Aspen HYSYS Property Packages

Overview and Best Practices for Optimum Simulations

Aspen Process Engineering Webinar
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Aspen HYSYS Property Packages

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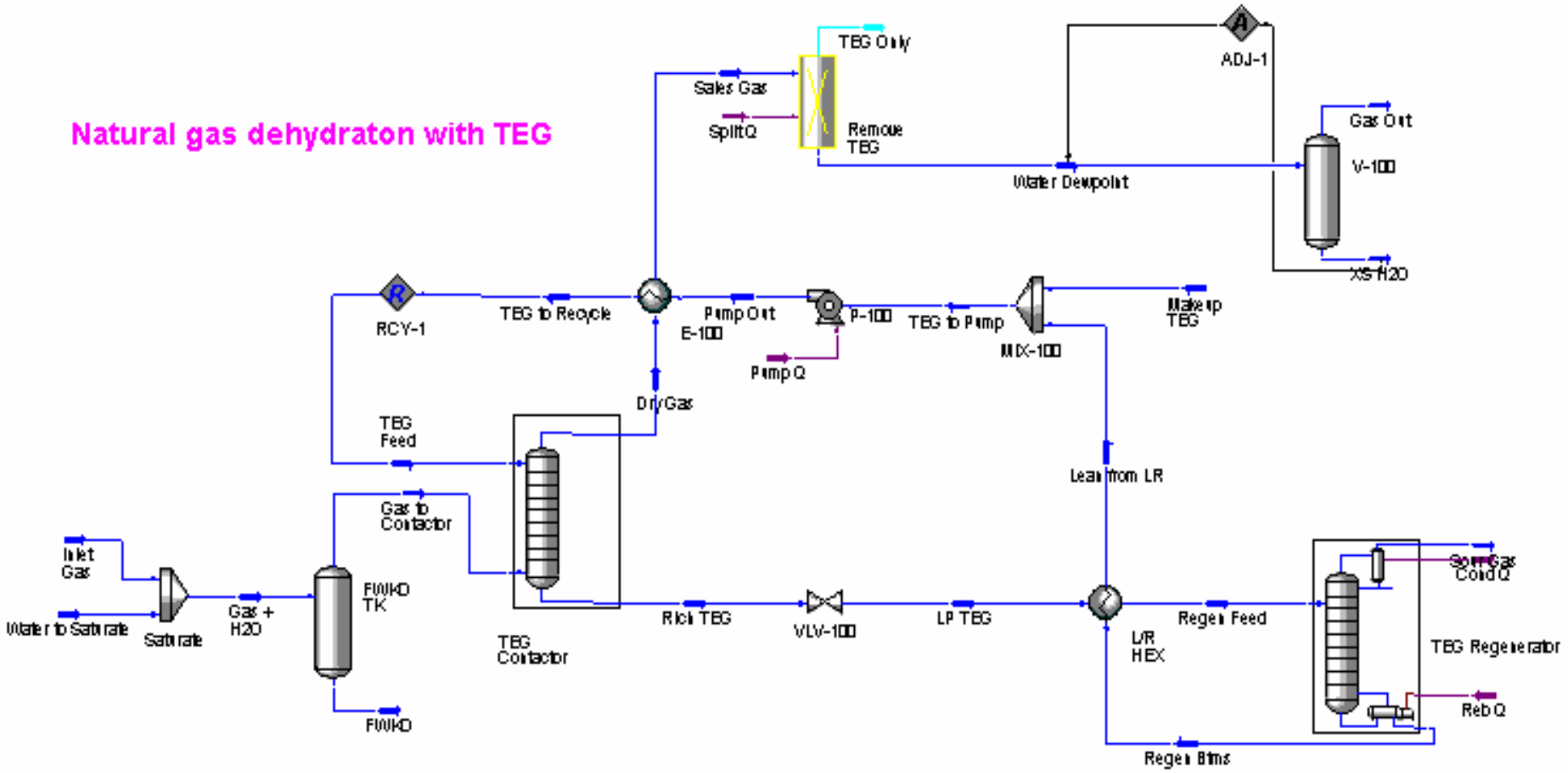
Agenda

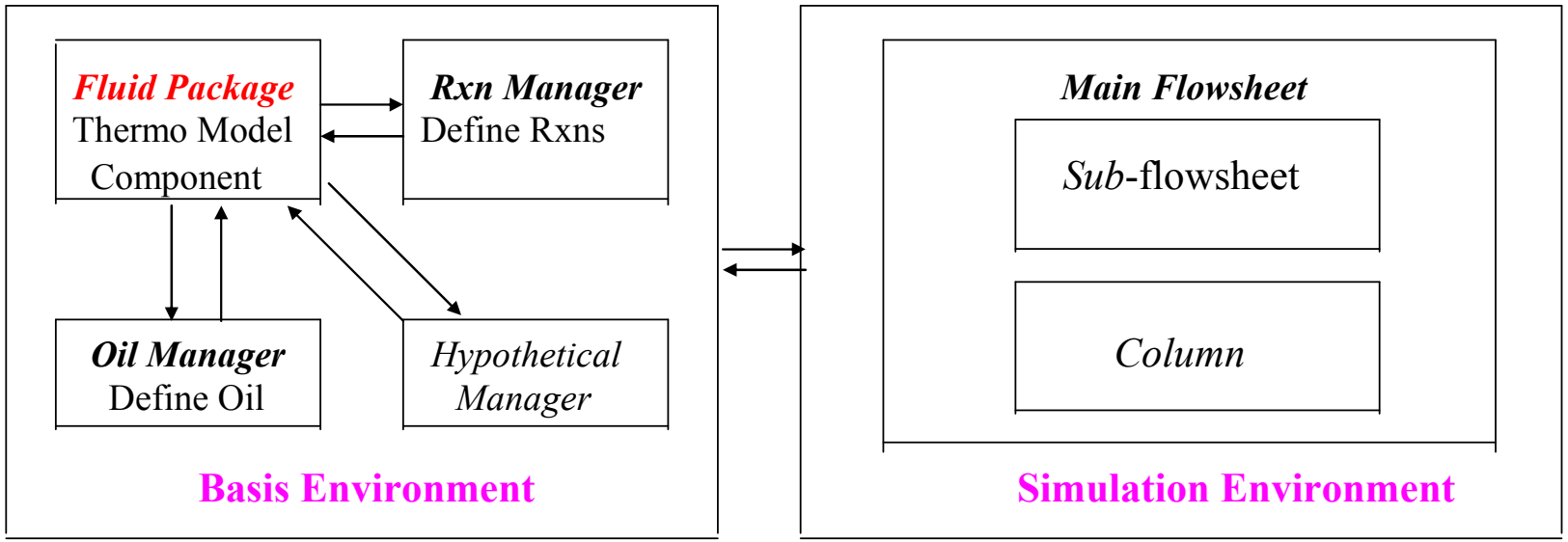
- Introduction
- Review of methods available in Aspen HYSYS
- Thermodynamics assistant in HYSYS 2006
- Recommendations and tips for applications in:
  - Oil & Gas
  - Refining
- Demonstration (as we go)
- Q & A

What is Process Simulation?



