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Selecting Fluid Packages for HYSYS Process Simulator

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Selecting Appropriate Fluid Packages in HYSYS

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Outline

- Importance of Selecting the Appropriate Prediction Method
- Principal Steps in Selecting the Appropriate Thermodynamics Package
- Sources of Information
- Issues in Selection of the Appropriate Thermodynamics Package
- Recommendations for the Selection of the Appropriate Thermodynamics Package
 - Eric Carlson's Recommendations
 - Professor Seader Recommendations
 - Hyprotech Recommendations
- Example: water and 1-propanol

Importance of Selecting the Appropriate Prediction Method

- Correct predictions of the physical properties of the mixture as a function of temperature and pressure.
- Each method is suitable only for particular types of components and limited to certain operating conditions.
- Choosing the wrong method may lead to incorrect simulation results.
- Particularly important for reliable computations associated with separation operations (distillation, LL extraction, etc.).

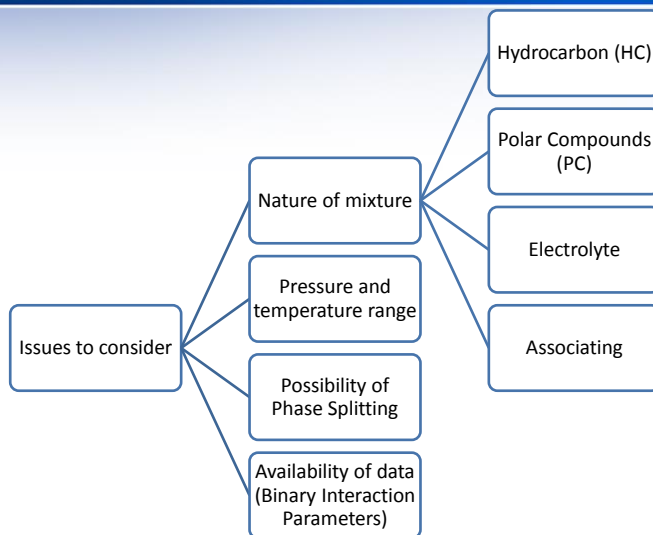
Principal Steps in Selecting the Appropriate Thermodynamics Package

1. Choosing the most suitable model/thermo method.
2. Comparing the obtained predictions with data from the literature.
3. Adding estimates for components that not available in the chosen thermo package. Can they be neglected?
4. Generation of lab data if necessary to check the thermo model.

Sources of Information

1. Publications and professional literature that deal with the process in question or with the components that participate in the process.
 - a) Journal of Chemical reference Data (NIST)
 - b) Journal of Chemical and Engineering Data
 - c) Journal of Chemical Thermodynamics
 - d) Journal of Fluid phase Equilibria
2. Simulator reference manual (HELP).
3. DATABANKS
 - a) DIPPR
 - b) DECHEMA (Dortmund)
4. Rules of thumb
 1. Look for Walas's design book
 2. Your textbook
 3. Brennan's rules of thumb (latest edition)
 4. Turton's Process Design textbook.

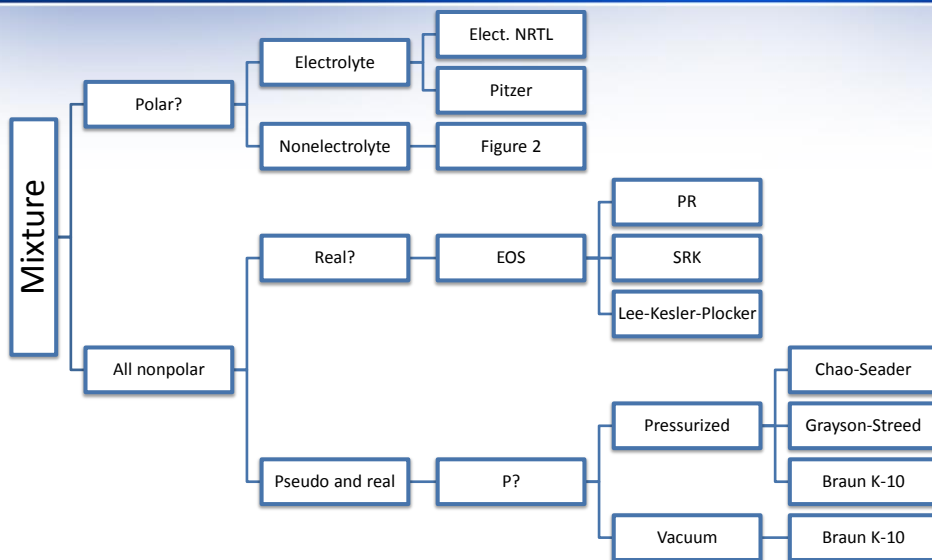
Issues in Selection of the Appropriate Thermodynamics Package



