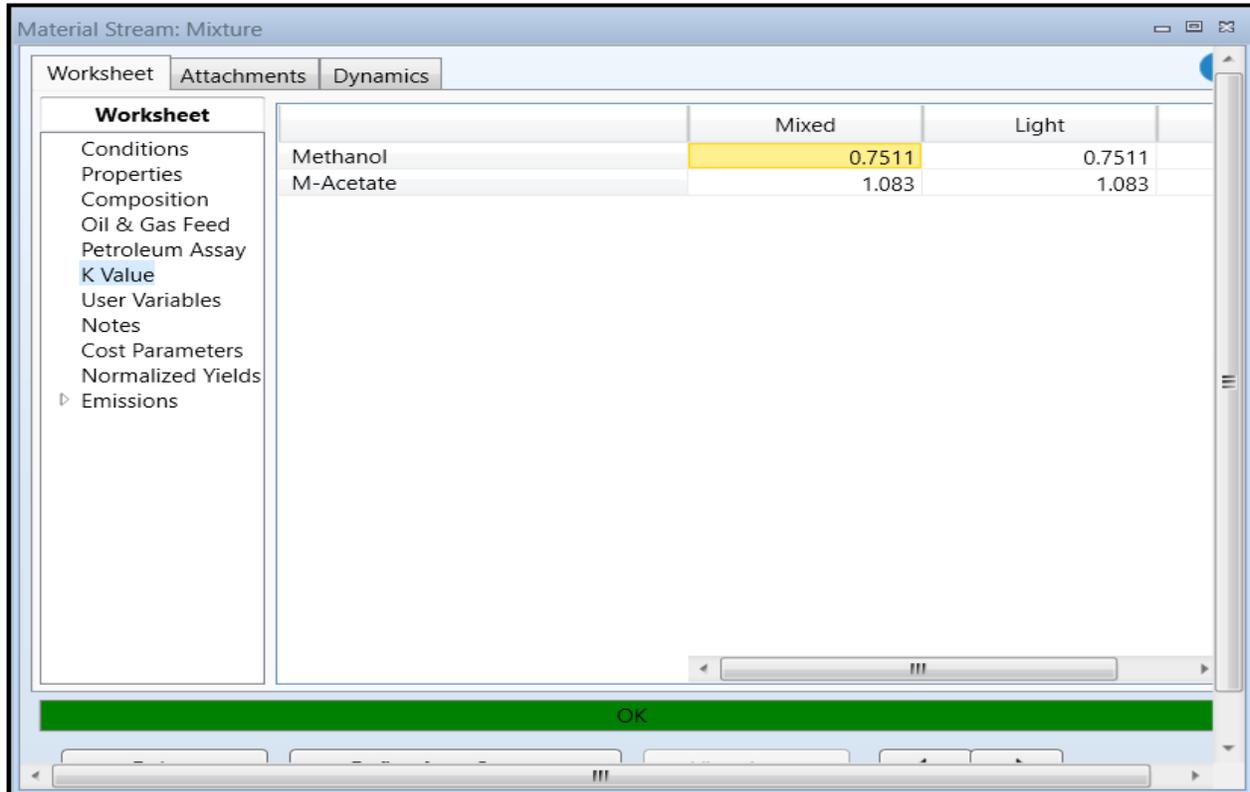
Material Stream: Mixture

Worksheet Attachments Dynamics

Worksheet	Stream Name	Mixture	Liquid Phase
Conditions	Vapour / Phase Fraction	0.0000	1.0000
Properties	Temperature [C]	45.00	45.00
Composition	Pressure [kPa]	61.36	61.36
Oil & Gas Feed	Molar Flow [kgmole/h]	1.000	1.000
Petroleum Assay	Mass Flow [kg/h]	63.57	63.57
K Value	Std Ideal Liq Vol Flow [m3/h]	6.922e-002	6.922e-002
User Variables	Molar Enthalpy [kJ/kgmole]	-3.896e+005	-3.896e+005
Notes	Molar Entropy [kJ/kgmole-C]	89.13	89.13
Cost Parameters	Heat Flow [kJ/h]	-3.896e+005	-3.896e+005
Normalized Yields	Liq Vol Flow @Std Cond [m3/h]	6.905e-002	6.905e-002
Emissions	Fluid Package	Basis-1	
	Utility Type		



8. To answer the second part, click on the K-value and the following window shows up:



To calculate the methanol fraction in gas phase, thermodynamic equation is applied:

$$Y_i = K_i \times X_i$$
$$Y_{\text{methanol}} = K_{\text{methanol}} \times X_{\text{methanol}}$$
$$Y_{\text{methanol}} = 0.7511 \times 0.25 = 0.1877$$

By this example you can not only understand but also feel it how selection of fluid package can impact results. To be honest, it is a simple example but imagine this for real and complex applications.



Comparison Table

	NRTL	PRSV
Pressure	72.71	61.36
K-Value	1.112	0.7511
Y_{methanol}	0.278	0.1877