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
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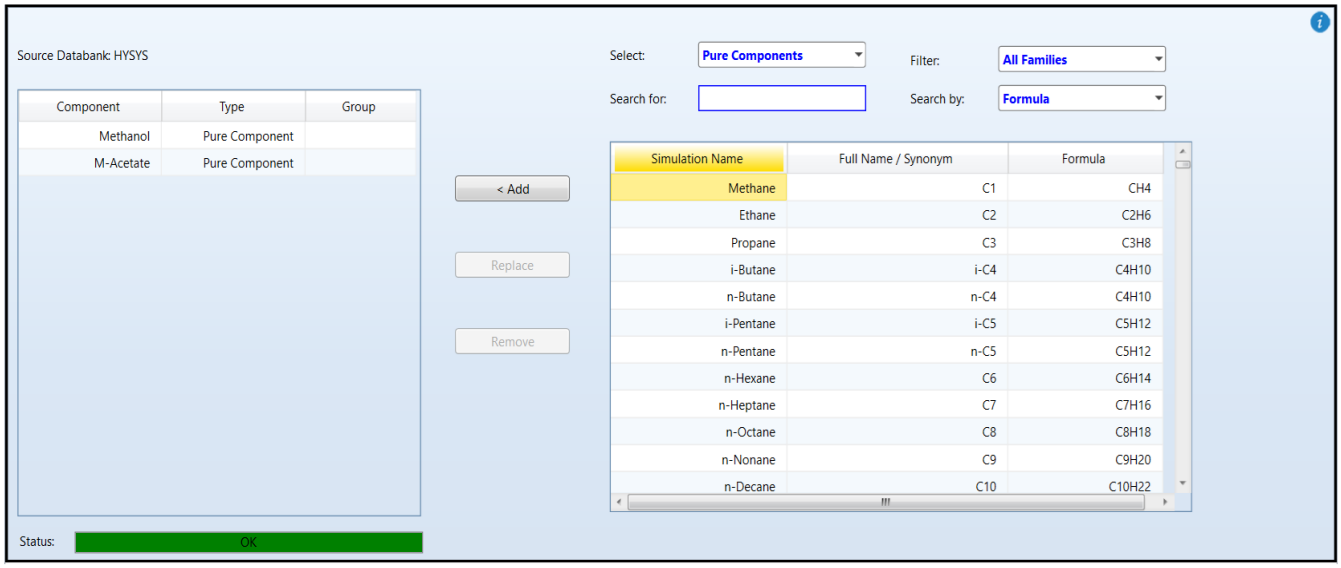
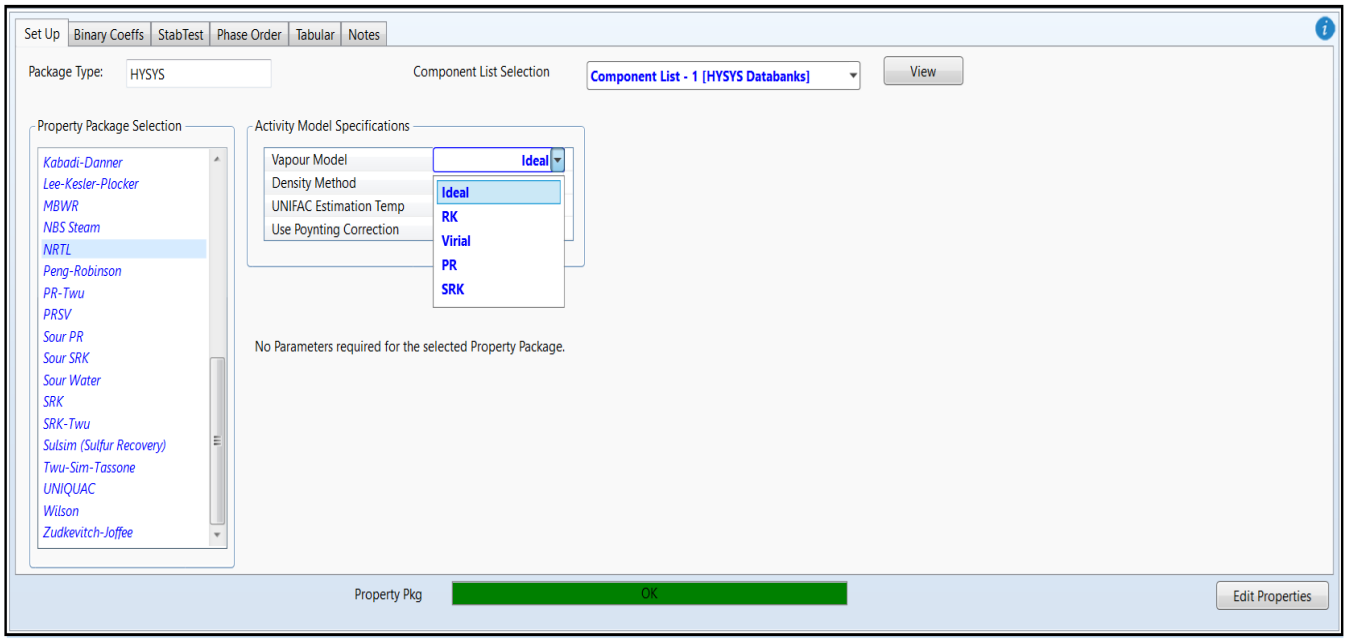
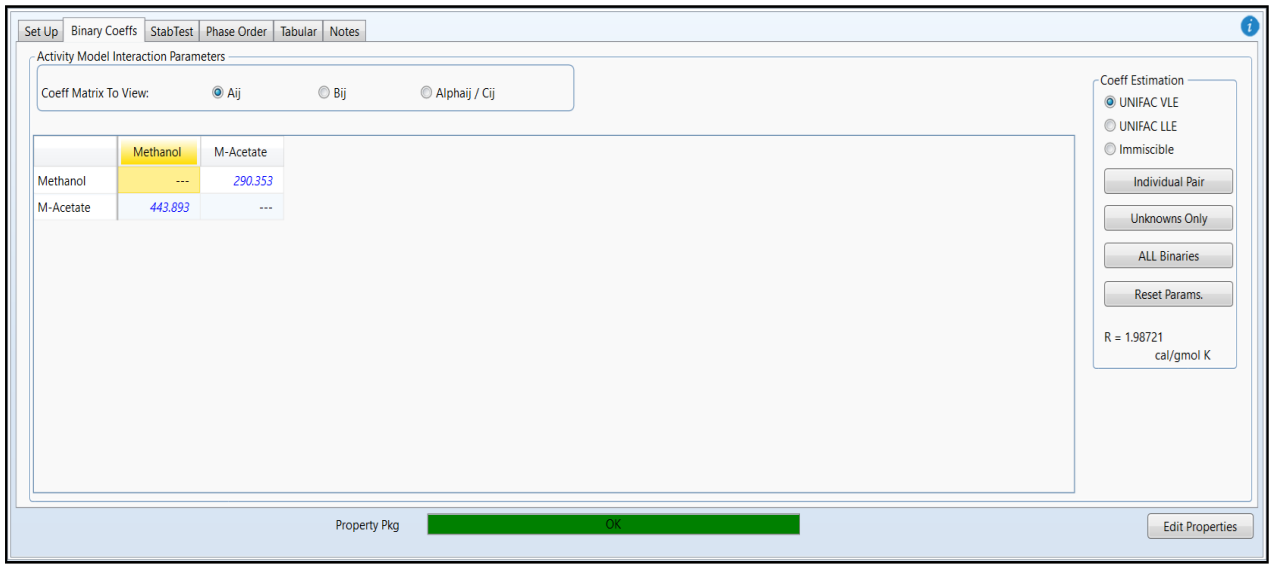
1.As first step we define the components