How Does Aspen HYSYS Work?

Thermodynamic models are used to represent the phase equilibrium behavior and energy level of pure compound and mixture systems.



Can We Believe Simulation Results?

In many cases, simulation results **DO NOT** reflect what is really happening in a plant

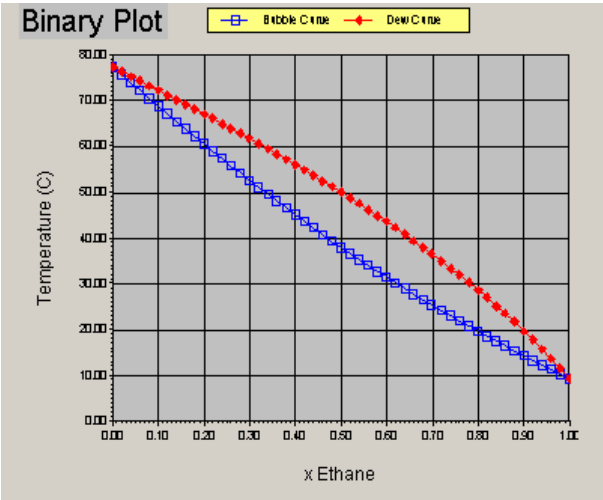
WHY?

- Improperly selected thermodynamic models
- Inadequate model parameters
- Incorrect hypothetical components generation
- Problems with plant data consistency

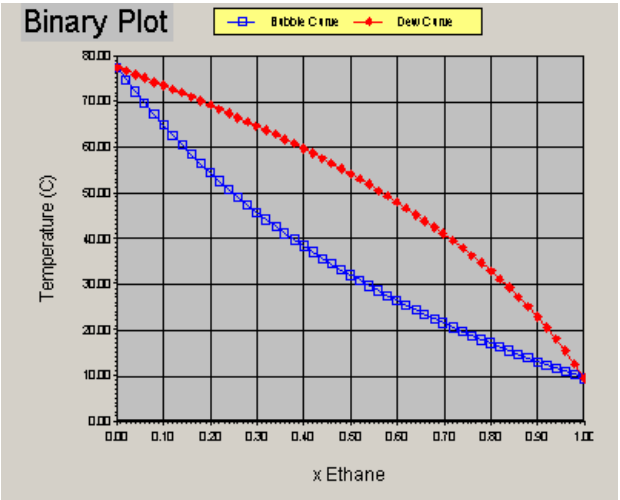
Different Models - Different Phase Behavior

Example:

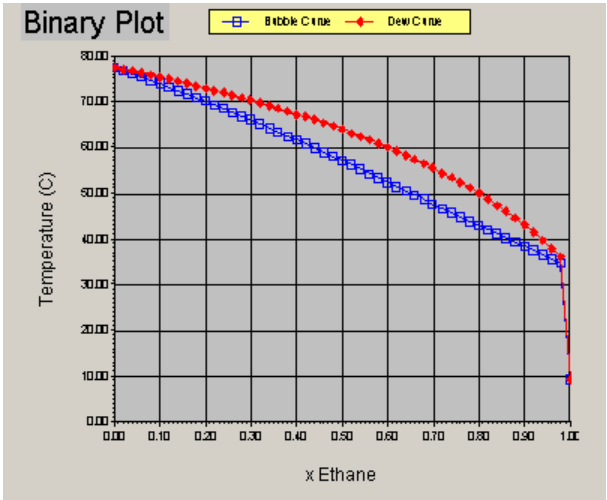
- A mixture of Ethane and Propane at 30 atm
- The PR Equation of State most closely represents the true phase behavior of the system



- Peng Robinson EOS
- Dew point 50.1 C



- Vapor Pressure model
- Dew point 54.3 C
- Good predictions at low pressures

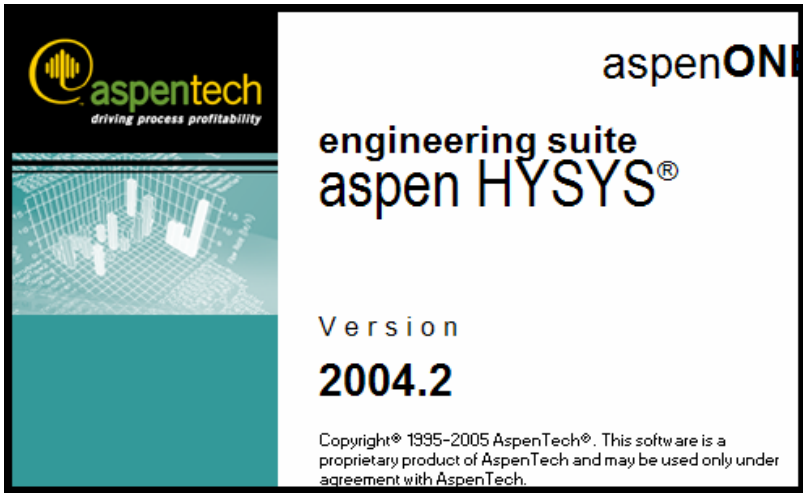


- NRTL Ideal

Thermodynamic Models in Aspen HYSYS

Aspen HYSYS contains over 30 thermodynamic models

- Equations of State
- Activity Coefficient Models
- Vapor Pressure Models
- Semi-Empirical Models
- Specialty Models
  - Steam Tables
  - Amines Package
  - Clean Fuels Package
  - Glycol Package
  - OLI
  - Neotec Black Oil
  - Infochem Multiflash
  - etc.



