Property Package Descriptions

Equations of State (EOS)

Equation of State models have proven to be very reliable in predicting the properties of most hydrocarbon based fluids over a wide range of operating conditions. Their application focuses on primarily non-polar or slightly polar components.

GCEOS

The GCEOS model allows you to define and implement your own generalized cubic equation of state including mixing rules and volume translation.

Kabadi Danner

The Kabadi Danner model is a modification of the original SRK equation of state, enhanced to improve the vapour-liquid-liquid equilibria calculations for water-hydrocarbon systems, particularly in dilute regions.

The model is an improvement over previous attempts which were limited in the region of validity. The modification is based on an asymmetric mixing rule, whereby the interaction in the water phase (with its strong H_2 bonding) is calculated based on both the interaction between the hydrocarbons and the H_2O, and on the perturbation by hydrocarbon on the H_2O-H_2O interaction (due to its structure).

The Kabadi Danner model uses the Kabadi Danner method to calculate VLE and uses SRK to calculate Enthalphy and Entropy.

Lee-Kessler Plocker

The Lee-Kesler Plocker model is the most accurate general method for non-polar substances and mixtures and is recommended for Ethylene Towers. LKP uses the Lee-Kesler-Plocker method to calculate VLE and uses the Lee Kesler method to calculate Enthalpy and Entropy.

Plöcker applied the Lee Kesler equation to mixtures, which itself was modified from the BWR equation.

Peng-Robinson

The Peng-Robinson (PR) model is ideal for VLE calculations as well as calculating liquid densities for hydrocarbon systems. Several enhancements to the original PR model were made to extend its range of applicability and to improve its predictions for some non-ideal systems. However, in situations where highly non-ideal systems are encountered, the use of Activity Models is recommended.

The PR property package rigorously solves any single-, two-, or three-phase system with a high degree of efficiency and reliability and is applicable over a wide range of conditions:

- Temperature Range > -271°C or -456°F
- Pressure Range < 100,000 kPa or 15,000 psia

The PR property package also contains enhanced binary interaction parameters for all library hydrocarbon-hydrocarbon pairs (a combination of fitted and generated interaction parameters), as well as for most hydrocarbon-non-hydrocarbon binaries. For non-library or hydrocarbon hypocomponents, HC-HC interaction parameters are generated automatically by HYSYS for improved VLE property predictions.

For Oil, Gas, or Petrochemical applications, the PR EOS is the generally recommended property package. The PR property package is generally used for the following simulations:

- TEG Dehydration
- TEG Dehydration with Aromatics
- Cryogenic Gas Processing
- Air Separation
- Atm Crude Towers
- Vacuum Towers
- High H2 Systems
- Reservoir Systems
- Hydrate Inhibition
- Crude Systems

PRSV

The PRSV model is a two-fold modification of the Peng-Robinson equation of state that extends the application of the original Peng-Robinson method for moderately non-ideal systems. This EOS is shown to match vapour pressures curves of pure components and mixtures more accurately than the PR method, especially at low vapour pressures. It is successfully extended to handle non-ideal systems giving results as good as those obtained using excess Gibbs energy functions like the Wilson, NRTL, or UNIQUAC equations.

The advantages of the PRSV equation are:

- It has the potential to more accurately predict the phase behaviour of hydrocarbon systems, particularly for systems composed of dissimilar components.
- It can be extended to handle non-ideal systems with accuracies that rival traditional activity coefficient models.

The only compromise for PRSV equation of state is the increased computational time and the additional interaction parameter that is required for the equation.

The PRSV equations of state perform rigorous three-phase flash calculations for aqueous systems containing H2O, CH3OH or glycols, as well as systems containing other hydrocarbons or non-hydrocarbons in the second liquid phase.

The PRSV property package generally used in the following simulations:

- Cryogenic Gas Processing
- Air Separation
- Chemical systems

- HF Alkylation

SRK

In many cases, the Soave-Redlich-Kwong (SRK) model provides comparable results to Peng-Robinson, but its range of application is significantly more limited:

- Temperature Range > -143°C or -225°F

- Pressure Range < 5,000 kPa or 35,000 psia

The SRK EOS should not be used for non-ideal chemicals such as alcohols, acids or other components. These chemicals are more accurately handled by the Activity Models (highly non-ideal) or the PRSV EOS (moderately non-ideal).
The SRK property package is generally used for the following simulations:

- TEG Dehydration
- Sour Water
- Cryogenic Gas Processing
- Air Separation
- Atm Crude Towers
- Vacuum Towers
- High H2 Systems
- Reservoir Systems
- Hydrate Inhibition
- Chemical systems
- HF Alkylation
- TEG Dehydration with Aromatics

The proprietary enhancements to the SRK property package allow the SRK equation of state (EOS) to correctly represent vacuum conditions and heavy components (a problem with traditional EOS methods), as well as handle the light ends and high-pressure systems.
The SRK property package contains enhanced binary interaction parameters for all library hydrocarbon-hydrocarbon pairs (a combination of fitted and generated interaction parameters), as well as for most hydrocarbon-nonhydrocarbon binaries. For non-library or hydrocarbon hypocomponent, HC-HC interaction parameters are generated automatically by HYSYS for improved VLE property predictions.