Recommendations for the Selection of the Appropriate Thermodynamics Package

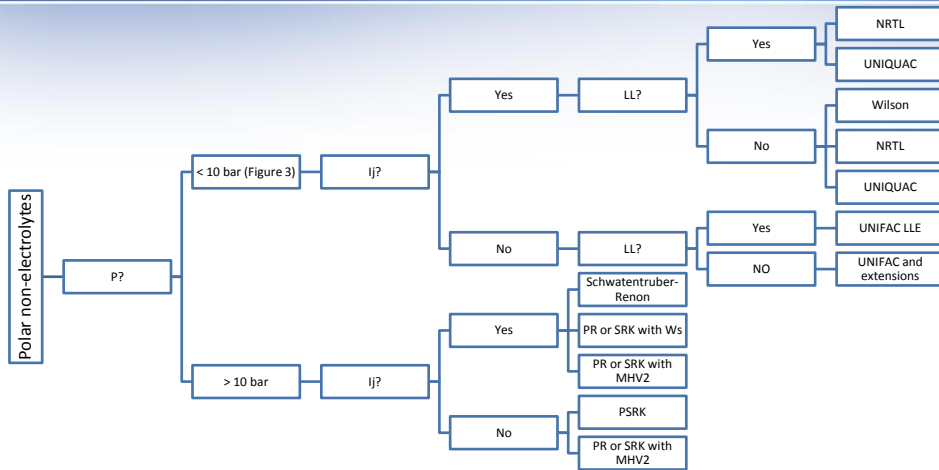
1. Eric Carlson, “**Don’t gamble with physical properties for simulations,**” Chemical Engineering Progress, October 1996, 35-46.
2. Prof J.D. (Bob) Seader, University of Utah
3. Hyprotech Recommendations