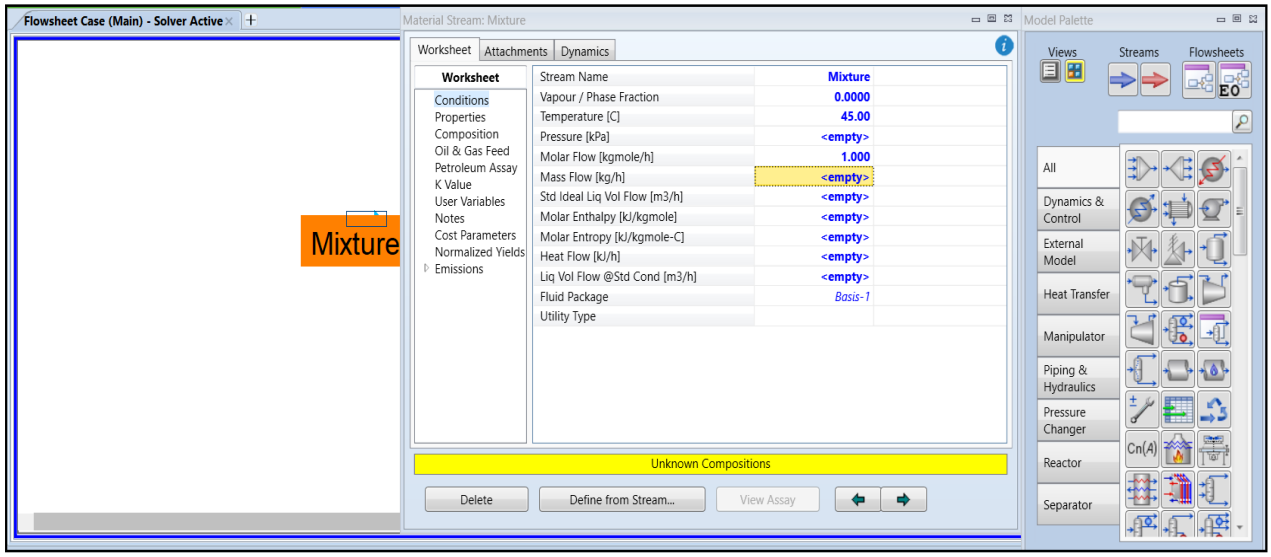
2.Select NRTL as the fluid package and for vapor model select Ideal



