Selection of Proper Fluid Package

Ref:
Aspen Property Package Descriptions, Aspen Technology, Inc., 2011.
Physical Property Methods and Models, Aspen Technology, Inc., 2011

Fluid Packages

- A Fluid Package consists of a component list you defined in the Components tab of the Basis Manager, and a property package.

Property Packages

- Property packages are collections of methods for calculating the properties of components in the simulation basis.
- When you have established a component list, you combine the component list with a property package.

Property Packages

- Thermodynamic properties:
  - Fugacity coefficient (or equivalent: chemical potential, K-value)
  - Enthalpy
  - Entropy
  - Gibbs energy
  - Volume
- Transport properties:
  - Viscosity
  - Thermal conductivity
  - Diffusion coefficient
  - Surface tension

Property Packages

- The classes of property Packages available are:
  - Equations of State (EOS)
  - Activity Models
  - Chao Seader & Grayson Streed Models
  - Vapour Pressure Models
  - Miscellaneous Types

EOS Method

- Equations of state can be used over wide ranges of temperature and pressure, including subcritical and supercritical regions.
- Thermodynamic properties for both the vapor and liquid phases can be computed with a minimum amount of component data.

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EOS Method

- Equations of state are suitable for modeling hydrocarbon systems with light gases such as CO_2, N_2 and H_2S.
- The assumptions in the simpler equations of state (SRK, PR, Lee-Kesler , ...) are not capable of representing highly non-ideal chemical systems, such as alcohol-water systems. Use the activity-coefficient options sets for these systems at low pressures. At high pressures, use the predictive equations of state.

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Activity Coefficient Method

- The activity coefficient method is the best way to represent highly non-ideal liquid mixtures at low pressures.
- You must estimate or obtain binary parameters from experimental data, such as phase equilibrium data.
- Binary parameters are valid only over the temperature and pressure ranges of the data.
- The activity coefficient approach should be used only at low pressures (below 10 atm).
- The Wilson model cannot describe liquid-liquid separation at all; UNIQUAC, UNIFAC and NRTL are suitable.

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Activity Coefficient Method

- Multicomponent vapor-liquid equilibria are calculated from binary parameters. These parameters are usually fitted to binary phase equilibrium data (and not multicomponent data) and represent therefore binary information. The prediction of multicomponent phase behavior from binary information is generally good.
- Multi-component liquid-liquid equilibria cannot be reliably predicted from binary interaction parameters fitted to binary data only. In general, regression of binary parameters from multi-component data will be necessary.

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Principle Steps in Selecting the Appropriate Property Packages

1. Choosing the most suitable Property Packages.
2. Comparing the obtained predictions with data from the literature.
3. Estimate or obtain binary parameters from experimental data if necessary.
4. Generation of lab data if necessary to check the property model.

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Eric Carlson's Recommendations