Equation of State (1)

- **Peng-Robinson (PR)**
  - Most enhanced model in Aspen HYSYS
  - Largest applicability range in terms of T and P
  - Special treatments for some key components
  - Largest binary interaction parameter database
- **PRSV**
  - Modified PR model
  - Better representation of vapor pressure of pure components and mixtures
  - Extends applicability of the original PR model to moderately non-ideal systems
- **SRK**
  - Modified RK model
  - Can provide comparable results to PR in many cases, but with a lot less enhancement in Aspen HYSYS

Equation of State (2)

- **PR-Twu**
- **SRK-Twu**
- **Twu-Sim-Tassone (TST)**
  - Modified equations of state models for hydrocarbon systems-non ideal systems (used for glycol package)
- **Generalized Cubic Equation of State (GCEOS)**
  - Provides a framework which allows users to define and implement their own generalized cubic equation of state including mixing rules and volume translation

Equation of State (3)

- **MBWR**
  - Modified BWR model
  - Having 32 parameters, this model works extremely well with a number of pure components within specified T and P ranges
- **Lee-Kesler-Plöcker**
  - Also a modified BWR model
  - Can be used for non-polar substances and mixtures
- **BWRS**
  - Modified BWR to handle multi components
  - Requires experimental data
- **Zudkevitch Joffee**
  - Modified RK model with better prediction of VLE for hydrocarbon systems, and systems containing hydrogen
- **Kabadi-Danner**
  - Modified SRK model with the enhancement to improve the VLE calculations for H2O-hydrocarbon systems, particularly in dilute regions
- **Sour PR/Sour SRK**
  - Used for sour water systems containing H2S, CO2, and NH3 at low to moderate pressures

Vapor Pressure Models

- **Modified Antoine Model**
  - Applicable for low pressure systems that behave ideally
- **Braun K10 Model**
  - Strictly applicable to heavy hydrocarbon systems at low pressures
- **Esso K Model**
  - Also strictly applicable to heavy hydrocarbon systems at low pressures

Semi-Empirical Models

- **Chao-Seader model**
  - Applicable to hydrocarbon systems in the range of T=0-500C, and P<10,000 kPa

- **Grayson-Streed model**
  - An extension to the Chao-Seader model with special emphasis on H2
  - Recommended for heavy hydrocarbon systems with high H2 content, such as hydrotreating units

Specialty Models (1)

- **Glycol Package**
  - For accurate representation of TEG circulation rates, purities of lean TEG, dew points and the water content of the gas stream used in natural gas dehydration process
- **Clean Fuels**
  - For systems containing thiols and hydrocarbons
- **OLI**
  - For electrolyte systems

Specialty Models (2)

- **Amines Models**
  - For modeling sour system sweetening processes using amines (DEA, TEA, MEA, MDEA, DGA and DIPA)

- **Steam Table Models**
  - **ASME Steam** – ASME 1967 Steam Tables
  - **NBS Steam** – NBS 1984 Steam Tables

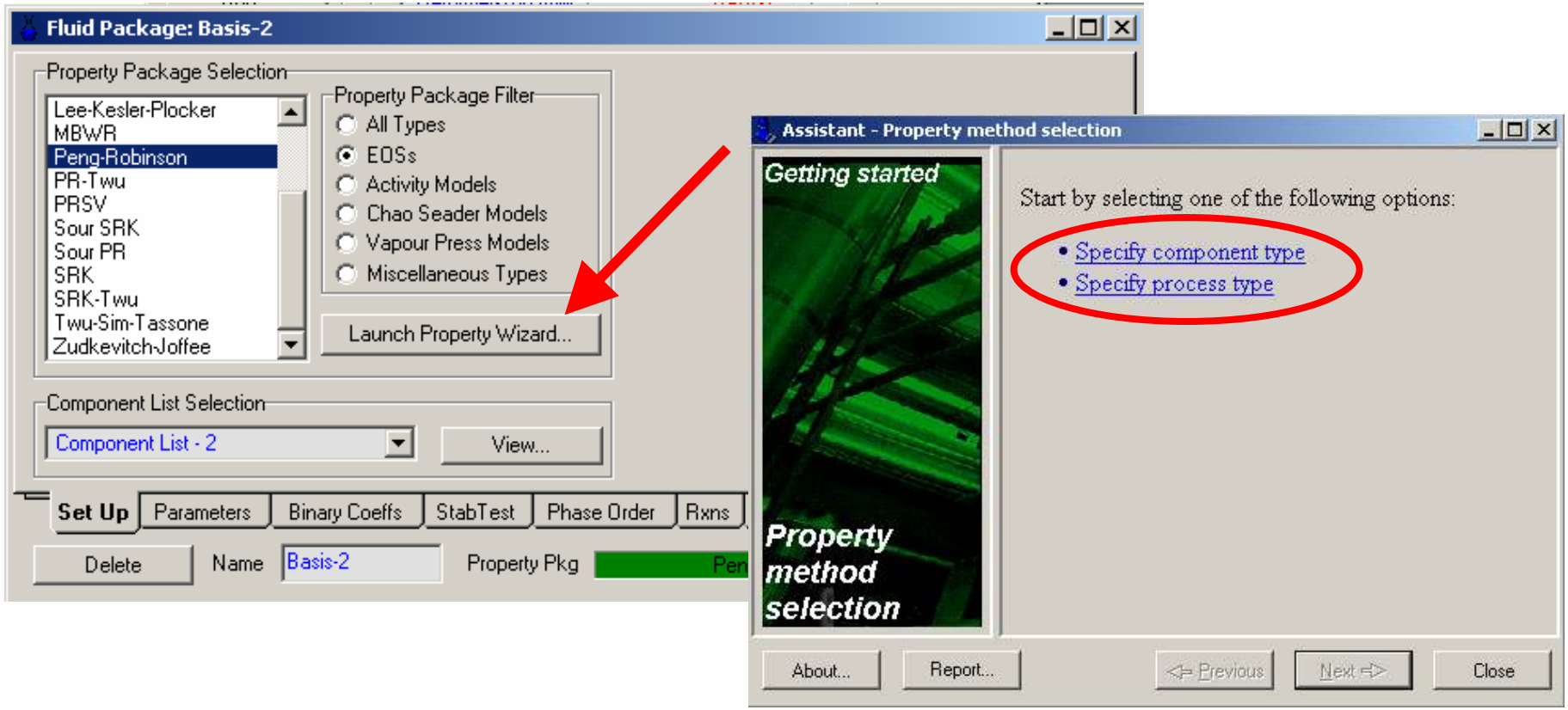
Binary Interaction Parameters (BIP)

- BIPs are needed for each pair
- Aspen HYSYS provides over 16,000 BIPs by default
- BIPs for hypo-components will be estimated based on boiling point and density
- Most of the BIPs are user modifiable, except those receiving special treatment

Thermo Selection Utility (1)