Sour PR

The Sour PR model combines the Peng-Robinson equation of state and Wilson's API-Sour Model for handling sour water systems and can be applied to sour water strippers, hydrotreater loops, crude columns, or any process containing hydrocarbons, acid gases, and H_2O.
In the Sour PR model, the K-values for the aqueous phase are calculated using Wilson's API-Sour method. This option uses Wilson's model to account for the ionization of the H_2S, CO_2, and NH_3 in the aqueous water phase. The aqueous model employs a

modification of Van Krevelen's original model with many of the key limitations removed. The K-value of water is calculated using an empirical equation, which is a function of temperature only.

The original model is applicable for temperatures between 20°C (68°F) and 140°C (285°F), and pressures up to 50 psi. Use of the PR equation of state to correct vapour phase non idealities extends this range, but due to lack of experimental data, exact ranges cannot be specified. The acceptable pressure ranges for the HYSYS model vary depending upon the concentration of the acid gases and H_2O. The method performs well when the H_2O partial pressure is below 100 psi.
Note: The flash calculation is much slower than the standard EOS because the method performs an ion balance for each K-value calculation.

More details of the model are available in the original API publication 955 titled "A New Correlation of NH_3, CO_2, and H_2S Volatility Data from Aqueous Sour Water Systems."

Sour SRK
The Sour SRK model combines the Soave Redlich Kwong and Wilson's API-Sour Model and can be be applied to sour water strippers, hydrotreater loops, crude columns, or any process containing hydrocarbons, acid gases, and H_2O.
This option uses Wilson's model to account for the ionization of the H_2S, CO_2, and NH_3 in the aqueous water phase. The aqueous model employs a modification of Van Krevelen's original model with many of the key limitations removed. The K-value of water is calculated using an empirical equation, which is a function of temperature only.

The original model is applicable for temperatures between 20°C (68°F) and 140°C (285°F), and pressures up to 50 psi. Use of the SRK equation of state to correct vapour phase non idealities extends this range, but due to lack of experimental data, exact ranges cannot be specified. The acceptable pressure ranges for the HYSYS model vary depending upon the concentration of the acid gases and H2O. The method performs well when the H2O partial pressure is below 100 psi.

Note: The flash calculation is much slower than the standard EOS because the method performs an ion balance for each K-value calculation.

More details of the model are available in the original API publication 955 titled "A New Correlation of NH_3, CO_2, and H_2S Volatility Data from Aqueous Sour Water Systems."

Zudkevitch Joffee
The Zudkevitch Joffee model is a modification of the Redlich Kwong equation of state. This model has been enhanced for better prediction of vapour-liquid equilibria for hydrocarbon systems, and systems containing Hydrogen. The major advantage of this model over the previous version of the RK equation is the improved capability of predicting pure component equilibria, and the simplification of the method for determining the required coefficients for the equation.
Enthalpy calculations for this model are performed using the Lee-Kesler model.

The Zudkevitch Joffee property package is generally used for High H_2 Systems.

BWRS
The Benedict-Webb-Rubin-Starling (BWRS) model is commonly used for compression applications and studies. It is specifically used for gas phase components that handle the complex thermodynamics that occur during compression, and is useful in both upstream and downstream industries.

The BWRS EOS calculates fugacity coefficients, enthalpy departure, entropy departure, and molar volume for both the vapour and the liquid phases. This EOS is a modification of the BWR EOS and uses eleven compound-specific coefficients along with binary interaction parameters.

The BWRS property package uses 11 pure-component parameters:

- B0   · A0
- C0   · Gamma
- b   · a
- alpha   · c
- D0   · D
- E0

Coefficients and binary interaction parameters are available for 15 compounds that are built-in to the property package and stored in the database.

- Methane   · I-Pentane
- Ethane   · n-Pentane
- Propane   · n-Hexane
- I-Butane   · n-Heptane
- n-Butane   · n-Octane
- N_2 · Ethylene
- CO_2 · Propylenen
- H_2S

These coefficients are obtained from multiproperty (vapor-liquid-equilibrium, enthalpy, PVT, etc.) data regressions. Coefficients for chemicals common to natural gas mixtures are available from Starling (K. E. Starling, "Fluid Themodynamic Properties for Light Petroleum Systems", Gulf Publishing Co., Houston, Texas (1973).). If pure-component coefficients are not supplied, they are automatically estimated using Tc, Vc and acentric factor with Han-Starling correlations proposed by Starling, or you can enter your own coefficients for each compound. Any compound without the coefficients will not be allowed in the Fluid Package.

