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Exercise 2

How to chose the best property prediction method for simulation ?

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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.).

Principle 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.
- 2. Simulator reference manual (HELP).
- 3. DATABANKS
- 4. Rules of thumb.

Issues in Selection of the Appropriate Thermodynamics Package

- Nature of mixture (e.g., hydrocarbon, polar, electrolyte, etc.)
- Pressure and temperature range
- Availability of data.

Recommendations for the Selection of the Appropriate Thermodynamics Package

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

Hyprotech Recommendations







Bob Seader's Recommendations



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Bob Seader's Recommendations



Figure 5



Figure 6



Hyprotech Recommendations

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 H2 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 H2O solubility in HC is important	Kabadi Danner
Systems with select gases and light hydrocarbons	MBWR

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Example

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

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Figure 6



$1-Propanol, H_2O$



1/3/13

20

TXY macro for HYSYS



1/3/13