Tool to help you select of the most appropriate thermodynamic method

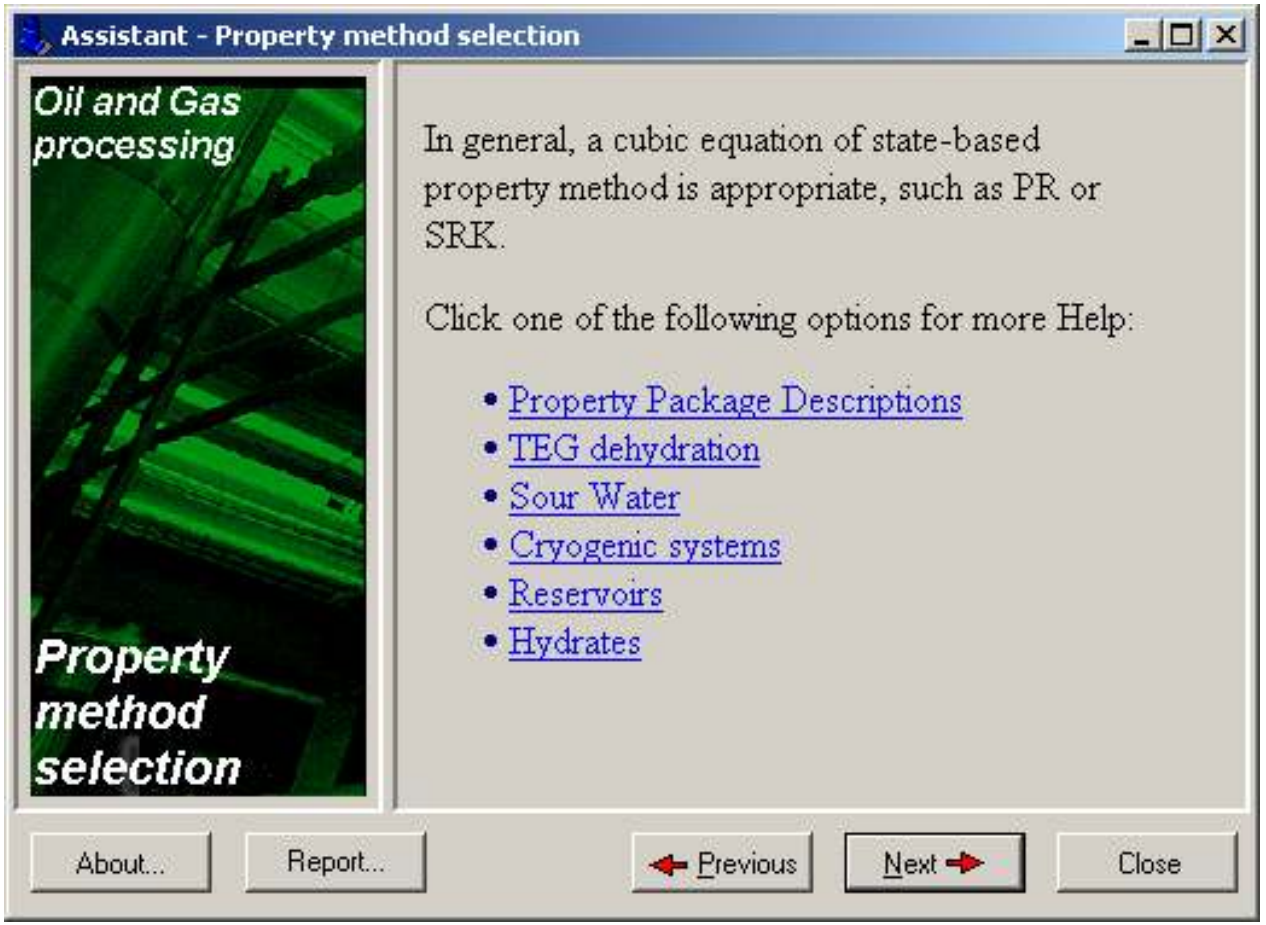
Available only with Version 2006



- Request to enter the components or the application type

Thermo Selection Utility (2)

- It will give a general suggestion of the most appropriate property packages to use.
- It will bring up the HYSYS specific documentation on the thermodynamic method.
- Any detailed question can be verified through AspenTech Technical Support.