Activity Models

The Activity Models handle highly non-ideal systems and are much more empirical in nature when compared to the property predictions in the hydrocarbon industry. Polar or non-ideal chemical systems are traditionally handled using dual model approaches. In this type of approach, an equation of state is used for predicting the vapour fugacity coefficients and an activity coefficient model is used for the liquid phase. Since the experimental data for activity model parameters are fitted for a specific range, these property methods cannot be used as reliably for generalized application.

Chien Null

The Chien Null model provides a consistent framework for applying existing Activity Models on a binary by binary basis. It allows you to select the best Activity Model for each pair in your case through the A, B, and C coefficient matrices.
The Chien Null property package is generally used for chemical systems with highly non-ideal chemicals.
Chien Null uses the following calculation methods:

For liquid:

- Chien Null method for VLE
- Cavett method for Enthalpy and Entropy

For vapour:

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for VLE
- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for Enthalpy and Entropy

Extended NRTL

The Extended NRTL is a variation of the NRTL model, allowing you to input values for the Aij, Bij, Cij, Alp1ij and Alp2ij parameters used in defining the component activity coefficients.
Apply this model to systems:

- with a wide boiling point range between components
- where you require simultaneous solution of VLE and LLE, and there exists a wide boiling point range or concentration range between components

Extended NRTL uses the following calculation methods:

For liquid:

- NRTL method for VLE
- Cavett method for Enthalpy and Entropy

For vapour:

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for VLE
- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for Enthalpy and Entropy

The Extended NRTL model enables you to enter values for the matrices of the Aij, Bij, Cij, Alp1ij and Alp2ij energy parameters.

General NRTL

This variation of the NRTL model allows you to select the equation format for equation parameters: t and x
Apply this model to systems:

- with a wide boiling point range between components
- where you require simultaneous solution of VLE and LLE, and there exists a wide boiling point or concentration range between components

General NRTL uses the following calculation methods:

For liquid:

- NRTL method for VLE
- Cavett method for Enthalpy and Entropy

For vapour:

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for VLE
- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for Enthalpy and Entropy

Margules

The Margules model was the first Gibbs excess energy representation developed. The equation does not have any theoretical basis, but is useful for quick estimates and data interpolation. HYSYS has an extended multicomponent Margules equation with up to four adjustable parameters per binary.
Margules uses the following calculation methods:

For liquid:

- Margules method for VLE
- Cavett method for Enthalpy and Entropy

For vapour:

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for VLE

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for Enthalpy and Entropy

Note: The equation should not be used for extrapolation beyond the range over which the energy parameters are fitted.

The four adjustable parameters for the Margules equation in HYSYS are the aij, aji (temperature independents), bij, and bji (temperature dependents). The equation uses parameter values stored in HYSYS or any user supplied value for further fitting the equation to a given set of data.

NRTL

The Non-Random-Two-Liquid (NRTL) equation is an extension of the Wilson equation. It uses statistical mechanics and the liquid cell theory to represent the liquid structure. It is capable of representing VLE, LLE, and VLLE phase behaviour.
The NRTL property package is used for chemical systems and HF Alkylation with highly non-ideal chemicals.
NRTL uses the following calculation methods:

For liquid:

- NRTL method for VLE
- Cavett method for Enthalpy and Entropy

For vapour:

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for VLE
- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for Enthalpy and Entropy

Like the Wilson equation, the NRTL is thermodynamically consistent and can be applied to ternary and higher order systems using parameters regressed from binary equilibrium data. It has an accuracy comparable to the Wilson equation for VLE systems.
The NRTL equation in HYSYS contains five adjustable parameters (temperature dependent and independent) for fitting per binary pair. The NRTL combines the advantages of the Wilson and van Laar equations.

- Like the van Laar equation, NRTL is not extremely CPU intensive and can represent LLE quite well.

- Unlike the van Laar equation, NRTL can be used for dilute systems and hydrocarbon-alcohol mixtures, although it may not be as good for alcohol-hydrocarbon systems as the Wilson equation.

- The five adjustable parameters for the NRTL equation in HYSYS are the aij, aji, bij, bji, and aij terms.

Note: Due to the mathematical structure of the NRTL equation, it can produce erroneous multiple miscibility gaps.

The equation uses parameter values stored in HYSYS or any user supplied value for further fitting the equation to a given set of data.

