Physical Properties estimation using Aspen Plus

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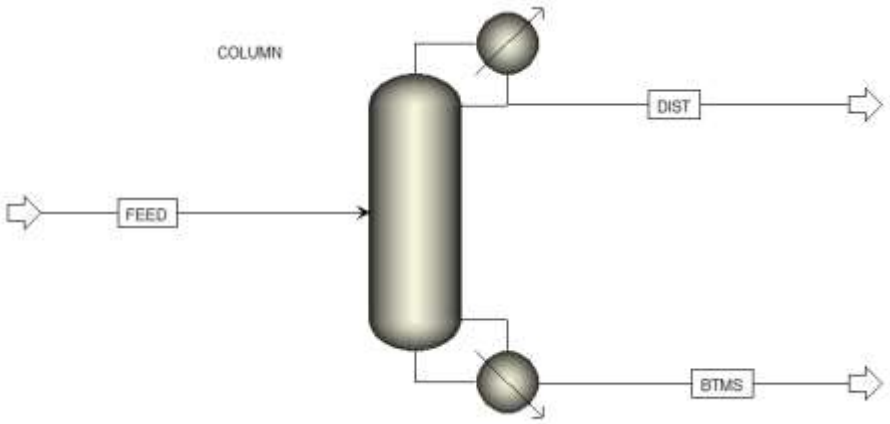
Agenda

- Physical properties estimation with ASPEN+
  - Property methods: selection guidelines
  - Property analysis
  - Property sets
  - Data regression

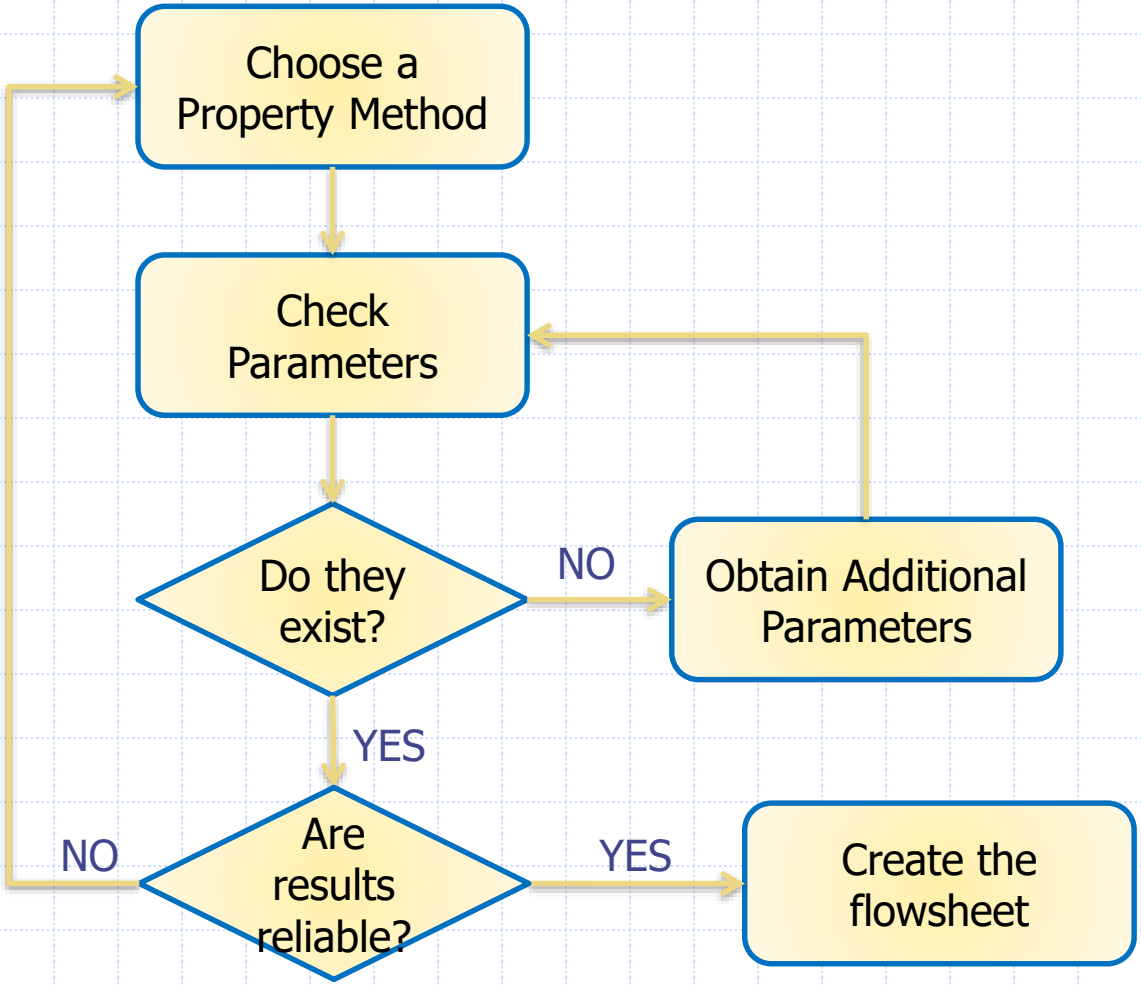
Ooops… the results are different!



