EQ-COMP : The VLE Simulator

The ultimate answer to all your vapor-liquid equilibrium needs

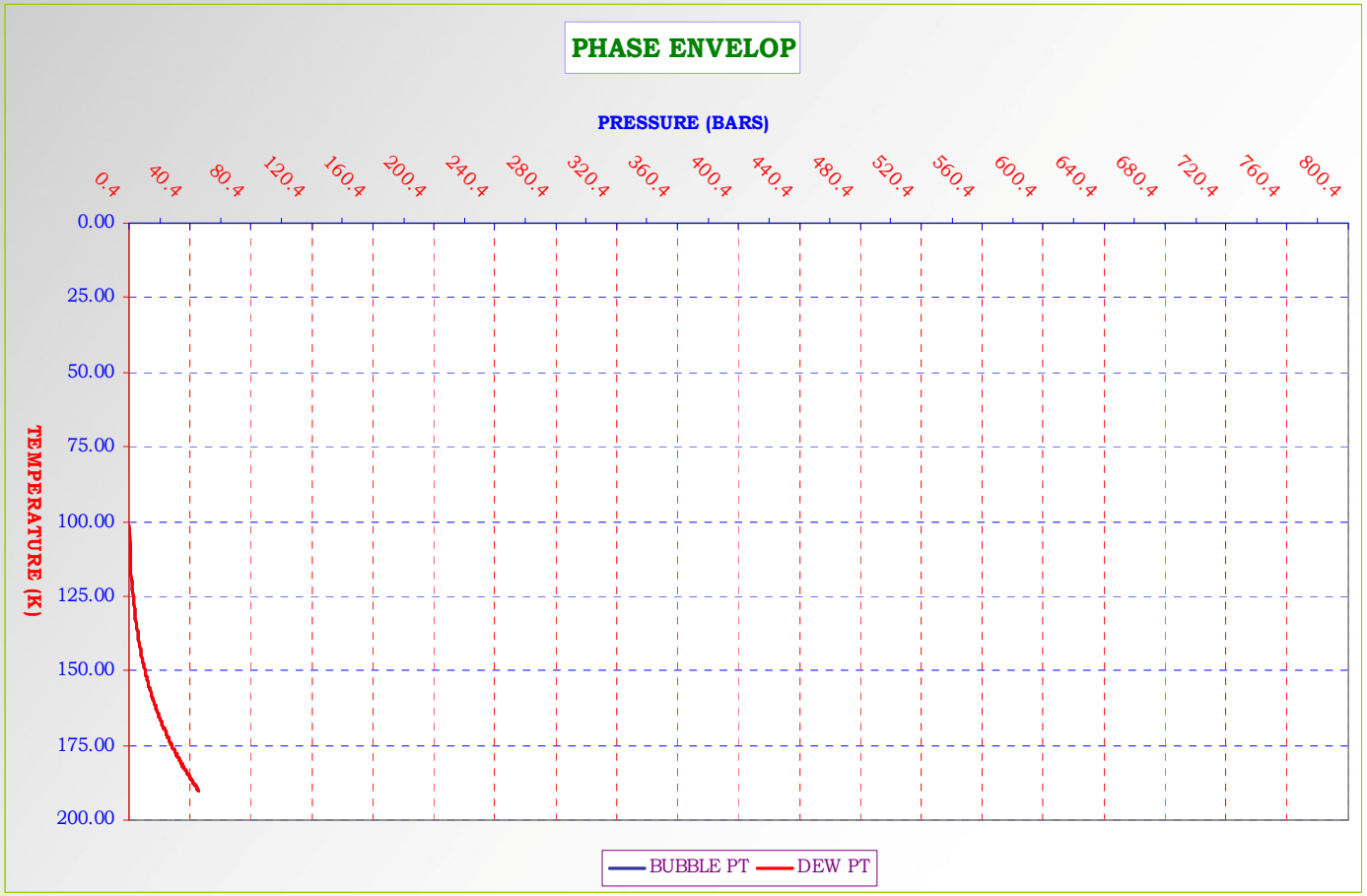
VAPOR-LIQUID EQUILIBRIUM CONCEPT

PURE COMPOUNDS

- Vapor-Liquid Equilibrium curves for pure compounds are Pressure-Temperature plots showing the variation of boiling/bubbling temperatures with pressures.
- These curves end at critical point corresponding to critical temperature and critical pressure
- The compound can be vaporized at a constant temperature lower than critical temperature from an initial pressure beyond critical pressure by decreasing the pressure.
- Similarly compound can be liquefied at a constant pressure below critical pressure from an initial temperature higher than critical temperature by decreasing the temperature
- The compound can not be liquefied or vaporized by variation of temperature at constant pressure or by variation of pressure at constant temperature incase the both the initial temperature and pressure of compound are higher than critical values.
- Beyond critical point, the compound can not be characterized as liquid or vapor thus resulting in absence of vapor-liquid equilibrium and VLE curve beyond critical point.

VAPOR-LIQUID EQUILIBRIUM CONCEPT

VLE CURVE OF A PURE COMPOUND



VLE curve of Methane (CH4)