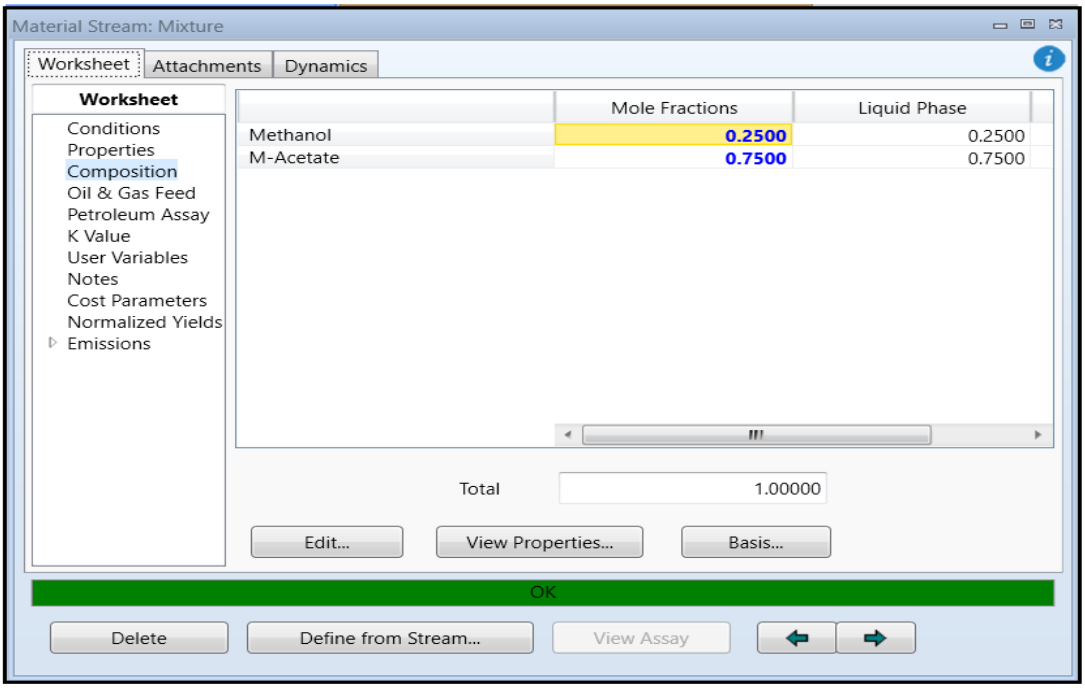
In Binary Coeffs tab you can see the binary parameters between methanol and M-acetate.