Specification:
- 30 stages
- Distillate rate 500 kmol/hr
- Reflux ratio 1.3

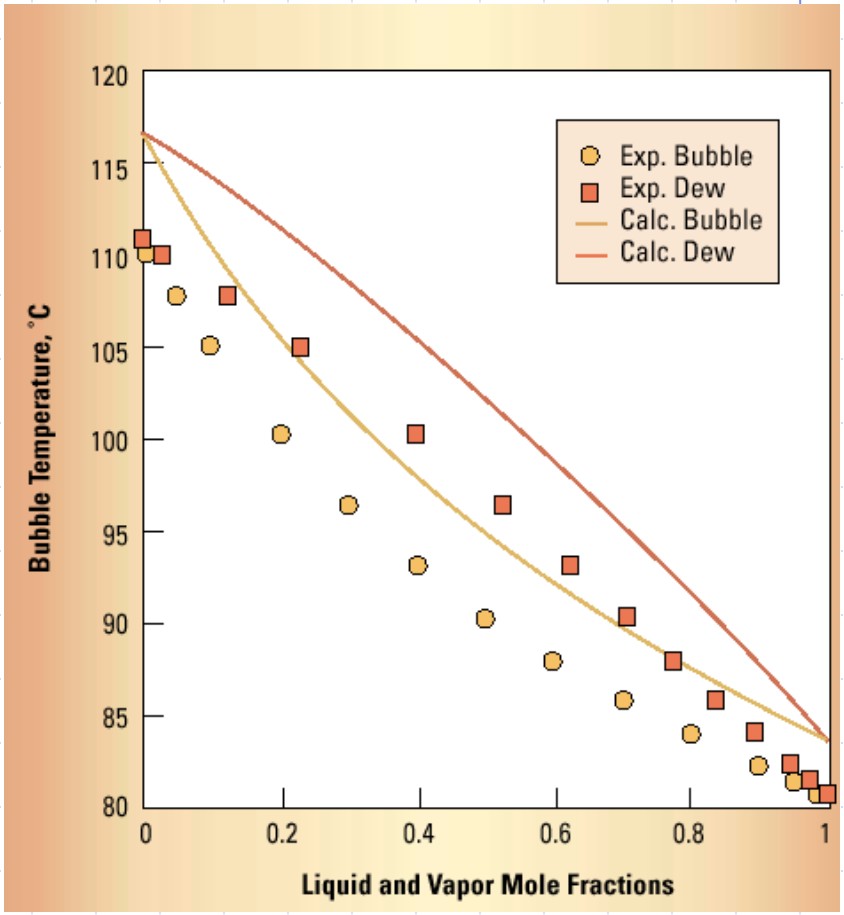
		IDEAL			NRTL		PENG-ROBINSON	
	Units	FEED	BTMS	DIST	BTMS	DIST	BTMS	DIST
– Mole Flows	**kmol/hr**	**2328.31**	**1828.31**	**500**	**1828.31**	**500**	**1828.31**	**500**
WATER	kmol/hr	1754.07	1691.96	62.1051	1753.92	0.147487	1754.05	0.0143418
METHANOL	kmol/hr	574.243	136.349	437.895	74.3909	499.853	74.2578	499.986
– Mole Fractions								
WATER		0.753365	0.925424	0.12421	0.959312	0.000294974	0.959384	2.86836e-05
METHANOL		0.246635	0.0745763	0.87579	0.0406884	0.999705	0.0406155	0.999971

How to establish Physical Properties



Vapor pressure is the king

- Simple EOS do not use Antoine constants
  - Do nor play around with w (entalpy is affected…)
- More complex EOS may or may not use vapor pressure
  - Always check vapor pressure
- Do not get careless if the problem is simple
  - Low pressure
  - Ideal system
  - Vapor pressure and vapor phase correction becomes important
- Use simple models to your advantage
  - Playing with vapor pressure
  - Playing with simple gamma models



Points of attention in using process simulators

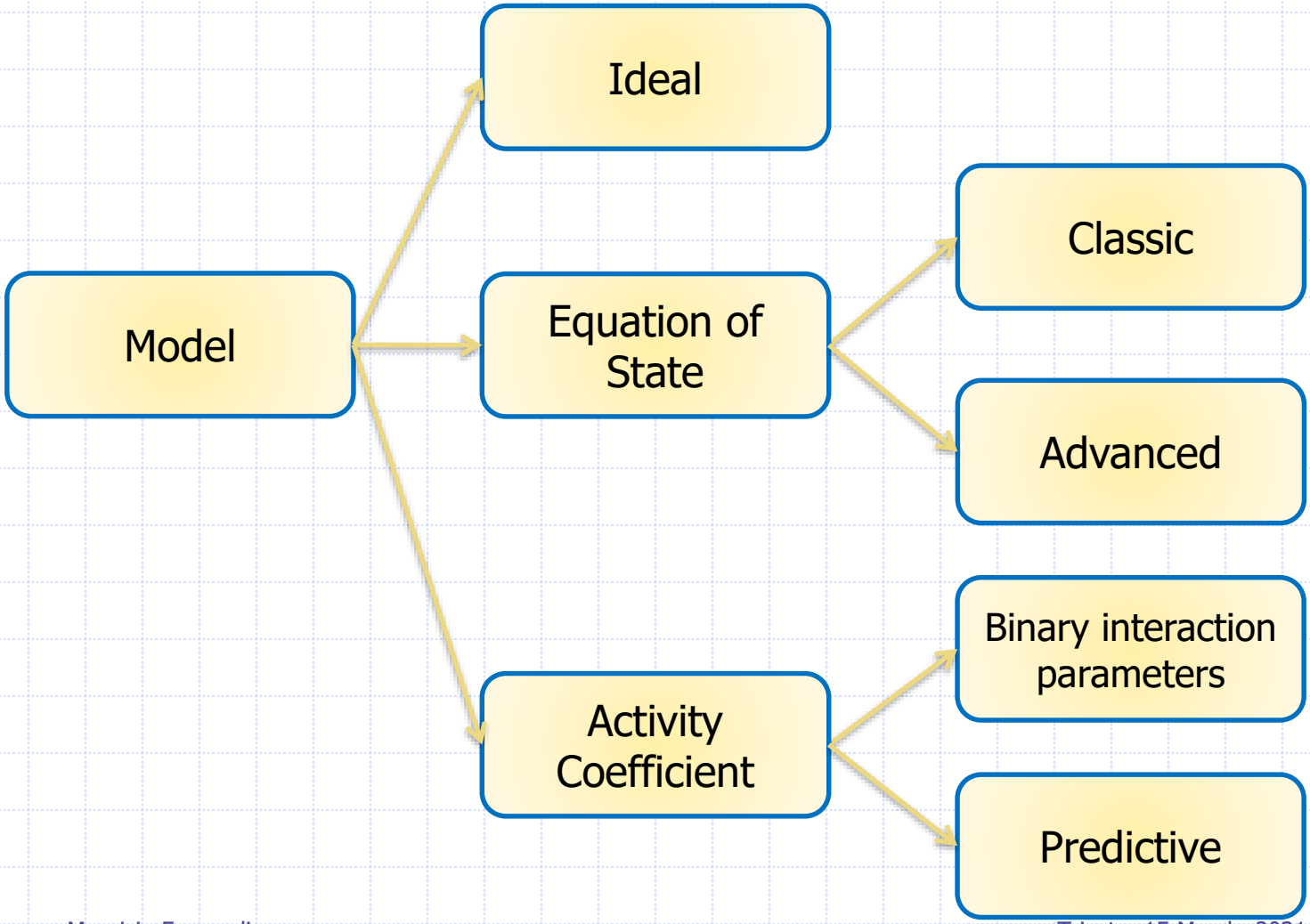
- Extrapolation and documentation
  - Simulation models tend to live longer than their creator ….
- Check your model also versus the 'less attractive area'
  - Density, entropy, enthalpy, viscosity, …
  - Find some data and check the models
- Accuracy vs. precision
  - Remember that Process Simulators are precise
  - Process simulators may NOT be accurate
  - Use error analysis
  - Consider the significant digits
- Henry's law is used to determine the amount of a supercritical component or light gas in the liquid phase
  - Declare any supercritical component or light gas (CO2, N2, etc) as Henry's component in the Properties Environment.
  - Remember to specify Henry's components ID in the thermodynamic method!