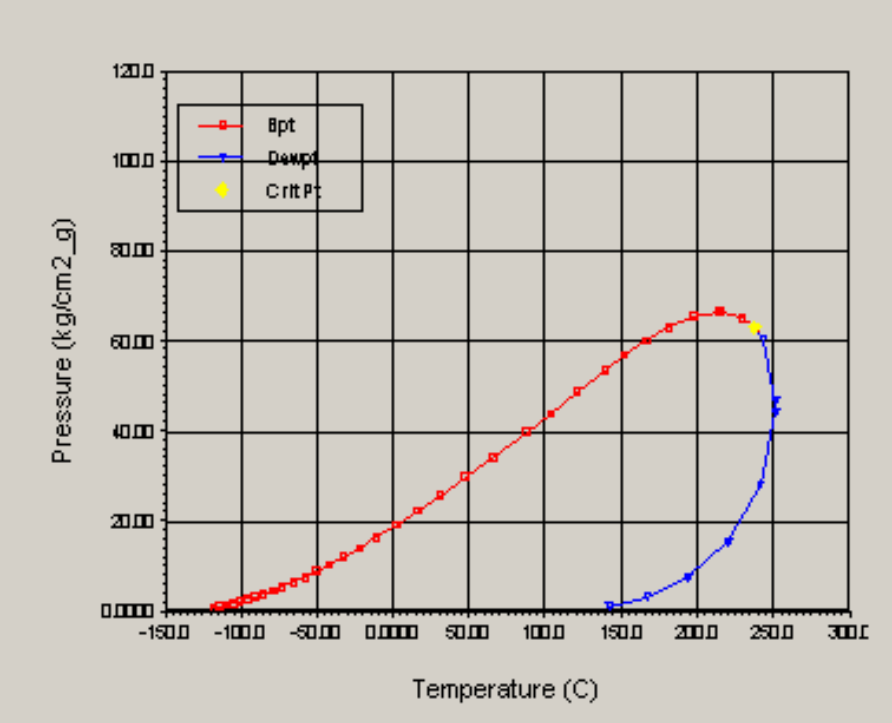


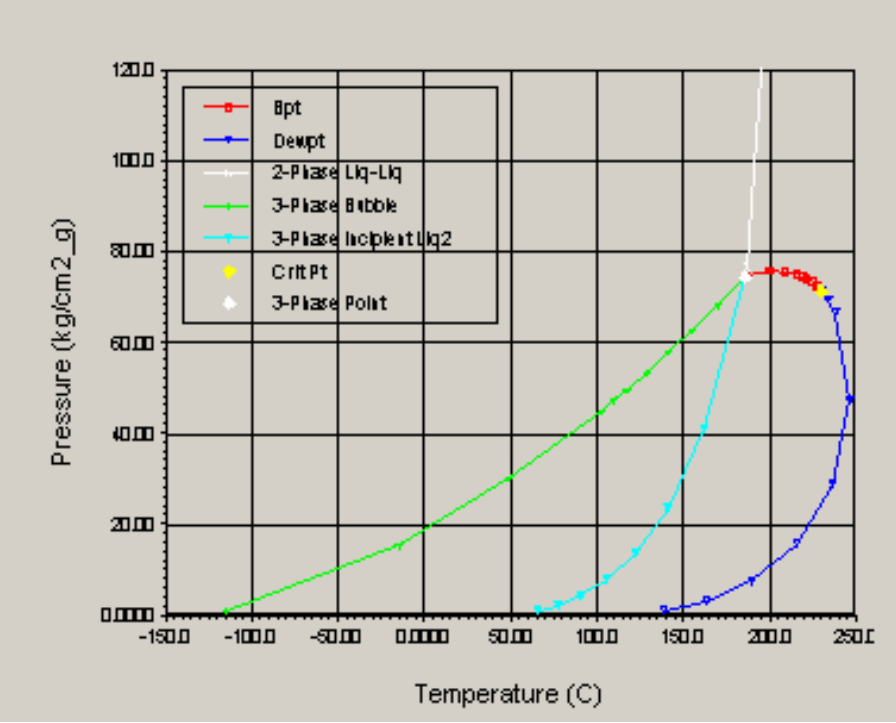
Aspen HYSYS Recommendations
Oil & Gas Applications

- Hydrocarbon systems – PR, SRK or any other EOS*
- Hydrate inhibition – PR (special fit of BIP)
- Natural gas dehydration with TEG – Glycol package
- Sour gas sweetening with amines
- Utility systems using H2O – Steam Table

Hydrocarbon Systems Phase Envelope

- **Two-phase envelope utility**
  - On dry basis (water is ignored)
  - Vapor-Liquid phase equilibrium
- **Three-phase envelope utility**
  - Vapor-Liquid, Liquid-Liquid, Vapor-Liquid-Liquid
  - Associated with COMThermo property package





Amines Models

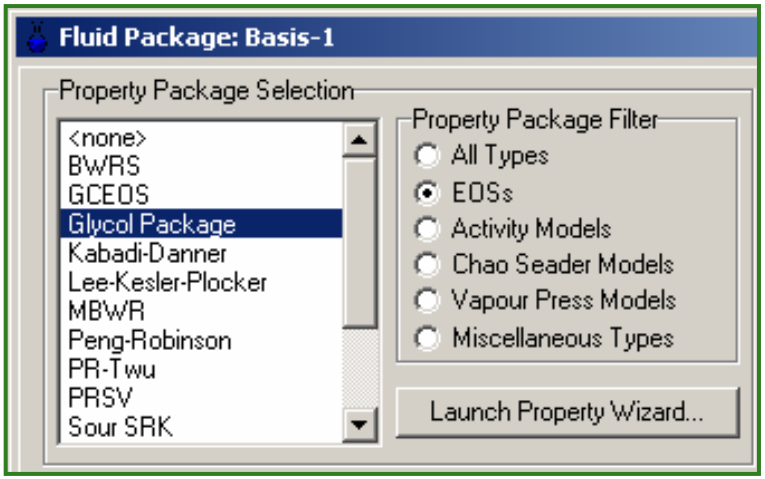
- **Amine Package**
  - Only applicable to the systems containing specified amines in fixed amine concentration, temperature, and pressure ranges

- **DBR Amine Package**
  - Incorporates the latest AMSIM version 7.2 from Schlumberger through COMThermo
    - Kent Eisenberg – Based on regression to experimental data
    - Lee Mather – Based on stronger thermodynamic foundation: recommended
    - Solvents: DEPG

Glycol Package

- **Based on TST Equation of State**
  - Internally combines the equation of state with an interaction coefficients method (NRTL) and …
  - … Some proprietary modifications
  - Adequately predicts phase equilibrium systems containing TEG and water.

- **PR**
  - Still applicable because of its internal fit of BIP's to accurately predict natural gas dehydration absorbers and TEG solutions regeneration.
  - But was giving strange behavior outside normal gas dehydration operating conditions.
  - Use **PR** for MEG and DEG



Aspen HYSYS Recommendations
Refining Applications

- Hydrocarbon systems up to distillate range hypo-components – PR, SRK or any other EOS*
- Vacuum columns – GS, PR or BK10
- Sour gas sweetening with Amines
- Sour water treatment process – Sour PR/SRK
- Clean fuels for sulfur components and hydrocarbons
- High H2 content systems – GS, PR
- Utility systems using H2O – Steam Table

Sour PR or Sour SRK

- Combines the Equation of State with the API Sour Model (Wilson)
- Will accurately predict desorption of H2S, NH3 and CO2 from sour waters
- The only limitation is that it does not report pH or any ionic species in water solution, i.e., CO2, not CO3=, etc.
- Takes into account any change in acidity of water solution, i.e., the addition of NaOH to the system