Eric Carlson’s Recommendations Figure 1: Global Perspective



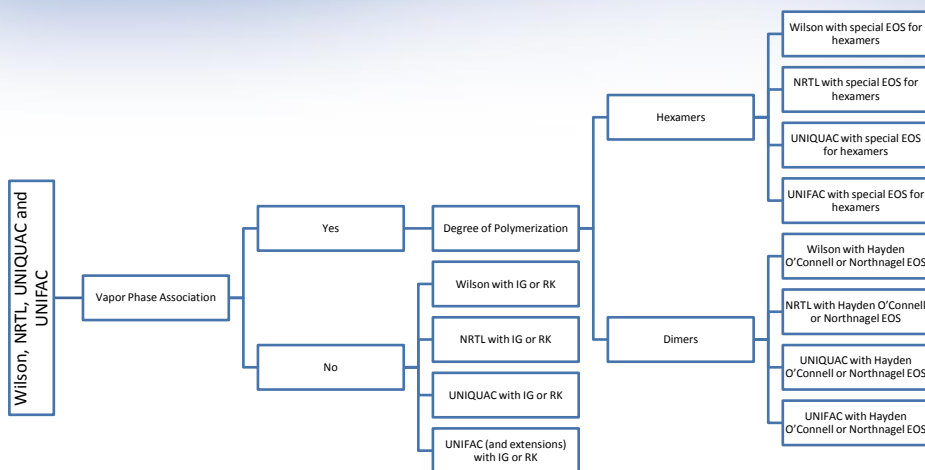
Eric Carlson's Recommendations

Figure 2: Case of Polar non-electrolytes

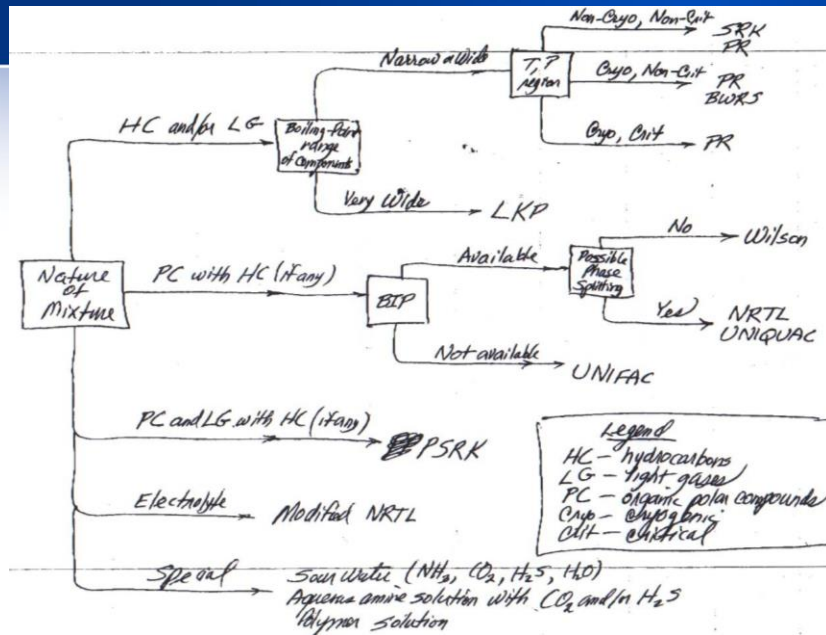


Eric Carlson's Recommendations

Figure 3: Case of Vapor Phase Association

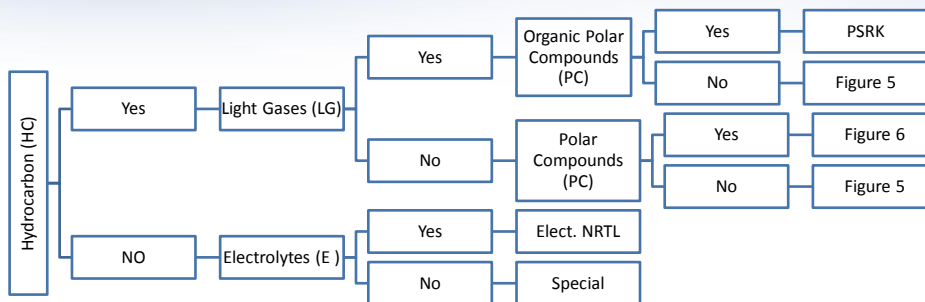


Bob Seader's Recommendations



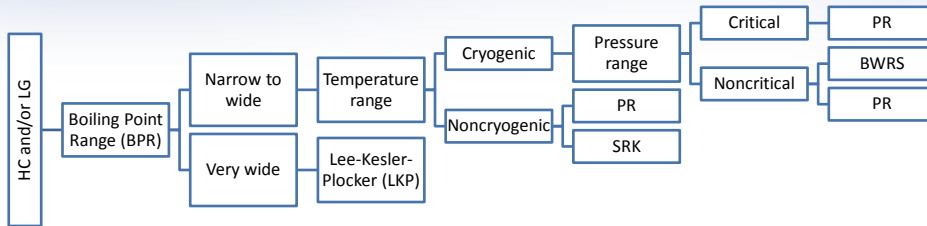
Bob Seader's Recommendations

Figure 4: Global Perspective

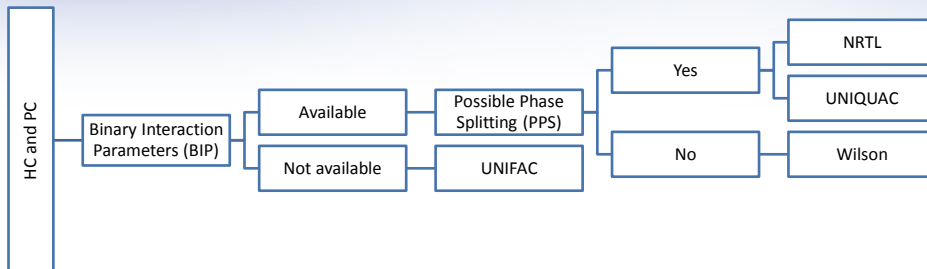


e.g., Sour Water (NH_3 , CO_2 , H_2S , H_2O), Aqueous amine solution with CO_2 and H_2S