UNIQUAC

The UNIversal QUAsi Chemical (UNIQUAC) equation uses statistical mechanics and the quasi-chemical theory of Guggenheim to represent the liquid structure. The equation is capable of representing LLE, VLE, and VLLE with accuracy comparable to the NRTL equation, but without the need for a non-randomness factor.
UNIQUAC uses the following calculation methods:

For liquid:

- UNIQUAC method for VLE
- Cavett method for Enthalpy and Entropy

For vapour:

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for VLE
- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for Enthalpy and Entropy

The UNIQUAC equation is significantly more detailed and sophisticated than any of the other activity models. Its main advantage is that a good representation of both VLE and LLE can be obtained for a large range of non-electrolyte mixtures using only two adjustable parameters per binary. The fitted parameters usually exhibit a smaller temperature dependence which makes them more valid for extrapolation purposes.
The UNIQUAC equation utilizes the concept of local composition as proposed by Wilson. Since the primary concentration variable is a surface fraction as opposed to a mole fraction, it is applicable to systems containing molecules of very different sizes and shape, such as polymer solutions. The UNIQUAC equation can be applied to a wide range of mixtures containing H_2O, alcohols, nitriles, amines, esters, ketones, aldehydes, halogenated hydrocarbons, and hydrocarbons.

HYSYS contains the following four-parameter extended form of the UNIQUAC equation. The four adjustable parameters for the UNIQUAC equation in HYSYS are the aij, aji (temperature independents), bij, and bji (temperature dependents).

Van Laar

The van Laar equation fits many systems, particularly for LLE component distributions. It can be used for systems that exhibit positive or negative deviations from Raoult's Law; however, it cannot predict maxima or minima in the activity coefficient. Therefore it generally performs poorly for systems with halogenated hydrocarbons and alcohols.

The van Laar property package uses the following calculation methods:

For liquid:

- van Laar method for VLE
- Cavett method for Enthalpy and Entropy

For vapour:

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for VLE
- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for Enthalpy and Entropy

The van Laar property package is used for chemical systems with highly non-ideal chemicals.

The van Laar equation was the first Gibbs excess energy representation with physical significance. The van Laar equation in HYSYS is a modified form described in "Phase Equilibrium in Process Design" by H.R. Null.

Note: Due to the empirical nature of the equation, caution should be exercised in analyzing multi-component systems. It also has a tendency to predict two liquid phases when they do not exist. The van Laar equation also performs poorly for dilute systems and cannot represent many common systems, such as alcohol-hydrocarbon mixtures, with acceptable accuracy.

The van Laar equation has some advantages over the other activity models in that it requires less CPU time and can represent limited miscibility as well as three phase equilibrium. HYSYS uses the following extended, multi-component form of the van Laar equation.

The four adjustable parameters for the van Laar equation in HYSYS are the aij, aji, bij, and bji terms. The equation will use parameter values stored in HYSYS or any user supplied value for further fitting the equation to a given set of data.

Wilson
The Wilson equation is the first activity coefficient equation to use the local composition model to derive the Gibbs Excess energy expression. It offers a thermodynamically consistent approach to predicting multi-component behaviour from regressed binary equilibrium data. However, the Wilson model cannot be used for systems with two liquid phases.
The Wilson property package is used for chemical systems with highly non-ideal chemicals.
Wilson uses the following calculation methods:

For liquid:

- Wilson method for VLE
- Cavett method for Enthalpy and Entropy

For vapour:

- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for VLE
- Ideal Gas, RK, Virial, Peng Robinson, and SRK methods for Enthalpy and Entropy

Although the Wilson equation is more complex and requires more CPU time than either the van Laar or Margules equations, it can represent almost all non-ideal liquid solutions satisfactorily except electrolytes and solutions exhibiting limited miscibility (LLE or VLLE). It performs an excellent job of predicting ternary equilibrium using parameters regressed from binary data only.

The Wilson equation gives similar results as the Margules and van Laar equations for weak non-ideal systems, but consistently outperforms them for increasingly non-ideal systems.

The Wilson equation in HYSYS requires two to four adjustable parameters per binary. The four adjustable parameters for the Wilson equation in HYSYS are the a_{ij} and a_{ji} (temperature independent) terms, and the b_{ij} and b_{ji} (temperature dependent) terms. Depending upon the available information, the temperature dependent parameters may be set to zero.

Note: Setting all four parameters to zero does not reduce the binary to an ideal solution, but maintains a small effect due to molecular size differences represented by the ratio of molar volumes.

The equation uses parameter values stored in HYSYS or any user supplied value for further fitting the equation to a given set of data.

Chao Seader & Grayson Streed Models

The Chao Seader and Grayson Streed methods are older, semi-empirical methods. The Grayson Streed correlation is an extension of the Chao Seader method with special emphasis on hydrogen. Only the equilibrium data produced by these correlations is used by HYSYS. The Lee-Kesler method is used for liquid and vapour enthalpies and entropies.