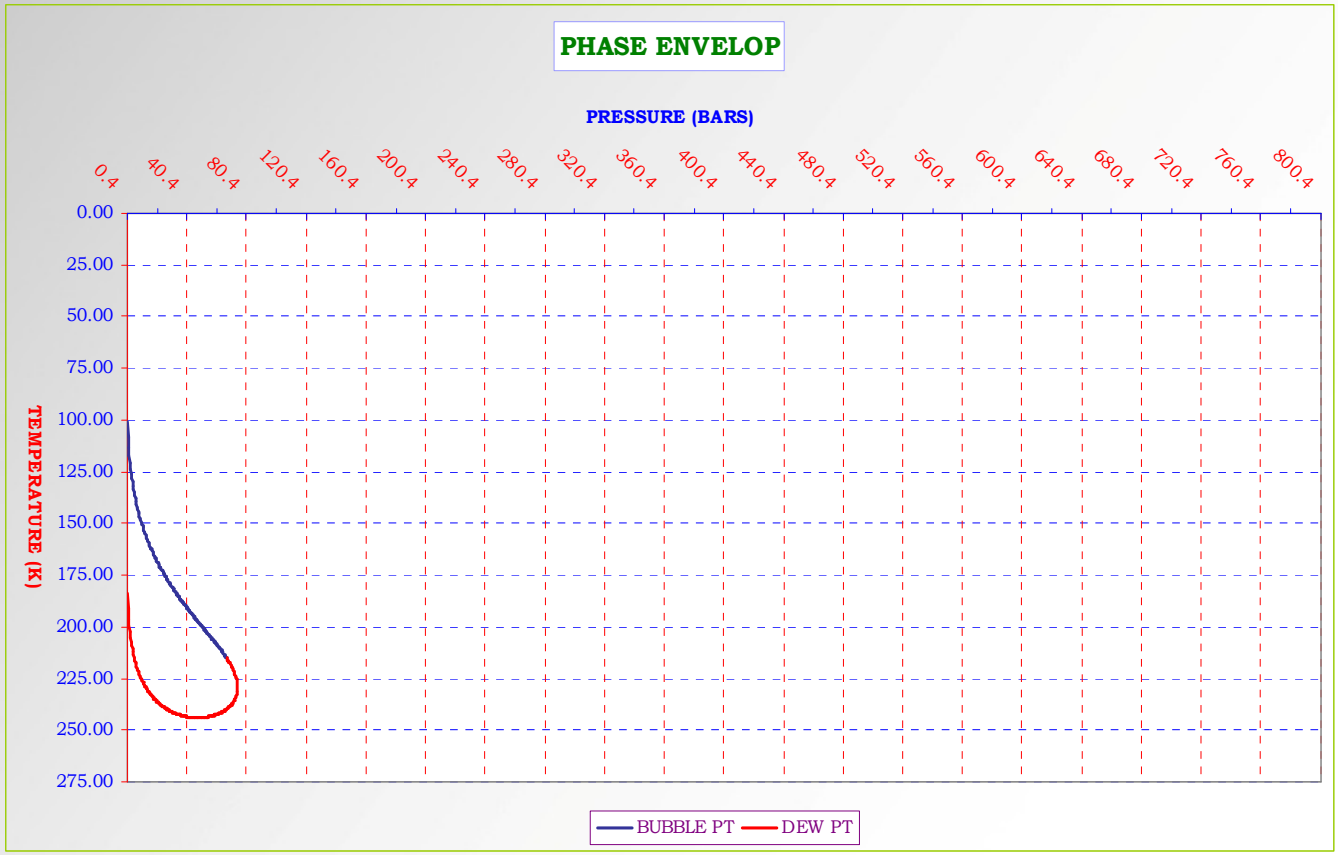
VAPOR-LIQUID EQUILIBRIUM CONCEPT

HYDROCARBON MIXTURES

- Vapor-Liquid Equilibrium curves for hydrocarbon mixtures are generally closed envelopes known as Phase envelopes comprising of bubble point curve and dew point curve.
- Bubble point curve is the plot of pressure of the mixture (bubble point pressure) with the temperature at which vaporization of the mixture starts/ first bubble of vapor is formed (bubble point temperature or initial boiling point temperature).
- Dew point curve is the plot of pressure of the mixture (dew point pressure) with the temperature at which vaporization of the mixture ends/ single drop of liquid remains (dew point temperature or final boiling point temperature).
- The meeting point of bubble point curve and dew point curve on phase envelope is the critical point of the hydrocarbon mixture.
- Inside the Phase envelope in general and between initial and final boiling temperatures in particular, the hydrocarbon mixture exists in two phases i.e. partially in liquid and partially in vapor phase.
- Unlike VLE curves for pure compounds, VLE curves for hydrocarbon mixtures extend beyond critical pressure to cricondenbar (point of maximum pressure on the phase envelope) and beyond critical temperature to cricondentherm (point of maximum temperature on the phase envelope).

VAPOR-LIQUID EQUILIBRIUM CONCEPT

PHASE ENVELOPE FOR A HYDROCARBON MIXTURES



Phase envelope of a typical Natural Gas composition

CH4 : 90 %, C2H6 : 6.2 %, C3H8 : 2.3 %, i-C4H10 : 0.4 %, n-C4H10 : 0.55 %, n-C5H12 : 0.03 %, N2 : 0.52 %

VLE PROPERTIES DETERMINATION AND ITS UTILITY

UTILITY OF VLE PROPERIES

VLE Properties like bubble point, dew point, two phase composition, critical point, cricondentherm, cricondenbar etc. form the basis of complete hydrocarbon industry and have immense usage in all kinds of hydrocarbon operations as well as in all other areas even remotely related to hydrocarbons. Some uses of VLE properties are:

- VLE Properties are required in designing of hydrocarbon plants like oil refineries, LPG plant, LNG liquefaction and gasification plants, Petrochemical plants etc.. They have roles in designing of all equipments of these plants like storage tanks, flash chambers, distillation towers, pumps etc.
- VLE Properties are required in all kinds of petroleum upstream calculations like oil and gas well simulation and designing of multiphase flow pipelines.