Figure 1

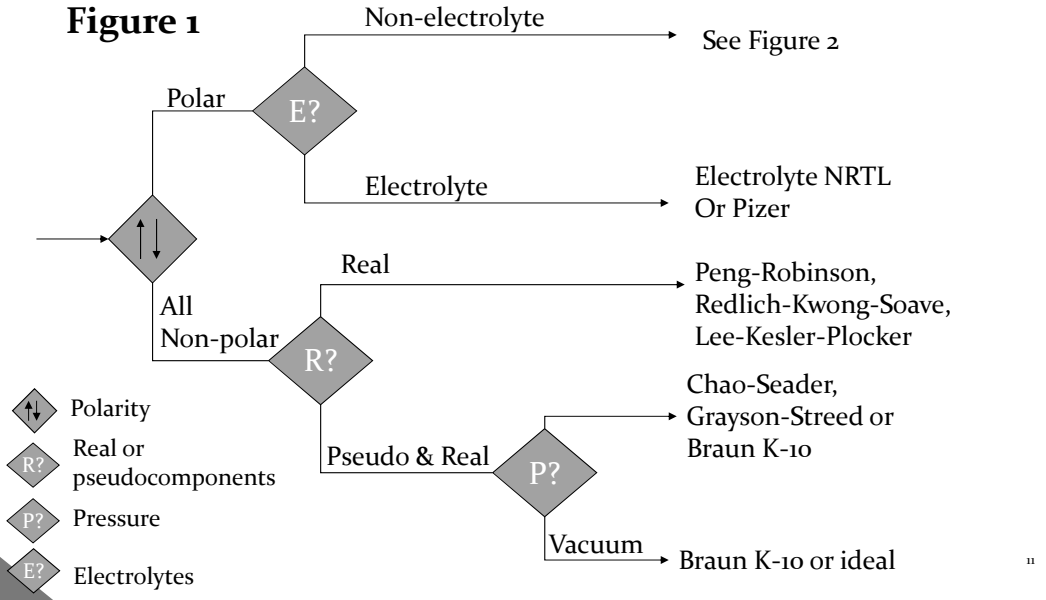

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Figure 2

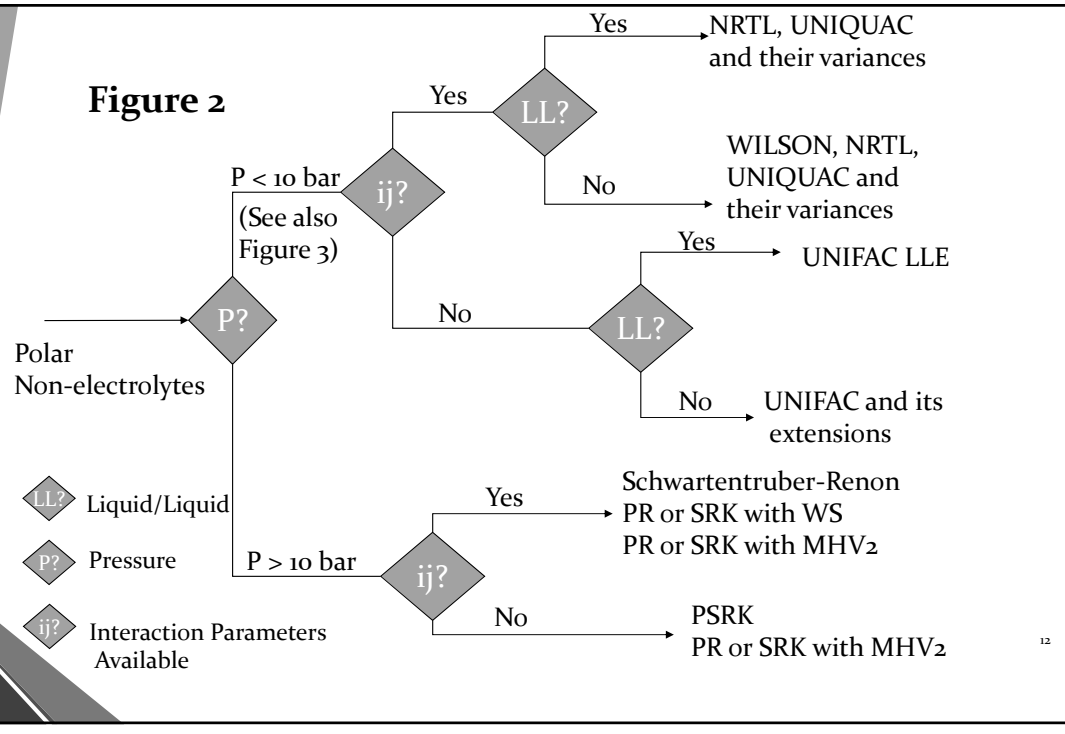

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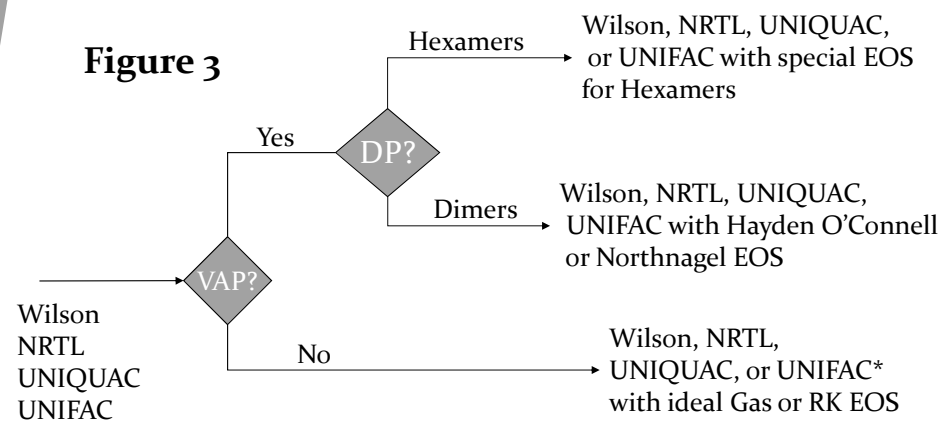
Figure 3



VAP? Vapor Phase Association

DP? Degrees of Polymerizatiom

UNIFAC* and its Extensions

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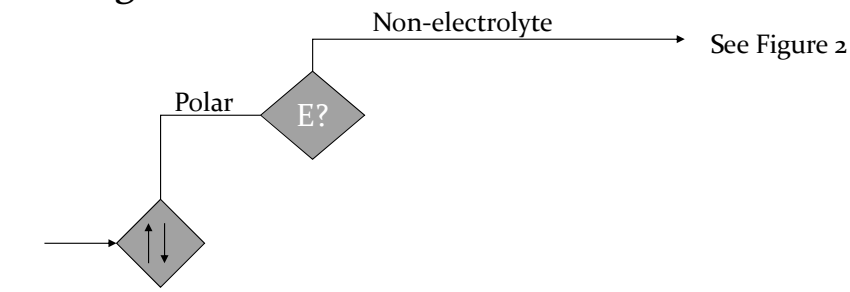
Eric Carlson's Recommendations