Chao Seader

Use the Chao Seader (CS) method for heavy hydrocarbons, where the pressure is less than 10342 kPa (1500 psia), and temperatures range between -17.78 and 260°C (0-500°F).
The CS property package is used for the steam systems. The CS property package can also be used for three-phase flashes, but is restricted to the use of pure H_2O for the second liquid phase.
The CS method, though limited in scope, may be preferred in some instances. For example, CS is recommended for problems containing mainly liquid or vapour H_2O because the property package includes special correlations that accurately represent the steam tables.

The following tables give an approximate range of applicability for CS method and under what conditions CS is applicable.

Method	Temp (°F)	Temp (°C)	Press (psia)	Press (kPa)
CS	0 to 500	-18 to 260	<1,500	<10,000

Conditions of Applicability:

For all hydrocarbons (except CH4):	$0.5<Tri<1.3$ and Prmixture <0.8
If CH_4 or H_2 is present:	molal average Tr <0.93
	CH4 mole fraction <0.3
	mole fraction dissolved gases <0.2

When predicting K values for:
Paraffinic or Olefinic Mixtures	liquid phase aromatic mole fraction <0.5
Aromatic Mixtures	liquid phase aromatic mole fraction >0.5

Chao-Seader (CS) uses the CS-RK method for calculating VLE and the Lee Kesler method for calculating Enthalpy and Entropy.
The vapour phase fugacity coefficients are calculated with the Redlich Kwong equation of state. The pure liquid fugacity coefficients are calculated using the principle of corresponding states. Special functions are incorporated for the calculation of liquid phase fugacities for N_2, CO_2 and H_2S. These functions are restricted to hydrocarbon mixtures with less than five percent of each of the above components.

As with the Vapour Pressure models, H_2O is treated using a combination of the steam tables and the kerosene solubility charts from the API Data Book. This method of handling H_2O is not very accurate for gas systems. Although three phase calculations are performed for all systems, it is important to note that the aqueous phase is always treated as pure H_2O with these correlations.

Grayson Streed

The GS correlation is an extension of the Chao-Seader method with special emphasis on H_2. Only the equilibrium results produced by these correlations are used by HYSYS. The Grayson-Streed correlation is recommended for use with systems having a high concentration of H_2 because of the special treatment given H_2 in the development of the model. The GS correlation can also be used for simulating topping units and heavy ends vacuum applications. This correlation may also be slightly more accurate in the simulation of vacuum towers.

The Grayson-Streed (GS) property package can be used for three-phase flashes, but is restricted to the use of pure H_2O for the second liquid phase.

The following tables gives an approximate range of applicability for the GS method and under what conditions the method is applicable:

Method	Temp (°F)	Temp (°C)	Press (psia)	Press (kPa)
GS	0 to 800	-18 to 425	<3,000	<20,000

Conditions of Applicability:

For all hydrocarbons (except CH_4): $0.5<Tri<1.3$ and Prmixture <0.8

If CH_4 or H_2 is present:
molal average Tr <0.93
CH_4 mole fraction <0.3
mole fraction dissolved gases <0.2

When predicting K values for:
Paraffinic or Olefinic Mixtures
liquid phase aromatic mole fraction <0.5
Aromatic Mixtures
liquid phase aromatic mole fraction >0.5

Grayson-Streed (GS) uses the GS-RK to calculate VLE and Lee-Kesler to calculate Enthalpy and Entropy.

The vapour phase fugacity coefficients are calculated with the Redlich Kwong equation of state. The pure liquid fugacity coefficients are calculated using the principle of corresponding states. Modified acentric factors are included in HYSYS' GS library for most components. Special functions are incorporated for the calculation of liquid phase fugacities for N_2, CO_2, and H_2S. These functions are restricted to hydrocarbon mixtures with less than five percent of each of the above components.

As with the Vapour Pressure models, H_2O is treated using a combination of the steam tables and the kerosene solubility charts from the API Data Book. This method of handling H_2O is not very accurate for gas systems. Although three phase calculations are performed for all systems, it is important to note that the aqueous phase is always treated as pure H_2O with these correlations.

Vapour Pressure Models

Vapour Pressure K-value models may be used for ideal mixtures at low pressures. Ideal mixtures include hydrocarbon systems and mixtures such as ketones and alcohols, where the liquid phase behaviour is approximately ideal. These equations are traditionally applied for heavier hydrocarbon fractionation systems and consequently provide a good means of comparison against rigorous models. The models may also be used as first approximations for non-ideal systems. They should not be considered for VLE (VAPOUR LIQUID EQUILIBRIUM) predictions for systems operating at high pressures or systems with significant quantities of light hydrocarbons.

Antoine

The Antoine model is applicable for low pressure systems that behave ideally. The equations are traditionally applied for heavier hydrocarbon fractionation systems and consequently provide a good means of comparison against rigorous models. They should not be considered for VLE predictions for systems operating at high pressures or systems with significant quantities of light hydrocarbons.