Ten Golden Rules

1. Check vapor pressure
2. Check pure and mixture densities – for aqueous mixtures excess volumes are important
3. Check pure and mixture enthalpy and heat capacities
4. Check transport properties (for heat exchangers and trays)
5. Check surface tension if you design trays
6. Azeotropes: check if they are present
7. Check trace components behavior versus infinite dilution activity coefficients
8. Talk to people, interact with chemists (new processes), talk to process simulators vendors
9. Beware of estimation methods for screening alternatives
10. Check the simulation results versus the reality, talk to the plant personnel, consider the reality (air leaks,…)

Models

The choice of model depends on degree of non-ideality, model parameters availability and operating conditions

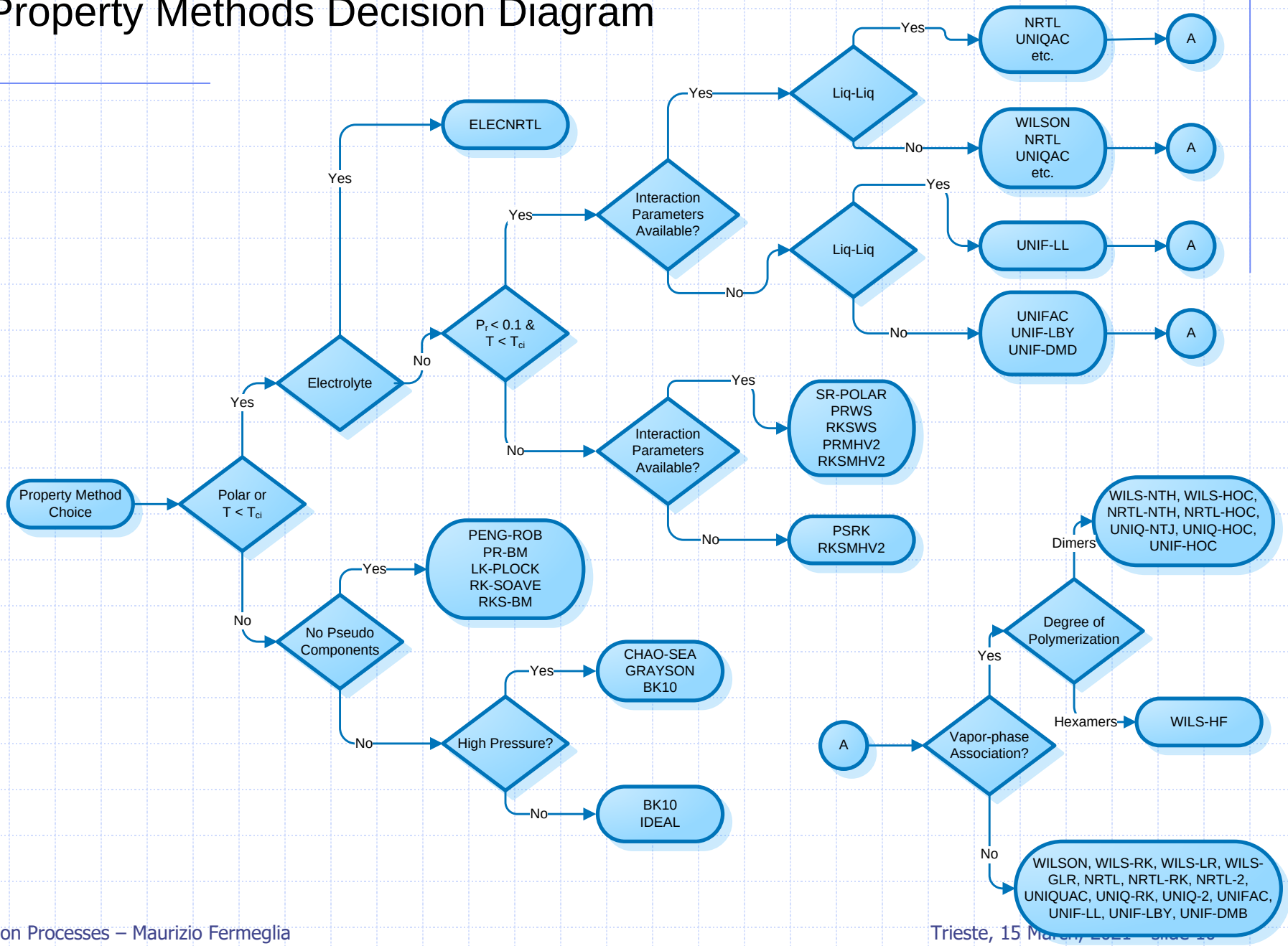


Equation of state vs Activity coefficient

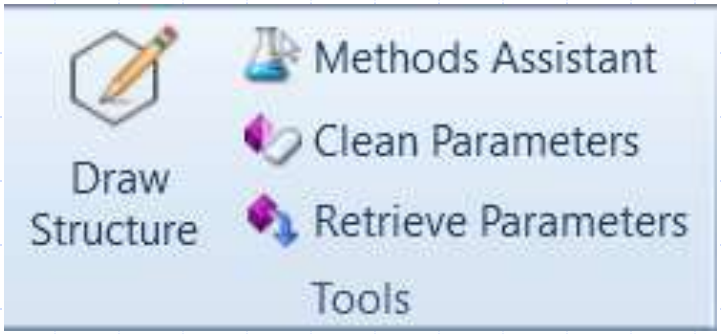
- Good for vapor phase modeling and liquids of low polarity
- Fewer binary parameters required
- Parameters extrapolated reasonably with temperature
- Consistent in critical region
- Typically limited in ability to represent non-ideal liquids
- Examples:
  - PENG-ROB
  - RK-SOAVE
  - PC-SAFT
  - PSRK