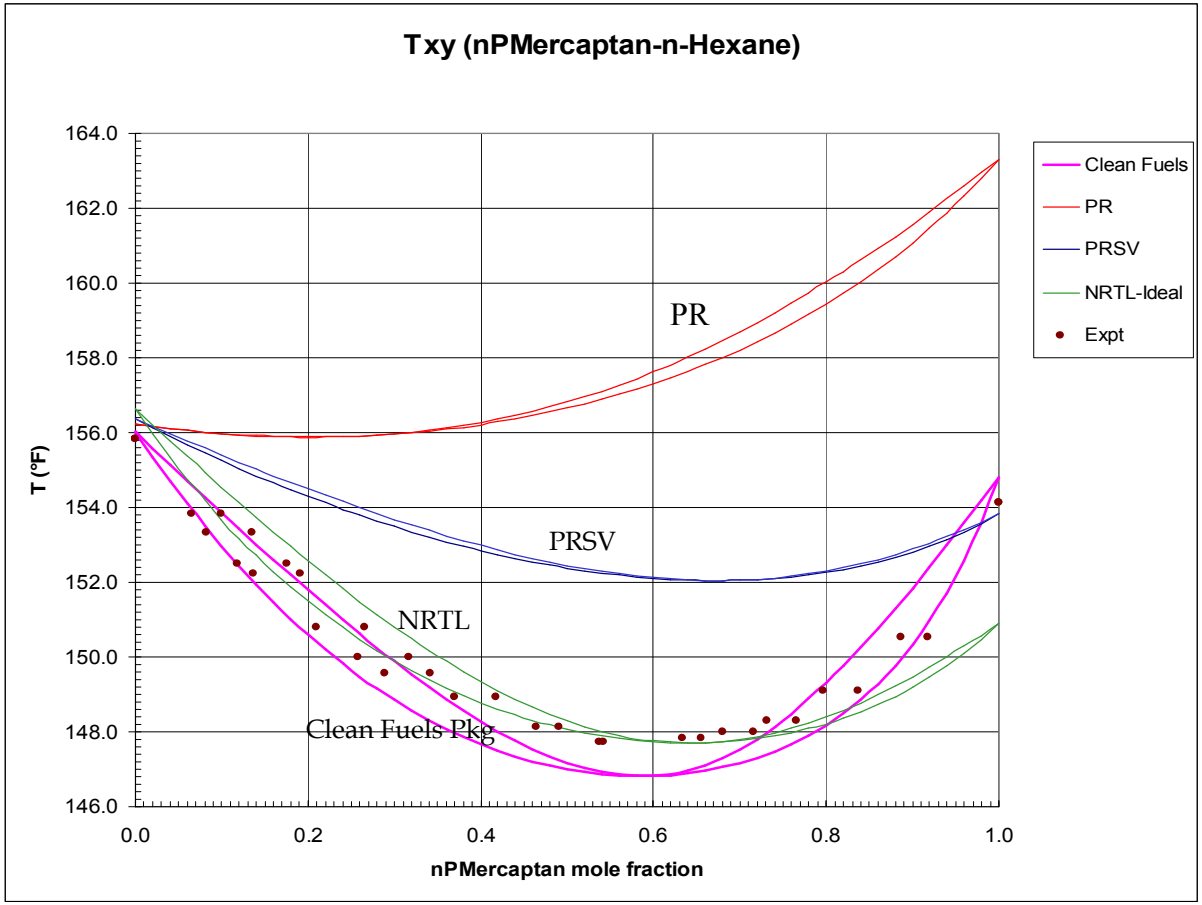
Clean Fuels Package (1)

- Used for FCC Naphtha Fractionation Complexes
- Thermodynamic package for thiols and hydrocarbons
- TST Equation of State with a modified NRTL is used
- 50+ sulphur components with physical properties
- 101 pairs of thiols – hydrocarbon regressed BIPs
- New thiol – hydrocarbon estimation method

Clean Fuels Package (2)

Typical FCC gasoline components distribution and their thermodynamic behavior

	Mass Fractions
2C3Mercaptan	0.000112
nPMercaptan	0.000100
Thiophene	0.000198
i-Butane	0.000733
i-Butene	0.025329
n-Butane	0.004336
i-Pentane	0.074980
1-Pentene	0.093101
2M-13-C4==	0.002759
Cyclopentene	0.004386
3M1C5=	0.004044
Cyclopentane	0.002129
23-Mbutane	0.009610
2-Mpentane	0.057180
2M1C5=	0.006024
1-Hexene	0.023015
n-Hexane	0.011229
NBP[0]122*	0.006781
NBP[0]149*	0.011306
NBP[0]174*	0.035812
NBP[0]195*	0.062678
NBP[0]222*	0.055974
NBP[0]247*	0.057187
NBP[0]273*	0.061747
NBP[0]298*	0.066964
NBP[0]323*	0.066918
NBP[0]347*	0.057256
NBP[0]374*	0.052163
NBP[0]399*	0.057738
NBP[0]420*	0.051857
NBP[0]450*	0.017791
NBP[0]475*	0.018565



Crude and Vacuum Distillation Columns

- **Crude Columns:**
  - **PR (or GS)**
  - Results practically equivalent
- **Vacuum Columns:**
  - **GS, PR, PR Options, BK-10 or Esso Tabular**
  - Product properties and yields will be the equivalent using PR or GS. The temperature profile and duties will be more closely matched with GS
    - Differences in duties of around 5-7%
    - Differences is temperature profile of ± 3ºC

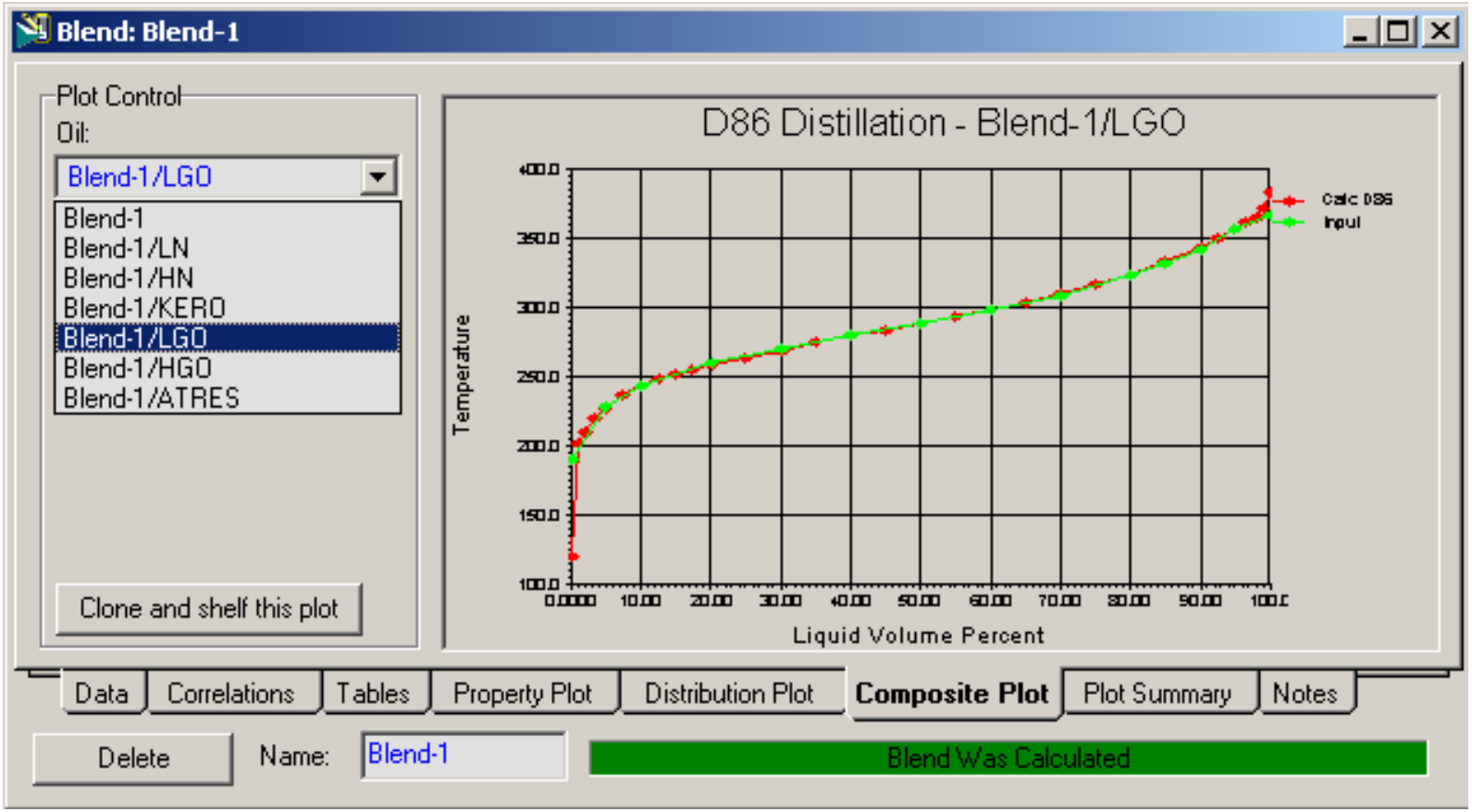
Crude and Vacuum Columns Typical Problems