Bob Seader's Recommendations
Figure 5: HC and/or LG



Bob Seader's Recommendation
Figure 6: HC and Polar Compounds PC



Hyprotech Recommendations
Hyprotech is HYSYS's original company

Type of System	Recommended Property Method
TEG Dehydration	PR
Sour Water	PR, Sour PR
Cryogenic Gas Processing	PR, PRSV
Air Separation	PR, PRSV
Atm Crude Towers	PR, PR Options, GS
Vacuum Towers	PR, PR Options, GS (<10 mm Hg), Braun K10, Esso K
Ethylene Towers	Lee Kesler Plocker
High H ₂ Systems	PR, ZJ or GS (see T/P limits)
Reservoir Systems	PR, PR Options
Steam Systems	Steam Package, CS or GS
Hydrate Inhibition	PR
Chemical systems	Activity Models, PRSV
HF Alkylation	PRSV, NRTL (Contact Hyprotech)
TEG Dehydration with Aromatics	PR (Contact Hyprotech)
Hydrocarbon systems where H ₂ O solubility in HC is important	Kabadi Danner
Systems with select gases and light hydrocarbons	MBWR

Example

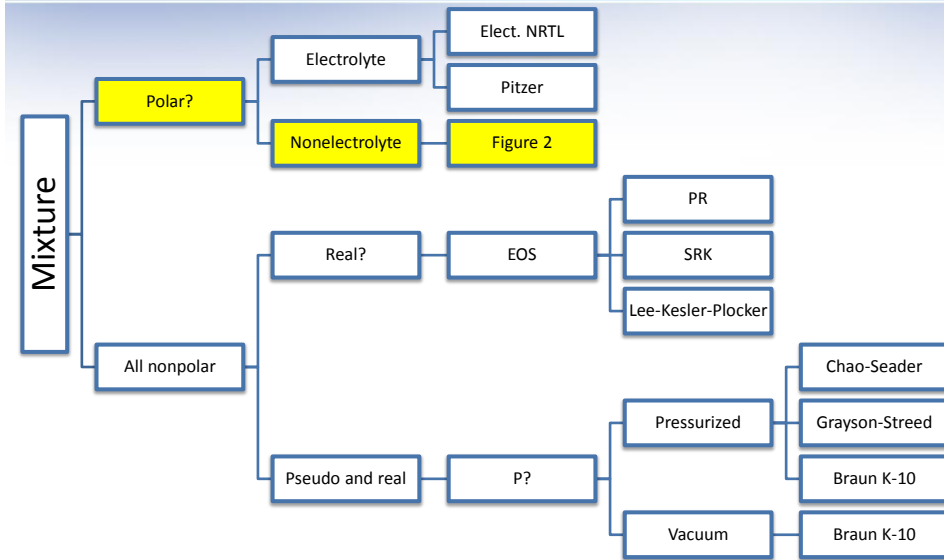
- Find the best thermodynamic package for 1-Propanol , H₂O mixture.

★ Eric Carlson, "Don't gamble with physical properties for simulations," Chem. Eng. Prog. October 1996, 35-46