- Good for liquid phase modeling only
- Many binary parameters required
- Binary parameters are highly temperature dependent
- Inconsistent in critical region
- Can represent highly non-ideal liquids
- Examples:
  - NRTL
  - UNIQUAC
  - WILSON
  - UNIFAC

Property Methods Decision Diagram

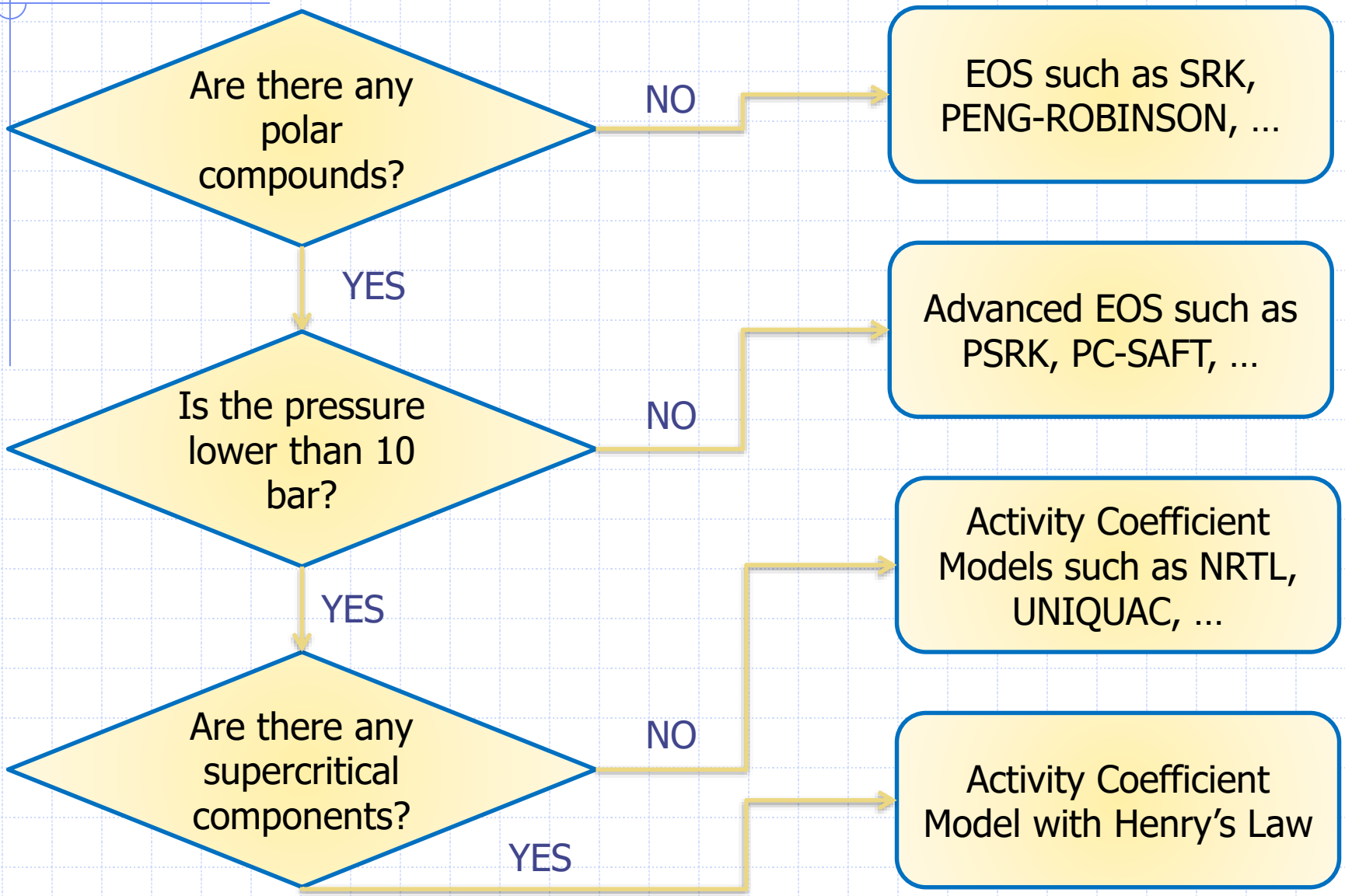


Property Method Selection Assistant



- The assistant will help you select the most appropriate property method by guiding you through a series of questions
- Search by components or process types
- At the end, the help topics for the recommended property methods are linked
- A report is also available that can be saved or printed