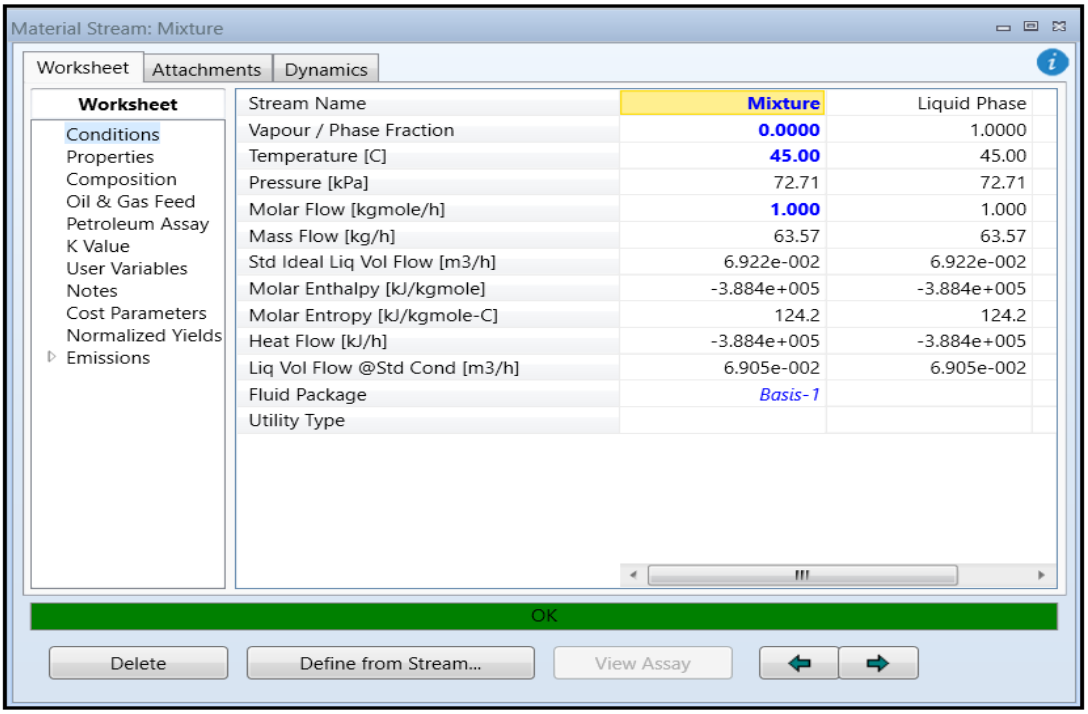
3.Enter simulation environment, enter 1 kmole/hr. as the flowrate, 45C as the operating temperature, and finally set the gas fraction to zero since we want to calculate the bubbling pressure.