- Main differences between simulation models and actual unit data rarely comes from bad selection of property package

- Most of the cases differences come from problems during oil characterization
  - Not enough hypo-components
  - Typing mistakes force bad fitting
  - Vacuum laboratory analysis entered as vacuum (laboratory normally reports at atmospheric conditions)
  - Density information not supplied with distillation
  - Not appropriate extrapolation method
  - Etc.

Crude and Vacuum Columns Typical Problems

Always review <u>Composite plots</u> before going to simulation

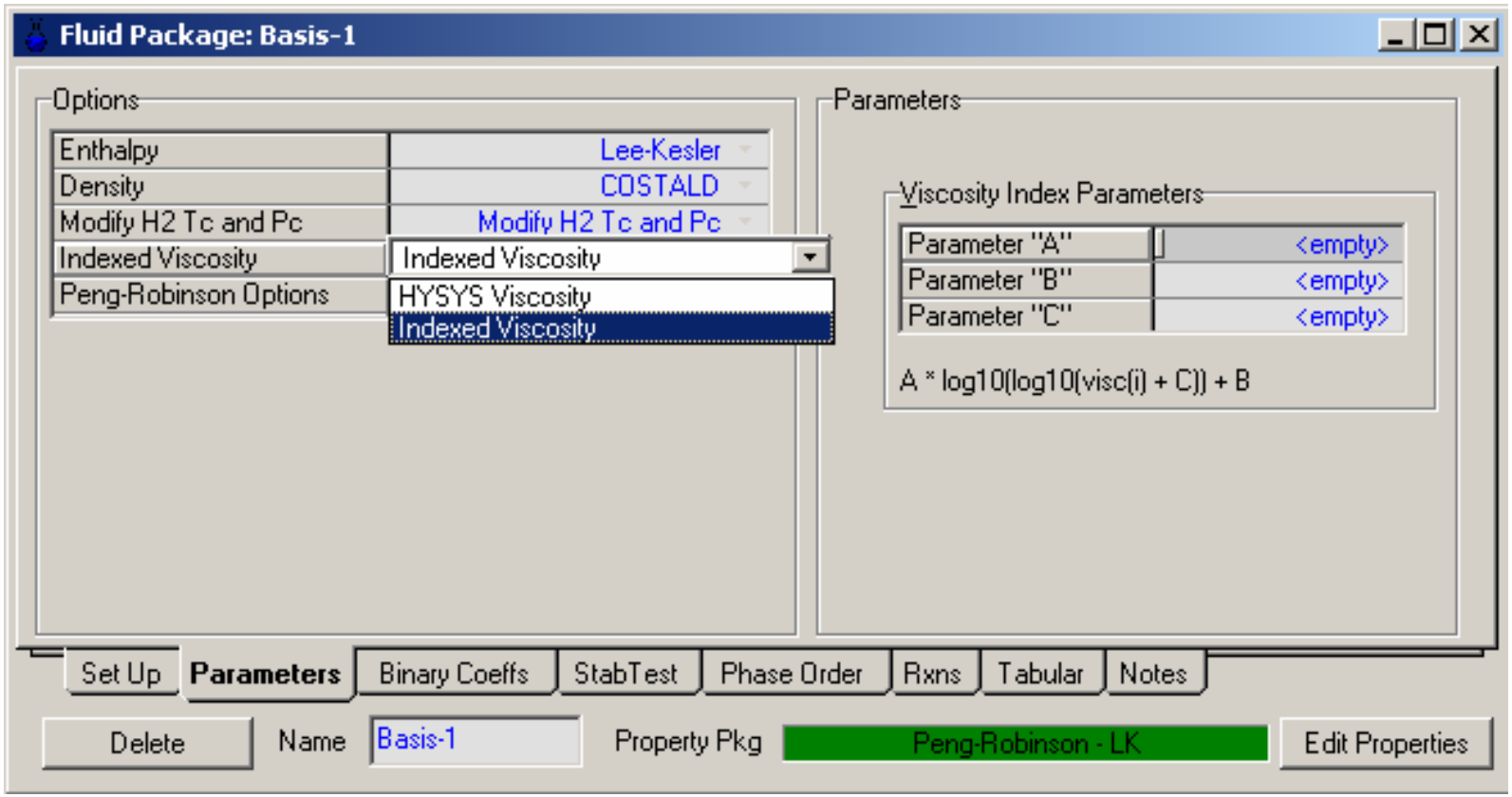


Viscosities for Oil Fractions

- Viscosity predictions always require experimental data for the feed streams.
- Viscosity is a property with an extremely non-linear behavior. Normally, indexed mixing rules are used for calculating viscosities.
- Aspen HYSYS 2006 incorporates the option to index viscosities if accurate prediction of viscosities for heavy streams is required.