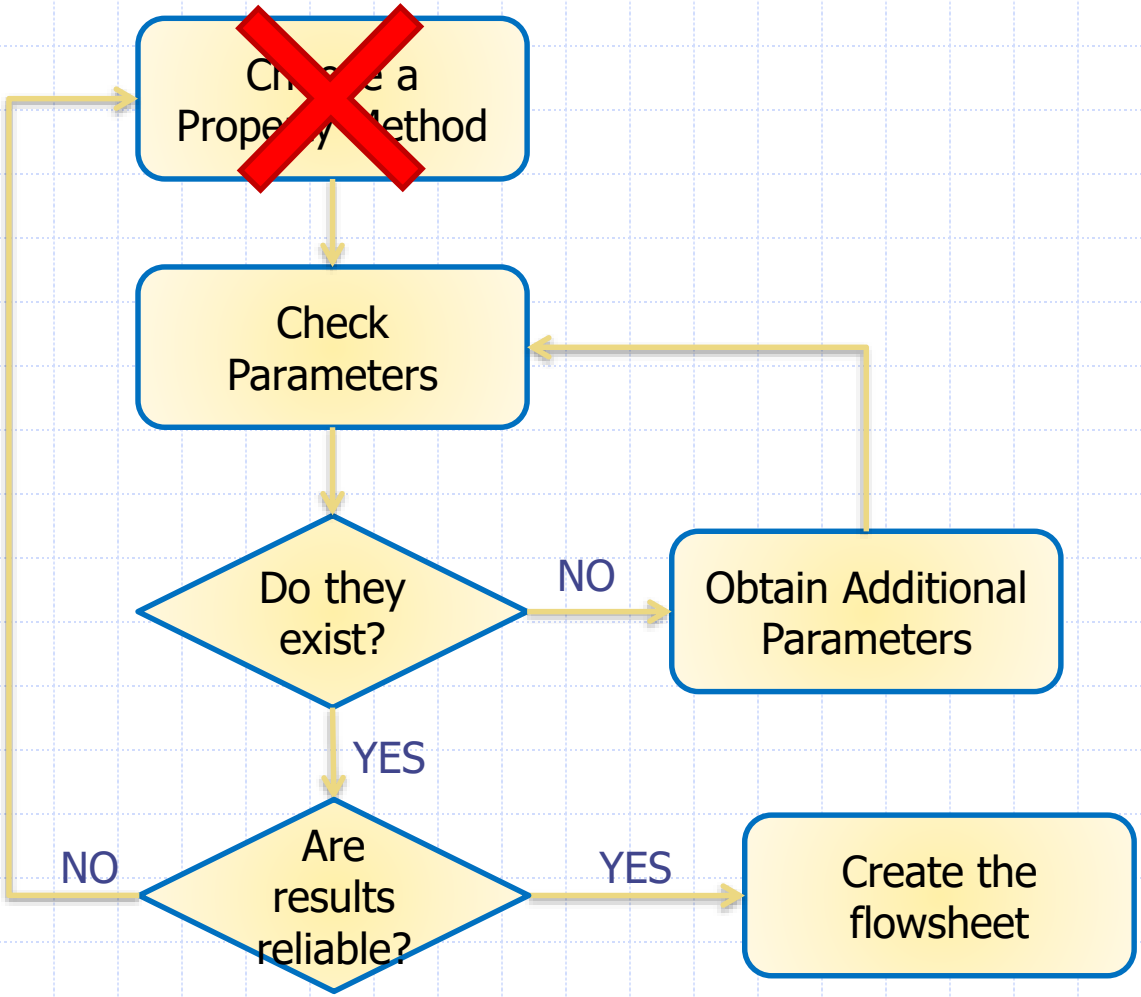
Choosing a Property Method



Choosing a Property Method - Examples

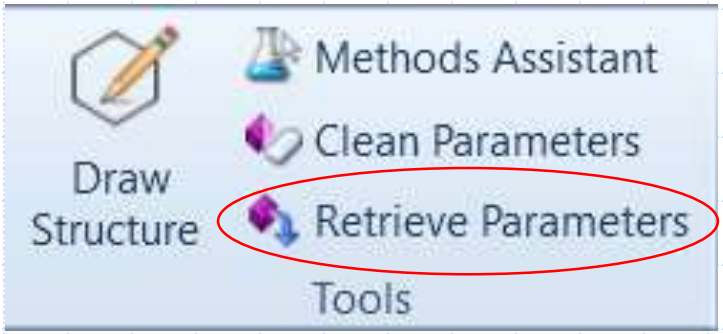
System @ 1 atm	Property Method
Propane, Ethane, Butane	EOS (SRK, PENG-ROB…)
Benzene, Water	AC (UNIQUAC, NRTL-RK, …)
Acetone, Water	AC (NRTL, WILSON, …)
Ethanol, Water	AC (NRTL,UNIFAC…)
Benzene, Toluene	EOS
Acetone, Water, Carbon Dioxide	AC+Henry
Ethane, Propanol	AC

How to establish Physical Properties



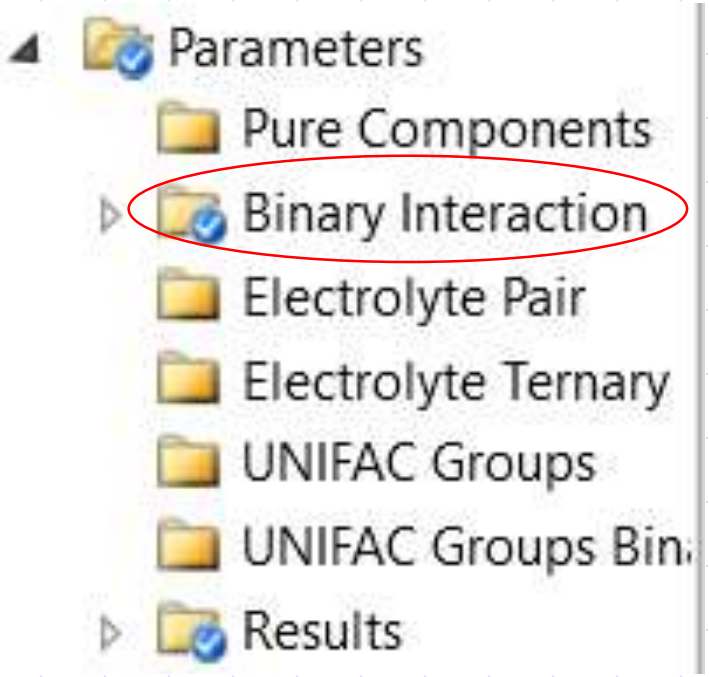
Pure components parameters

- Represent attributes of a single component
- Stored in databanks such as (PURE, AQUEOUS, SOLIDS, ...)
- Scalar: MW, ACENTRIC FACTOR, …
- Temperature-dependent: PLXANT for parameters in the extended Antoine vapor pressure model