Antoine property package is applicable to the following ranges:

Temperature	Press (psia)	Press (kPa)
<1.6 Tci	<100	<700

The modified Antoine equation assumes the form as set out in the DIPPR data bank.

$$\ln P_{vap} = A + \frac{B}{T + C} + D \ln T + E T^F$$

Where:
A, B, C, D, E, F = fitted coefficients
Pvap = the pressure in kPa
T = the temperature in K

These coefficients are available for all HYSYS library components. Vapour pressure coefficients for hypocomponent can be entered or calculated from either the Lee-Kesler correlation for hydrocarbons, the Gomez-Thodos correlation for chemical compounds, or the Reidel equation.
All enthalpy and entropy calculations are performed using the Lee-Kesler model.
This model is applicable for low pressure systems that behave ideally. For hydrocarbon components that you have not provided vapour pressure coefficients for, the model converts the Lee-Kesler vapour pressure model directly. As such, crude and vacuum towers can be modeled with this equation.

When using this method for super-critical components, it is recommended that the vapour pressure coefficients be replaced with Henry's Law coefficients. Changing Vapour

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Pressure coefficients can only be accomplished if your component is being installed as a Hypothetical.

Braun K10

The Braun K10 model is strictly applicable to heavy hydrocarbon systems at low pressures. The model employs the Braun convergence pressure method, where, given the normal boiling point of a component, the K-value is calculated at system temperature and 10 psia (68.95 kPa). The K10 value is then corrected for pressure using pressure correction charts. The K values for any components that are not covered by the charts are calculated at 10 psia using the modified Antoine equation and corrected to system conditions using the pressure correction charts.

The K10 value is then corrected for pressure using pressure correction charts. The K values for any components that are not covered by the charts are calculated at 10 psia using the modified Antoine equation and corrected to system conditions using the pressure correction charts.

Accuracy suffers with this model if there are large amounts of acid gases or light hydrocarbons. All three phase calculations assume that the aqueous phase is pure H_2O and that H_2O solubility in the hydrocarbon phase can be described using the kerosene solubility equation from the API Data Book.

Braun property package is applicable to the following ranges:

Temperature	Press (psia)	Press (kPa)
0°F (-17.78°C)<1.6 Tci	<100	<700

Braun K10 uses the Braun K10-Ideal Gas method to calculate VLE and the Lee-Kesler method to calculate Enthalpy and Entropy.

Esso Tabular

The Esso Tabular model is strictly applicable to hydrocarbon systems at low pressures. The model employs a modification of the Maxwell-Bonnel vapour pressure model.

Esso Tabular property package is applicable to the following system:

Temperature	Press (psia)	Press (kPa)
<1.6 Tci	<100	<700

For heavy hydrocarbon systems, the results are comparable to the modified Antoine equation since no pressure correction is applied. For non-hydrocarbon components, the K value is calculated using the Antoine equation. Accuracy suffers if there is a large amount of acid gases or light hydrocarbons. All three phase calculations are performed assuming the aqueous phase is pure H_2O and that H_2O solubility in the hydrocarbon phase can be described using the kerosene solubility equation from the API Data Book.

The Lee-Kesler model is used for enthalpy and entropy calculations for all components with the exception of H_2O which is treated with the steam tables.

Miscellaneous Types

The Miscellaneous group contains Property Packages that are unique and do not fit into the groups previously mentioned.

Amine Pkg

The Amine Package contains thermodynamic models developed by D.B. Robinson & Associates for their proprietary amine plant simulator, AMSIM. Their amine property package is available as an option with HYSYS giving you access to a proven third party property package for reliable amine plant simulation, while maintaining the ability to use HYSYS' powerful flowsheeting capabilities. Contact your AspenTech representative for further information.
For the Amines property method, the vapour phase is modeled using the PR model.

The chemical and physical property data base is restricted to amines and the following components:

Component Class	Specific Components
Acid Gases	CO_2, H_2S, COS, CS_2
Hydrocarbons	CH_4, C_7H_{16}
Olefins	C2=, C3=
Mercaptans	M-Mercaptan, E-Mercaptan
Non Hydrocarbons	H_2, N_2, O_2, CO, H_2O

The equilibrium acid gas solubility and kinetic parameters for the aqueous alkanolamine solutions in contact with H_2S and CO_2 are incorporated into their property package. The amines property package is fitted to extensive experimental data gathered from a combination of D.B. Robinson's in-house data, several unpublished sources, and numerous technical references.