- Prediction of these properties is useful in simulating various planetary atmospheres which contain varying proportions of hydrocarbons like methane, ethane and propane and some inorganic gases like N2, H2S, H2 and CO2.

VLE PROPERTIES DETERMINATION AND ITS UTILITY

DETERMINATION OF VLE PROPERIES

VLE Properties like bubble point, dew point, two phase composition, critical point, cricondentherm, cricondenbar etc. for binary mixtures are easy to calculate but determination of these properties for multicomponent mixtures require complex calculations involving complex equations. Optimization of these calculations to include maximum number of components and plotting of correct phase envelopes for multicomponent mixtures presents further challenge. These calculations can only be calculated using latest computers. These calculations further require complex computer programs to automate them so that the results can be generated at the click of a button.

INTRODUCTION TO EQ-COMP

- EQ-COMP is a VLE calculation software that can accurately calculate various VLE properties like bubble point, dew point, two phase compositions, critical point, cricondentherm, cricondenbar etc. for multicomponent hydrocarbon mixtures.
- EQ-COMP is one of its kind software in the world which is made single-handedly with basic infrastructure using very basic software tool like MS excel but gives results comparable to other such world class softwares made using most advanced software tools, vast infrastucture and large teams of scientists and developers.
- EQ-COMP is a very complex combination of macro programs of MS excel written using Visual Basic for Applications programming language for calculating multicomponent vapor-liquid equilibrium properties automatically at the click of a button.
- EQ-COMP is useful in finding out vapor-liquid equilibrium properties for a hydrocarbon mixture for any composition. It has been optimised to include any number of non-polar or slightly polar compounds subject to a maximum limit of 112 compounds.
- Various modules of EQ-COMP can be used to find out various VLE properties even in retrograde region and for compositions involving high proportions of non-condensables.
- The phase envelope generated using EQ-COMP consists of equilibrium temperature values at a specified interval of 0.4 bars clearly marking the critical point of mixture with easily locatable cricondenbar and cricondentherm.