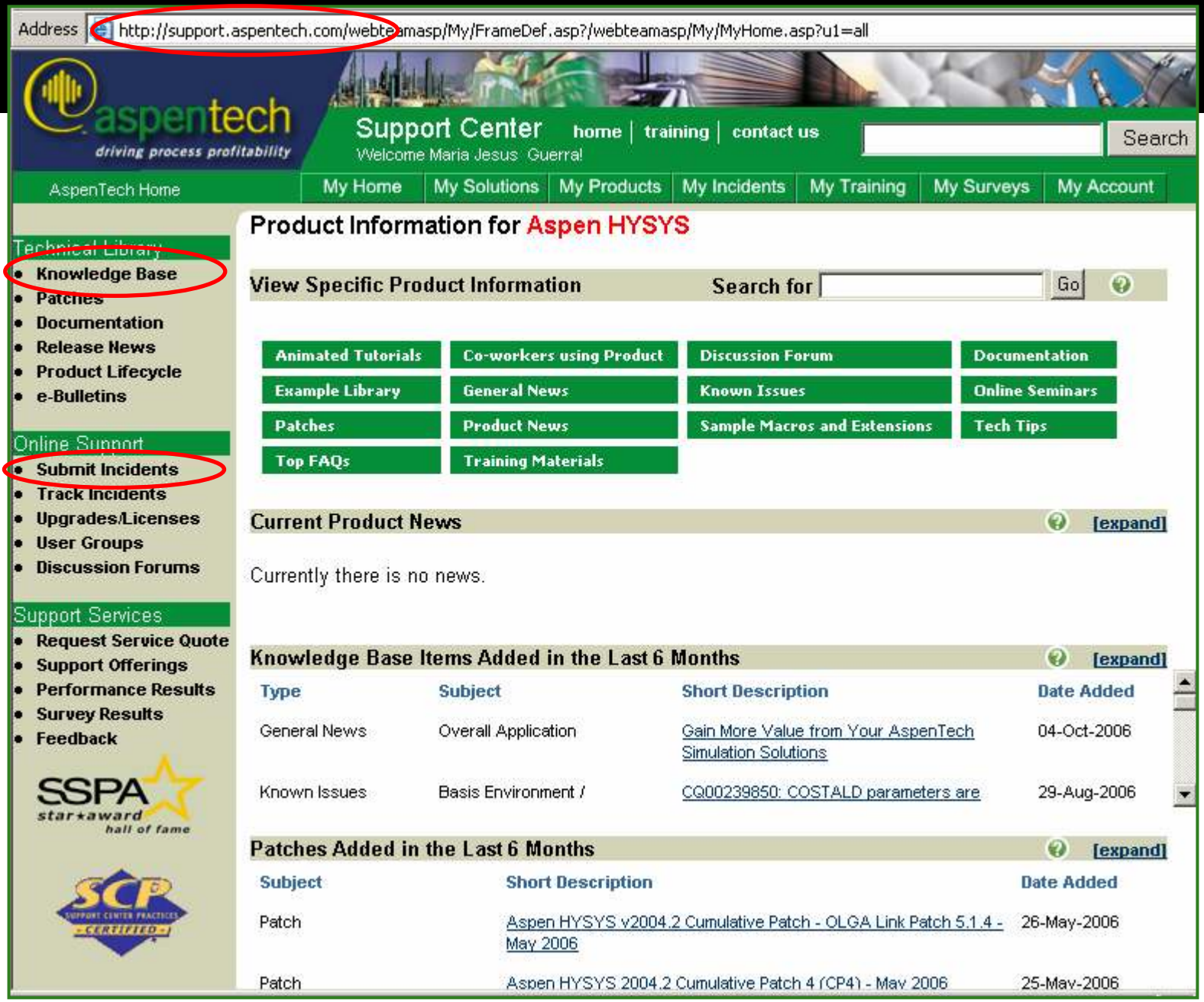
Viscosities for Oil Fractions

- **Use Viscosity Index Parameters:**
  - C = 0.7
  - A and B from experimental data regression (log-log V vs. T)
  - *From Twu and Bulls, Hydrocarbon Processing, 1981*



Aspen HYSYS Property Packages
Summary

- Selection of the appropriate thermodynamic method is key to producing accurate simulations
- PR is the most widely used thermodynamic package as it applies to all applications involving hydrocarbons
- Special packages should be used when simulation involves non-hydrocarbon components: TEG, amines, sour water, etc.
- Methanol for hydrate prevention has special fit of BIPs in PR equation of state
- In refinery models, review oil characterization before suspecting thermodynamics
- Contact AspenTech's Technical Support in case of any questions



AspenTech Online Support Center

aspenONE Process Engineering Webinars

Schedule for next 2 months

Topic	Date & Time
Aspen HYSYS Property Packages: Overview and Best Practices	Oct. 17, 2006 @ 11 am ET (US) ***Today!***
Efficient Engineering Workflow for Process Data Packages: Aspen HYSYS to Aspen Zyqad	Nov. 14, 2006 @ 3 pm ET (US)
Add Value to Aspen HYSYS Models with Rigorous HX Modeling: Aspen HTFS+ Update and Integration of Aspen Tasc+ and Acol+ with HYSYS	Dec. 12, 2006 @ 11 am ET (US)

To Register:
www.aspentech.com/webseminars/webseminars.cfm

aspenONE Process Engineering

On-Demand Webinars (Recordings of Recent Webinars)

Topic	Date
Develop and Evaluate Cost Effective Conceptual Designs: Integrate Aspen HYSYS Models with and Aspen Icarus Process Evaluator (IPE) to Quickly Evaluate Design Options with Consistent Cost Estimates	Sep. 26, 2006
Aspen Simulation Workbook: Integrate Simulation Models with Excel Leverage the Value of Simulation Models across Your Enterprise	Sep. 12, 2006
Aspen HYSYS Upstream Overview: Optimize O&G Asset Performance with Integrated Production and Facilities Modeling	August 29, 2006
Improve Safety, Reliability and Operability: Dynamic Modeling with Aspen HYSYS Dynamics	August 16, 2006
Maximize Your Flare System Efficiency: Evaluate your flare systems for revamps and expansions with Aspen Flarenet	July 18, 2006
Enhancing Refinery Models with Aspen RefSYS: Advanced Refinery Simulation for Integrating Process Modeling and Planning	June 8, 2006
Modeling Distillation Columns in Aspen HYSYS: Use Process Models to Make Better Decisions	May 9, 2006

- Available on AspenTech's eSupport Site to Registered Users
- http://support.aspentech.com
- Recordings of other topics are also available

Aspen HYSYS Property Packages

Overview and Best Practices for Optimum Simulations

- **Q & A**
- **For more information, contact support:**
  - http://support.aspentech.com
  - eSupport@aspentech.com
  - North America: +1 888 996 7100, press 4 then 2
  - Europe: +32 2 701 95 55
  - Your host: sanjeev.mullick@aspentech.com
  - Your presenter: maria.guerra@aspentech.com
- **Additional References:**
  - Aspen HYSYS Insight Newsletters
  - http://www.aspentech.com/newsletter/aspen_hysys_insights_june_2006.html
  - http://www.aspentech.com/newsletter/aspen_hysys_insights_august_2006.html
  - Next issue: October 31, 2006
- **Suggestions and feedback:** aspenHYSYS.Innovation@aspentech.com
- **For more info on Aspen HYSYS:** www.aspentech.com/hysys