The Amines method does not allow any hypotheticals.
The following table gives the equilibrium solubility limitations that should be observed when using this property package:

Alkanolamine	Alkanolamine Concentration (wt%)	Acid Gas Partial Pressure (psia)	Temperature (°F)
Monoethanolamine, MEA	0 - 30	0.00001 - 300	77 - 260
Diethanolamine, DEA	0 - 50	0.00001 - 300	77 - 260
Triethanolamine, TEA	0 - 50	0.00001 - 300	77 - 260
Methyldiethanolamine, MDEA*	0 - 50	0.00001 - 300	77 - 260
Diglycolamine, DGA	50 - 70	0.00001 - 300	77 - 260
DIsoPropanolAmine, DIsoA	0 - 40	0.00001 - 300	77 - 260

* The amine mixtures, DEA/MDEA and MEA/MDEA are assumed to be primarily MDEA, so use the MDEA value for these mixtures.

The data is not correlated for H_2S and CO_2 loadings greater than 1.0 mole acid gas/mole alkanolamine.

The absorption of H_2S and CO_2 by aqueous alkanolamine solutions involves exothermic reactions. The heat effects are an important factor in amine treating processes and are properly taken into account in the amines property package. Correlations for the heats of solution are set up as a function of composition and amine type. The correlations were generated from existing published values or derived from solubility data using the Gibbs-Helmholtz equation.

The amines package incorporates a specialized stage efficiency model to permit simulation of columns on a real tray basis. The stage efficiency model calculates H_2S and CO_2 component stage efficiencies based on the tray dimensions given and the calculated internal tower conditions for both absorbers and strippers. The individual component stage efficiencies are a function of pressure, temperature, phase compositions, flow rates, physical properties, mechanical tray design and dimensions as well as kinetic and mass transfer parameters.

Since kinetic and mass transfer effects are primarily responsible for the H_2S selectivity demonstrated by amine solutions, this must be accounted for by non unity stage efficiencies.

Amines Pkg uses the following methods of calculation:

- Liquid: VLE (vapour liquid equilibrium) = Mod Kent Eisenberg
- Vapour: VLE (vapour liquid equilibrium) = PR
- Enthalpy/Entropy = Curve Fit

DBR Amine Package

The DBR Amine Package is similar to the Amine Pkg, but is independently coded and maintained by DBR; it can be updated anytime AMSIM thermo features and capabilities are updated. Features include advanced solving and flowheet-composing capabilities through HYSYS, physical solvent simulation capability by DEPG, and improved thermodynamic model predictions based on newly availaby experimental data.

ASME Stream

The ASME Steam property package is restricted to a single component, namely H_2O. It accesses the ASME 1967 steam tables. The limitations of this steam package are the same as those of the original ASME steam tables:

- Pressures less than 15,000 psia
- Temperatures greater than 32°F (0°C) and less than 1,500°F.

The basic reference is "Thermodynamic and Transport Properties of Steam" - The American Society of Mechanical Engineers - Prepared by C.A. Meyer, R.B. McClintock, G.J. Silvestri and R.C. Spencer Jr.

Glycol PPkg
The Glycol property package contains the TST (Twu-Sim-Tassone) equation of state to determine the phase behaviour more accurately and consistently for the TEG-water mixture. The property package contains the necessary pure component and binary interaction parameters for components commonly encountered in natural gas dehydration process. The property package is tuned to represent accurately, the phase behaviour of these components, especially that for the TEG-water binary system.

The TST equation of state can accurately predict:

- activity coefficients of the TEG-water solutions within the average absolute deviation of 2%
- dew point temperatures within an average error of ±1°C.
- water content of gas within the average absolute deviation of 1%

The Glycol property package should be applicable over the range of temperatures, pressures, and component concentration encountered in a typical TEG-water dehydration system: between 15°C to 50°C and between 10 atm to 100 atm for the gas dehydrator, and between 202°C to 206°C and 1.2 atmospheres for the glycol regenerator.
The accuracy of predicted solubility of hydrocarbons in aqueous phase is expected to be within the experimental uncertainty.
The table below displays the prediction of equilibrium water content in lbH2O/MMSCF for a gas stream in contact with 99.5 weight percent TEG, using the Glycol property package.

| T dew (K) | Reported by: | | Predicted from TST (EOS): | |
	McKetta2	Bukacek1	Water Content	Pressure (Pa)
277.59	390	396	393	838
266.48	170	176	174	370
255.37	70	72	71	151
244.26	28	27	26	56.1
233.15	9.2	9.1	9	18.7
222.04	2.4	2.8	2.6	6

The BIP databank for the Glycol property package will be updated in future releases of HYSYS. Currently, there may be some limitations or missing BIP for certain component pairs. For example, heavy hydrocarbons or hypothetical components which may not have any interaction parameters available.

Glycol Calculation Methods:

For the Glycol property package, three alpha function parameters are used to correlate the vapor pressure of the component in the HYSYS component database. The alpha function parameters are: L, M, and N parameters that are unique for each component.