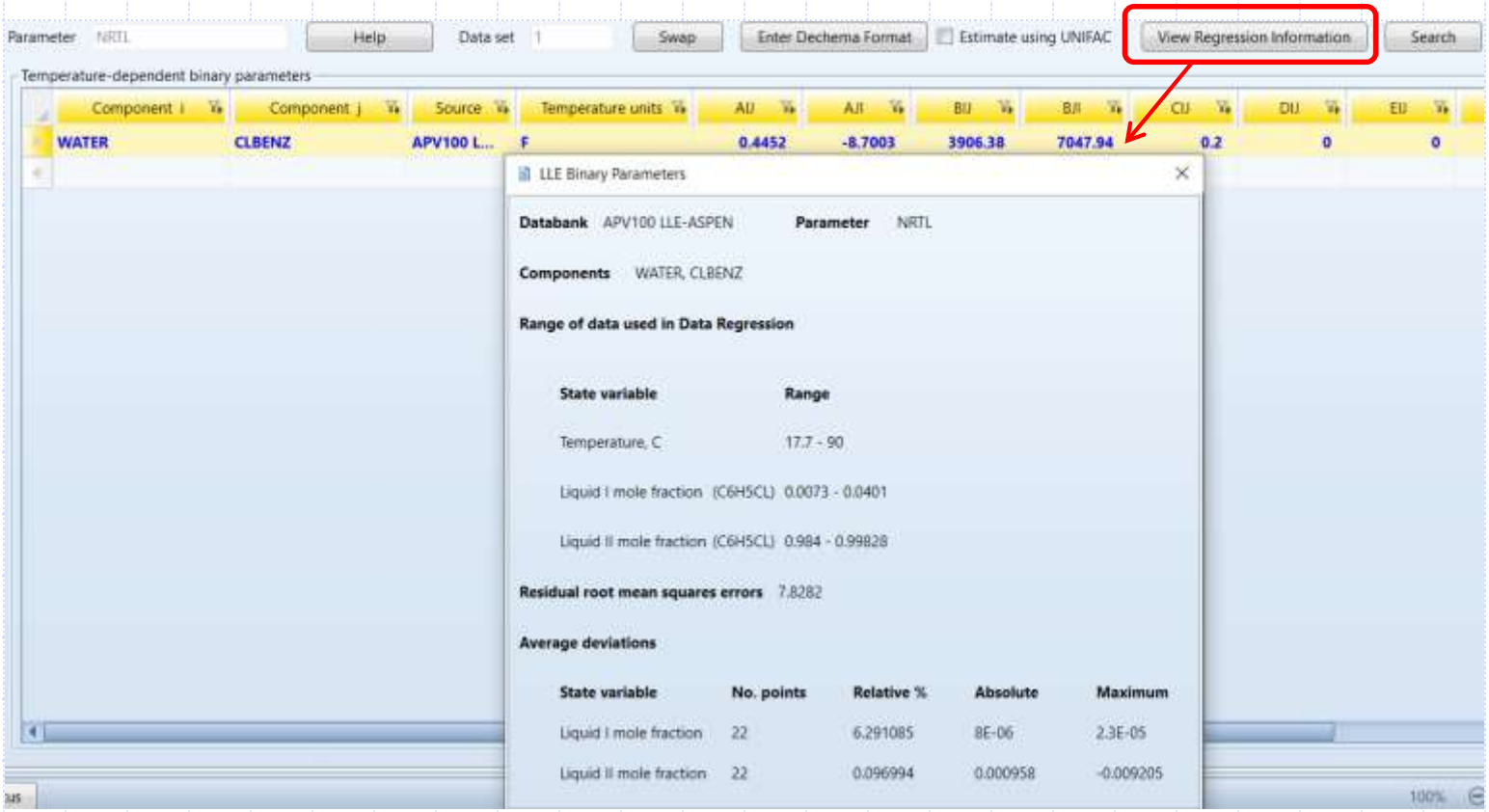
Binary Interaction parameters

- Used to describe interactions between two compounds
- Stored in binary databanks such as APV VLE-IG, APV LLE-ASPEN
- Parameters values from the databanks are visible automatically through the graphical user interface
- Examples:
  - Scalar: RKTKIJ-1 for Rackett model
  - Temperature-dependent: NRTL-1 for parameters in NRTL model