for 1-Propanol ,H_2O mixture

Figure 1



Polarity

R? Real or pseudocomponents

P? Pressure

E? Electrolytes

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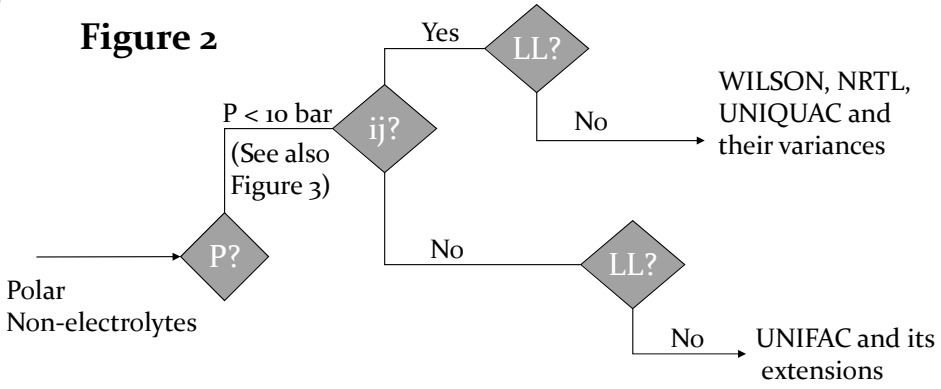
Figure 2


Yes
LL?
No
WILSON, NRTL, UNIQUAC and their variances
P < 10 bar
(See also Figure 3)
ij?
No
LL?
No
UNIFAC and its extensions
P?
Polar
Non-electrolytes
LL? Liquid/Liquid
P? Pressure
ij? Interaction Parameters Available

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