For Glycol property package, three adjustable parameters are used to correlate Vapor-Liquid-Equilibrium (VLE) mixture data. The parameters corresponding to the TST (Twu-Sim-Tassone) AE mixing rules are: Aij, Aji, and aij binary interaction parameters in the NRTL equation.

The Glycol property package uses the Cavett model for enthalpy and entropy calculations.

NBS Stream

The NBS Steam property package is restricted to a single component, namely H2O. It uses the NBS 1984 Steam Tables, which reportedly have better calculations near the Critical Point than ASME 1967 steam tables.

MBWR

The MBWR property package is a modified version of the original Benedict/Webb/Rubin equation. This 32-term equation of state model is applicable for only a specific set of components and operating conditions.

The Modified BWR (MBWR) property package is recommended for systems with select gases and light hydrocarbons.

The modified BWR is applicable only for the following pure components:

Component	Temp (K)	Temp (R)	Max Press (MPa)	Max Press (psia)
Ar	84 - 400	151.2 - 720	100	14,504
CH_4	91 - 600	163.8 - 1,080	200	29,008
C_2H_4	104 - 400	187.2 - 720	40	5,802
C_2H_6	90 - 600	162. - 1,080	70	10,153
C_3H_8	85 - 600	153. – 1080	100	14,504
i-C_4	114 - 600	205.2 - 1,080	35	5,076
n-C_4	135 - 500	243 - 900	70	10,153
CO	68 - 1,000	122.4 - 1,800	30	4,351
CO_2	217 - 1,000	390.6 - 1,800	100	14,504
D_2	29 - 423	52.2 - 761.4	320	46,412
H_2	14 - 400	25.2 - 720	120	17,405
o-H2	14 - 400	25.2 - 720	120	17,405
p-H2	14 - 400	25.2 - 720	120	17,405
He	0.8 - 1,500	1.4 - 2,700	200	29,008
N_2	63 - 1,900	113.4 - 3,420	1,000	145,038
O_2	54 - 400	97.2 - 720	120	17,405
Xe	161 - 1,300	289.8 - 2,340	100	14,504

Note: The mixtures of different forms of H2 are also acceptable. The range of use for these components is shown in the preceding table.

OLI_Electrolyte

The OLI Electrolyte property package was developed by OLI Systems Inc. and used for predicting the equilibrium properties of a chemical system including phase and reactions in a water solution.

Simplified aqueous modeling and computational approaches using approximation are usually ineffective and can be potentially dangerous when applied to real process applications. Aqueous systems often behave in complex and unpredictable ways, introducing great risk into plant design and operation if they are not adequately understood and accounted for. On the other hand, reliable electrolyte models can ultimately provide tremendous insight, process alternatives, efficiencies in plant design, trouble-shooting, and optimization. This improves process economics, reliability, versatility, and meets environmental constraints.

The HYSYS OLI Interface package is based on OLI Systems software that provides clients with a theoretical framework, databases, data regression techniques, and applications software that comprehensively and accurately simulates and predicts electrolyte systems.

OLI_Electrolyte Calculation Methods

The OLI_Electrolyte property package can model complex chemical phenomena, including:

- Intraphase Equilibria between aqueous, organic, vapour and solid phases
- Intraphase Equilibria including redox and speciation reactions

The OLI_Electrolyte property package uses a highly advanced thermodynamic and mathematical framework for predicting the equilibrium properties of a chemical system. This predictive framework is based upon:

- The revised Helgeson equation of state for predicting the standard state thermodynamic properties of all species, including organics, in water.
- The Bromley-Zemaitis framework for the prediction of excess thermodynamic properties.
- The Pitzer and Setschenow formulation for the prediction of the excess thermodynamic properties of molecular species in water.
- The enhanced SRK equation of state for the prediction of vapour and non-aqueous liquid phase thermodynamic properties. This enhanced equation of state applies to organics which are sparingly soluble in water, and which form a second liquid phase that is nearly ideal.

OLI_Electrolyte Components

All electrolyte features are accessed through the HYSYS interface. This package does not use the HYSYS component databases, but rather accesses the OLI databases, which include information required for generating the chemistry models. There are two databases available with this package. Each database offers identical HYSYS functionality but differs with regard to the number of available components.

- **Limited**. The standard 1,000 component databank. Components in this database are of most interest to the process industries. The electrolytes limited database is a subset of the Full database.

- **Full**. An extended 3,000 component electrolyte database. The Full database also includes the GEOCHEM (mineral components) electrolytes database.

The following functions are not supported in HYSYS when using the OLI_Electrolyte property package compared to the traditional components.

- Classification of components is based on their type; all components are classified as miscellaneous (you can not use the family filter).
- The Synonym, formula, and name columns in the component selection form are the same.
- Oil mixtures and hypothetical components are not available. To add hypothetical components, a private database must be created and specified in the Private User Database option.

Note: If water is not added or selected as a component, HYSYS will add it automatically.