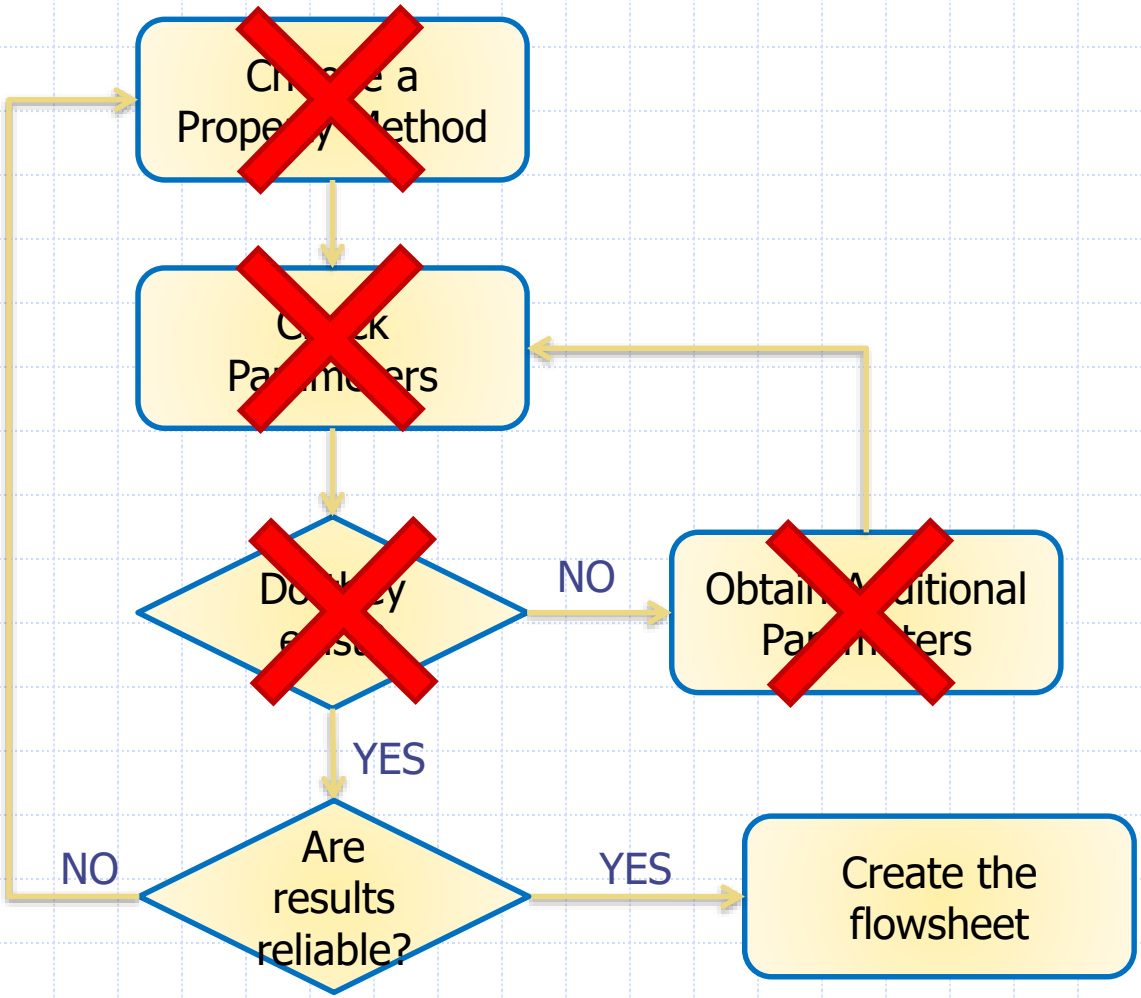


Binary Interaction parameters

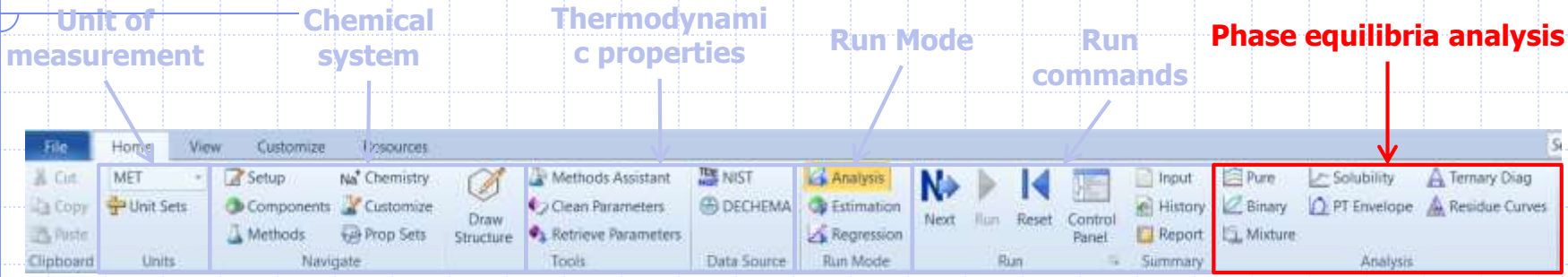
- Properties Parameters Binary Interaction NRTL-1 Form
  - Press the Regression Info button to display the regression data for each component pair



How to establish Physical Properties



Property Analysis



- Used to generate simple property diagrams to validate physical property models and data
- Diagram types:
  - Pure component, i.e. vapor pressure vs temperature
  - Binary, i.e. Txy, Pxy
  - Mixture
  - Ternary Residue Maps
  - Ternary Phase diagrams
  - PT envelope

Property Analysis - Review

1. Choose property method, based on:
   - Components present in simulation
   - Operating conditions in simulation
   - Available data or parameters for components
2. Check parameters:
   - Determine availability of parameters in Aspen Plus databanks, obtain additional parameters if necessary
3. Confirm Results:
   - Verify choice of Property Method and physical property data using Property Analysis plotting tool

Property Analysis – Hands on A+

Consider the binary mixtures:

- Methanol – Propanol
- Water - Ethanol
- Ethanol – Toluene
- Toluene – Water

Check vapor pressure of pure components

For each binary system create Txy, xy graph at 1 and 5 bar

Compare ideal with NRTL model

Compare with experimental data at P= 1 bar

Property Analysis - Exercise

- Objective: simulate a two-liquid phase settling tank and investigate the physical properties of the system

- A chemical plant has a settling tank that they use to decant off the water from a mixture of water and chlorobenzene; the inlet stream to the tank also contains some carbon-dioxide and nitrogen; the tank and feed are at ambient conditions (25 °C, 1 atm) and have the following flow rates:
  - Water: 230 kg/hr
  - Chlorobenzene: 2000 kg/hr
  - CO2: 340 kg/hr
  - N2: 20 kg/hr