★ Prof J.D. (Bob) Seader,
University of Utah

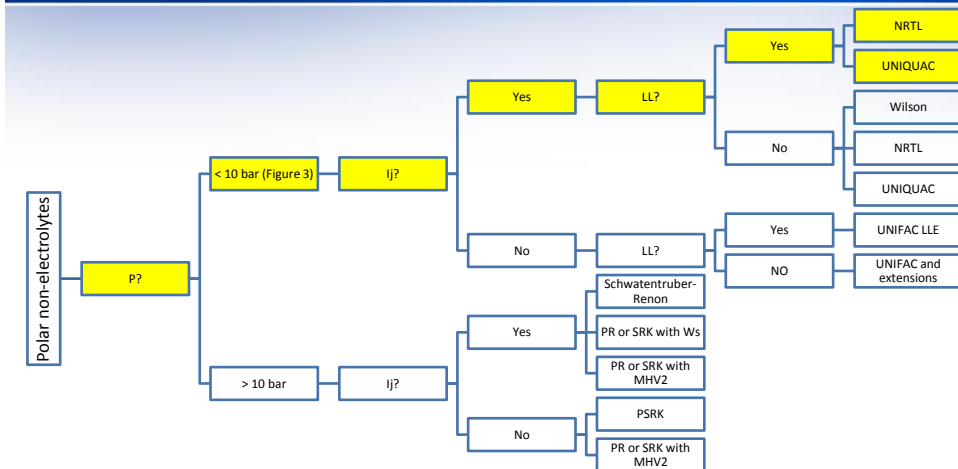
Eric Carlson's Recommendations

Figure 1: Global Perspective

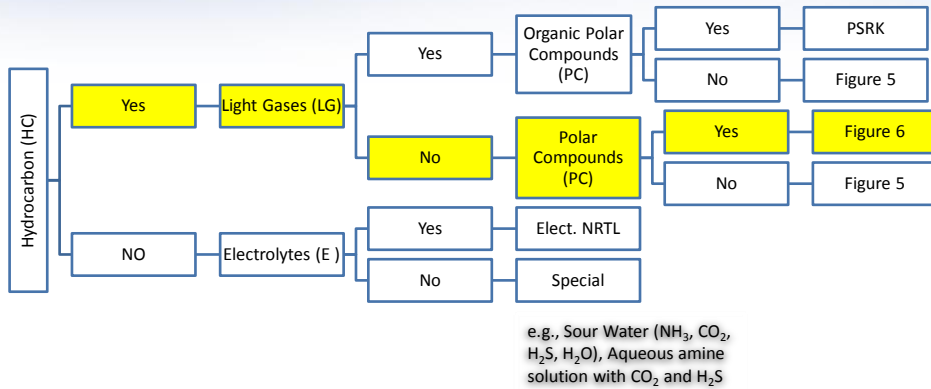


Eric Carlson's Recommendations

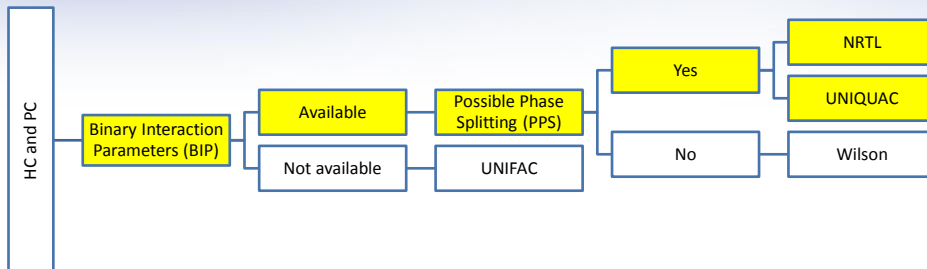
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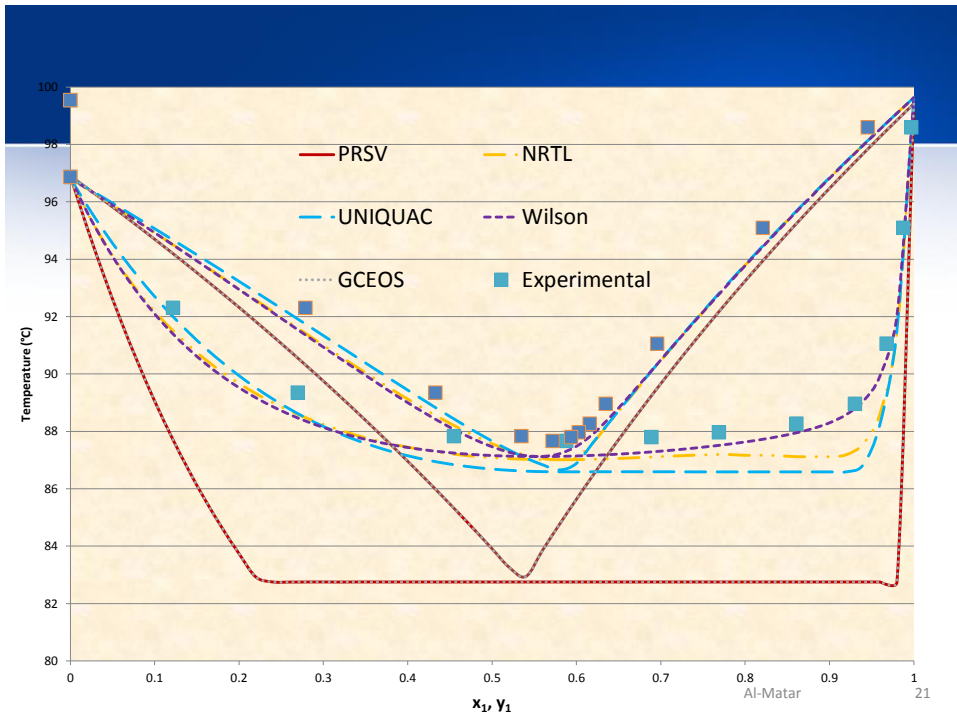


Bob Seader's Recommendations
Figure 4: Global Perspective



Bob Seader's Recommendation
Figure 6: HC and Polar Compounds PC





Exercise

- Select an appropriate fluid package for the following systems
 - Benzene, toluene, and xylene at $P = 8$ bar.
 - Water, NaCl.
 - Hydrogen, methane, benzene and toluene.

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