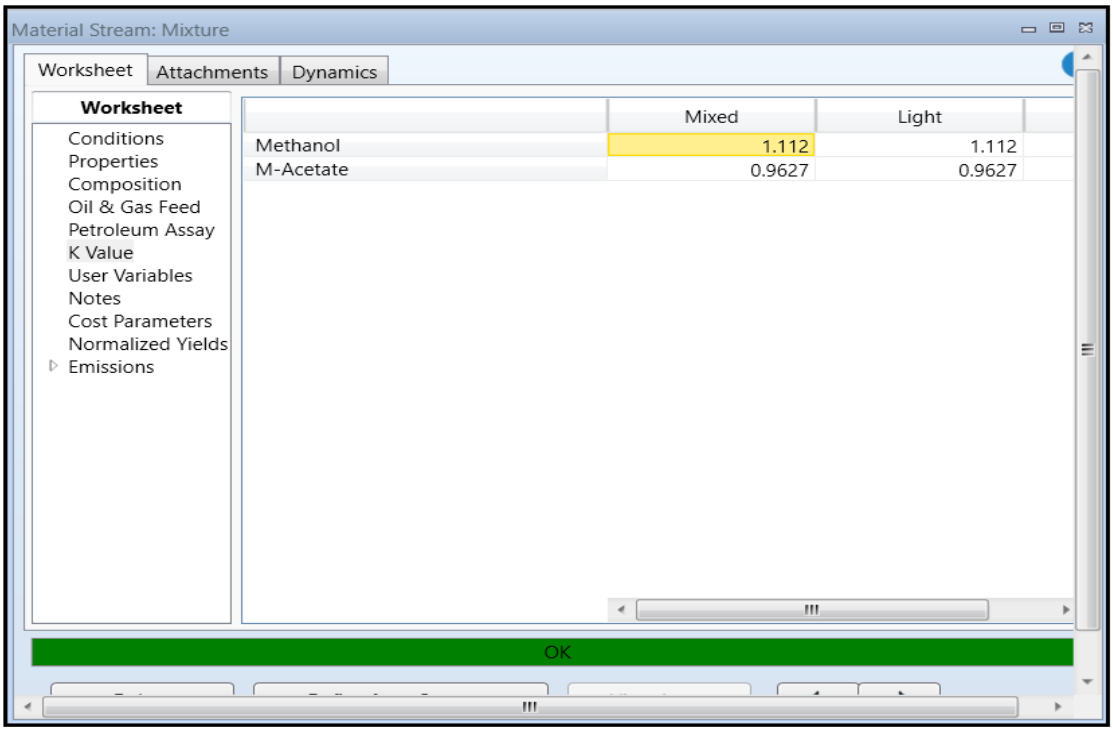
4.Enter the composition: 0.25 for methanol and 0.75 for methyl acetate.



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



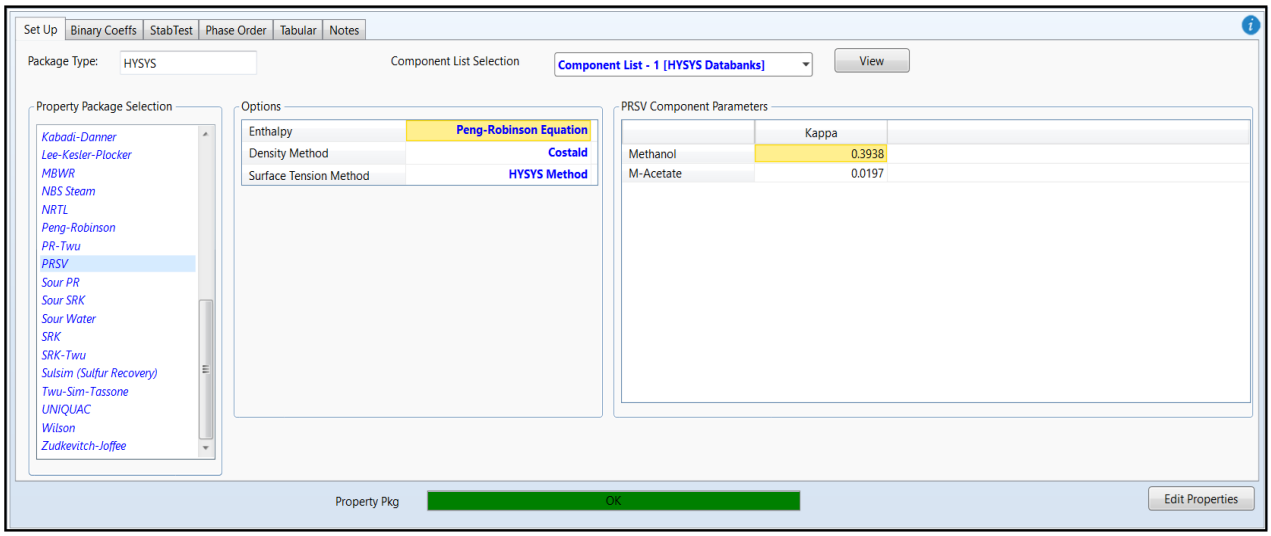
5.To answer the second part, click on the K-value and the following window shows up:



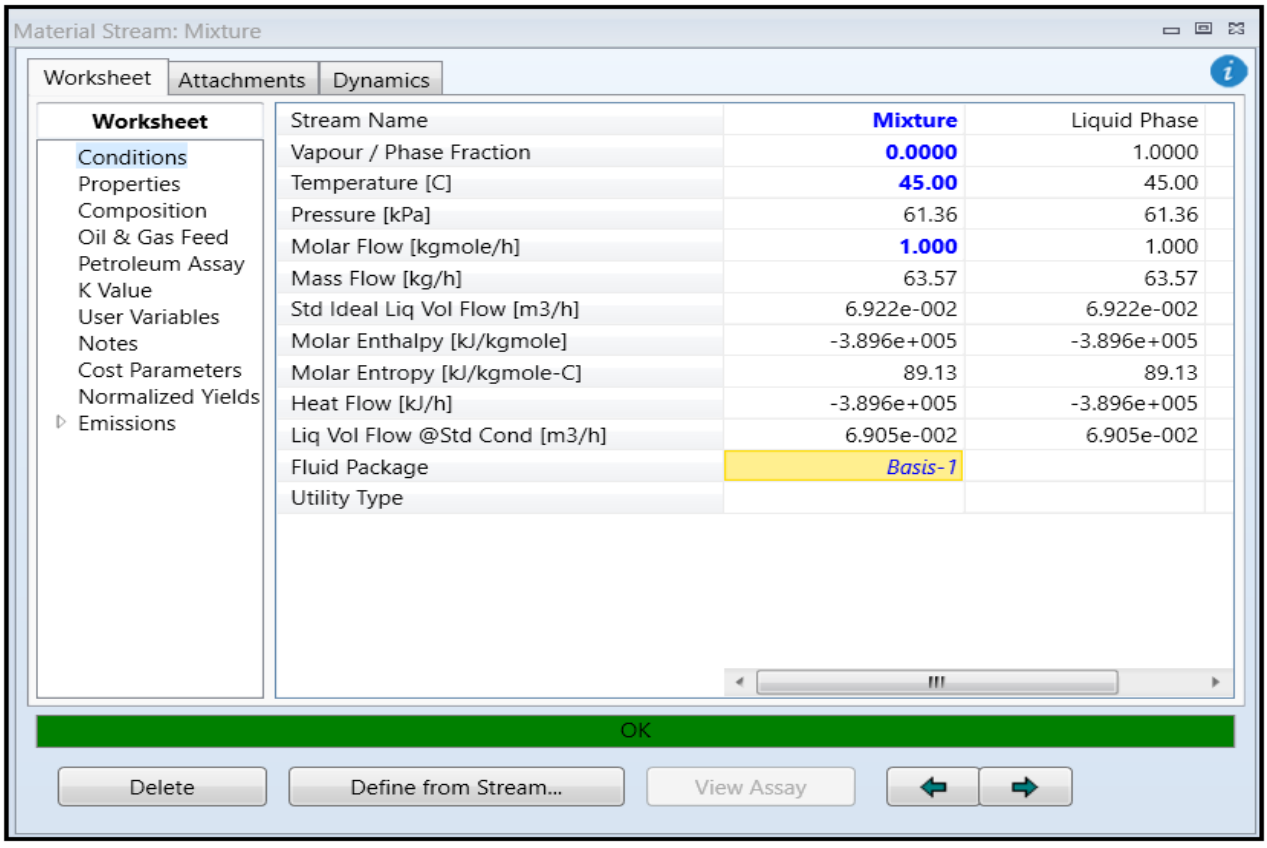
To calculate the methanol fraction in gas phase, thermodynamic equation is applied:

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

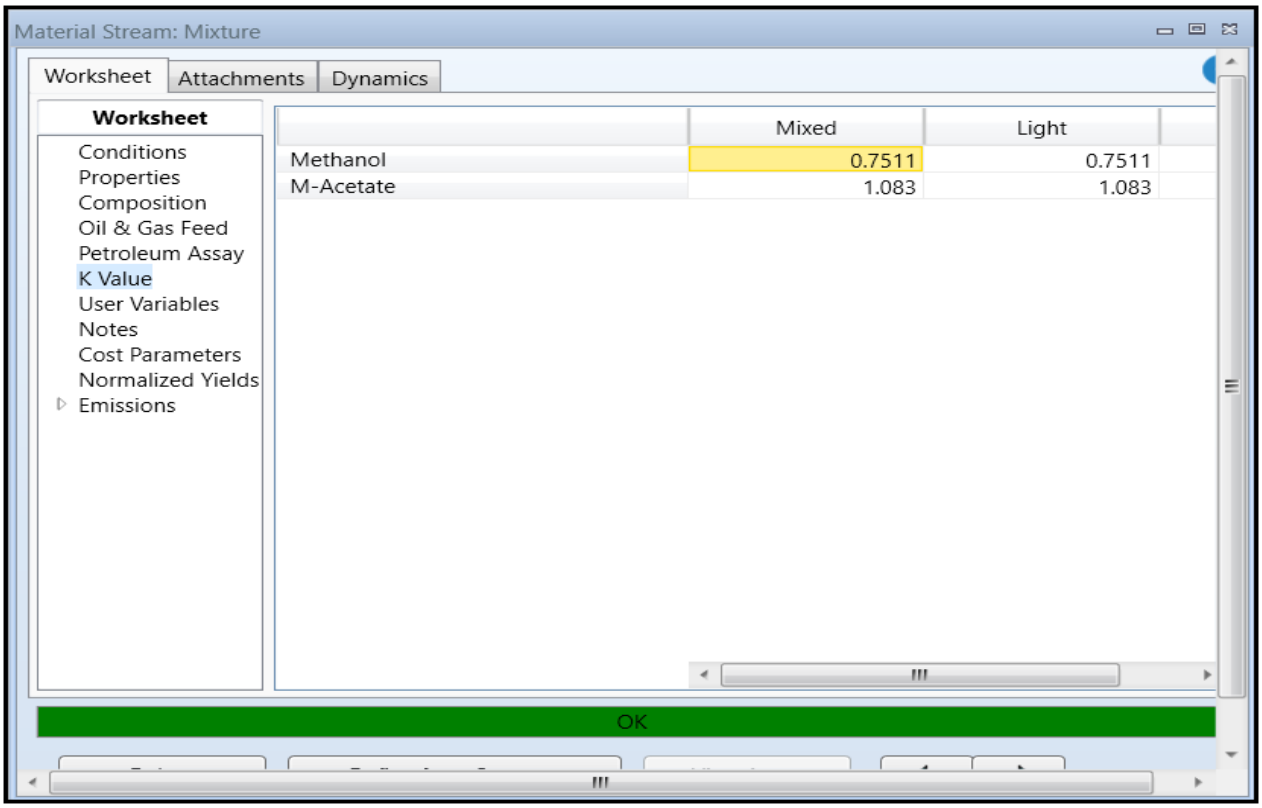
6.At this stage, we start the procedure again for PRSV package. Go to Properties/Fluid package and select PRSV.



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



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:

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

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