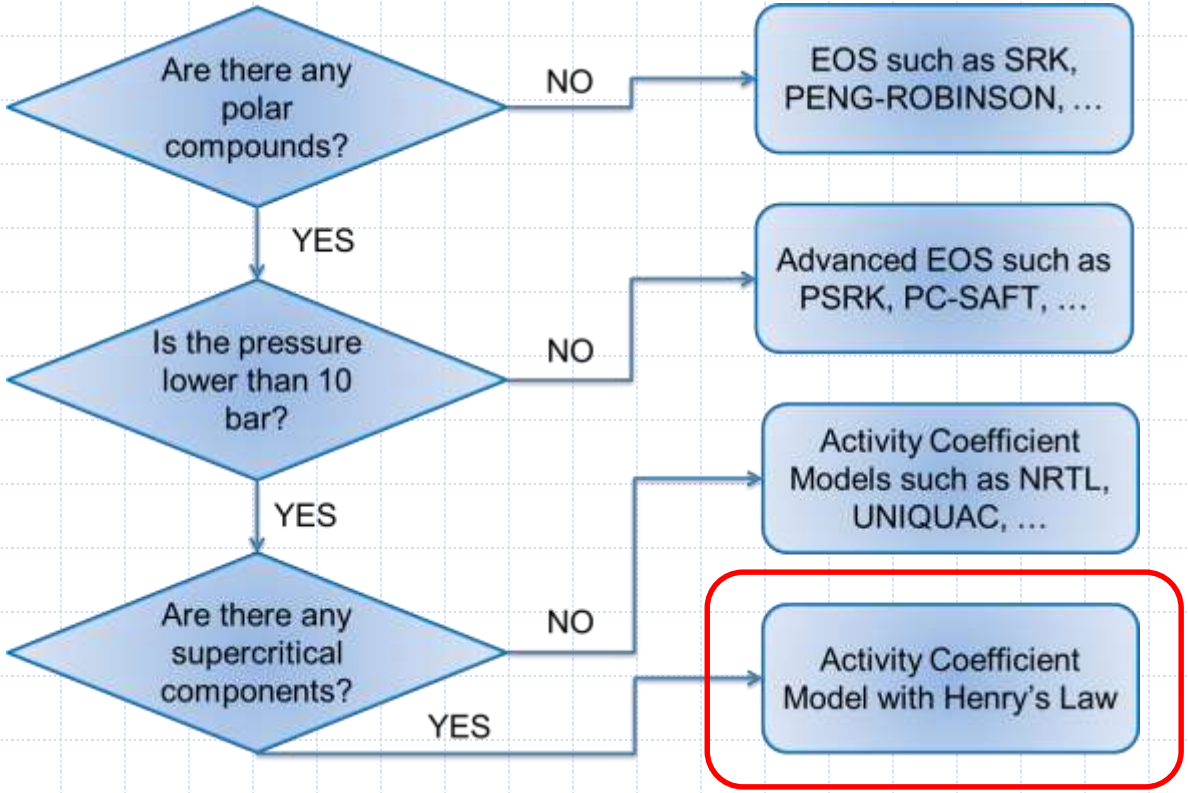
  Water and Chlorobenzene form two-liquid phases under the conditions in the tank

Property Analysis - Exercise

1. Choose an appropriate Property Method to represent the system. Parameters available?
2. Retrieve the Tc for CO2 and water
3. Use the binary isotherm analysis to investigate the phase equilibrium of the liquid mixture @ 1 atm
4. Set up the flowsheet to model the settling tank using a flash drum

Property Analysis - Exercise

1. Choose an appropriate Property Method to represent the system.

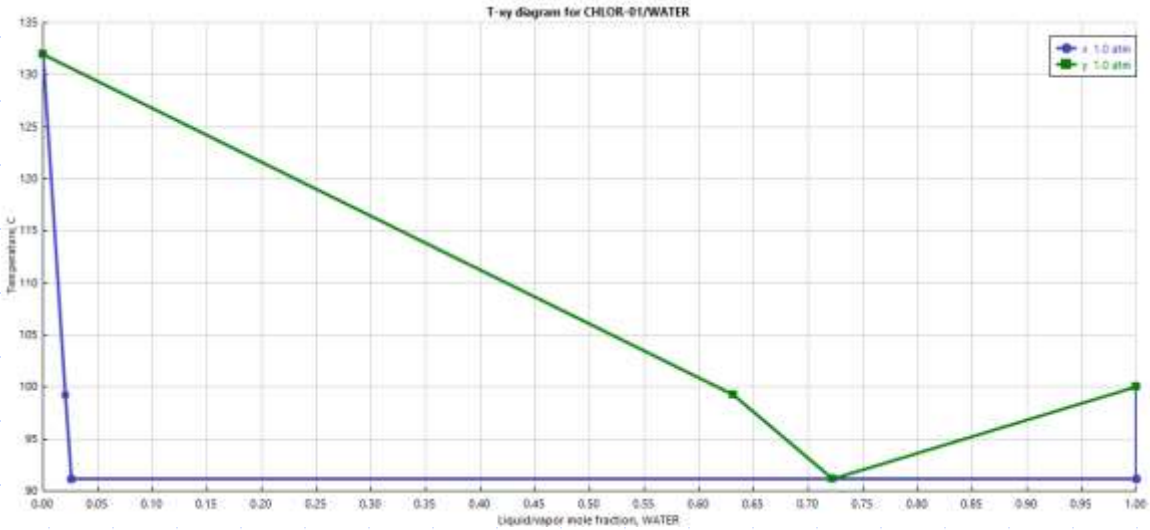


Property Analysis - Exercise

1. Choose an appropriate Property Method to represent the system.
   NRTL, UNIQUAC with Henry's components
2. Retrieve the Tc for CO_2 and water

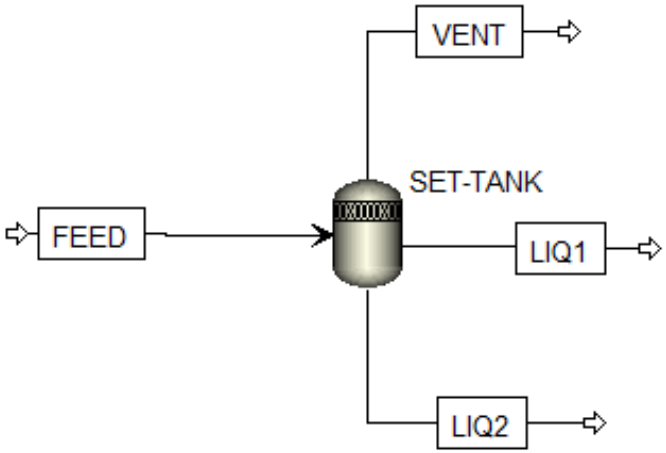
	Parameters	Units	Data set	Component WATER	Component CLBENZ	Component CO2
▶	TC	C	1	373.946	359.2	31.06

3. Use the binary isotherm analysis to investigate the phase equilibrium of the liquid mixture @ 1 atm



Property Analysis - Exercise

1. Set up the flowsheet to model the settling tank using a flash drum



2. Modify the stream report to include the constant pressure heat capacity (CPMX) for each phase (Vapor, Liquid 1 and Liquid 2), and the fraction of L1 to total liquid for a mixture (BETA)
3. Display Total stream mass density as Global Data on the Flowsheet