CALCULATIONS & EQUATIONS USED IN EQ-COMP

- EQ-COMP calculates VLE properties using Peng-Robinson cubic equation of state which is the preferred equation for such calculations for non-polar and slightly polar compounds
- EQ-COMP uses modified version of Peng-Robinson equation published in 1978
- In designing of EQ-COMP, trends of various phase envelop curves for different compositions developed using first principles have been carefully studied and generalized to fit other compositions.
- EQ-COMP does not use any popular converging method but uses long and un-conventional for such calculations but tried and tested and very reliable first principle approach and basic but standard calculation tools like MS excel for carrying out the calculations. So EQ-COMP may sometimes take long time in generating results but the chances of the results being incorrect under the preview of Peng-Robinson cubic equation of state is almost nil.
- Binary interaction parameters values can be included in the calculations in EQ-COMP to increase the accuracy of the VLE results.
- EQ-COMP is among the very few similar software in the world which have included temperature dependent binary interaction parameters as per Predictive Peng Robinson 78 (PPR 78) equation in its calculations. These parameters are specifically used for calculating reasonably accurate water dew point values and curves for hydrocarbon mixtures.
- EQ-COMP can include constant binary interaction parameters calculated using critical volumes of interacting hydrocarbons.

EXCLUSIVE FEATURES OF EQ-COMP

Some of the exclusive features and results possible with EQ-COMP are:

- Phase equilibrium curve with temperature-pressure data for any pure non-polar or mildly polar compound with known critical temperature, critical pressure accentricity factor.
- VLE properties like bubble point temperature, bubble point pressure, dew point temperature, dew point pressure, two phase composition, bubble point composition, dew point composition etc. for almost any hydrocarbon mixture involving any number of non-polar or mildly polar hydrocarbons.
- Complete phase envelope for almost any hydrocarbon mixture with critical point, cricondenbar, cricondentherm and multiple critical points.
- VLE properties in the retrograde region.
- VLE properties and Phase envelope for hydrocarbon mixtures involving high concentration of non-condensables.
- Prediction of state of hydrocarbon mixture (liquid, vapour, two phase or super critical) at a particular temperature and pressure.
- Customisation of software to include any other non-polar or mildly polar hydrocarbon in the calculations as per client's requirement.
- Inclusion of values of binary interaction parameters provided by the client to generate results.
- Inclusion of constant binary interaction parameters in case desired by the client.

EXCLUSIVE FEATURES OF EQ-COMP

Continued

- Generation of liquid and vapour compressibility factors for any hydrocarbon mixture over a range of temperatures and pressures.
- Generation of x-y, T-x-y, H-x-y and critical point profile for any binary mixture comprising of non-polar or mildly polar hydrocarbons.
- Calculation of enthalpy change from standard conditions, entropy change from standard conditions, gibbs free energy change from standard conditions, heat capacity at constant pressure (Cp), heat capacity at constant volume (Cv), heat capacity ratio (Cp/Cv) and Sonic speed for any hydrocarbon mixture at a given pressure and corresponding bubble and dew point temperatures and throughout the phase envelope at increments of 0.4 bars.
- Calculation of binary and multi-component distillation column design including number of stages in rectification and stripping section, minimum reflux ratio, q value of feed, liquid and vapour compositions in various stages and temperature in various stages using rigorous stage by stage calculation.
- Calculation of gas hydrate equilibrium curve for any mixture comprising of non-polar or mildly polar hydrocarbons with atleast one hydrate former alongwith types of hydrate formed, liquid-vapour-hydrate equilibrium compositions and fractional filing of large and small cavities.

APPLICATIONS OF EQ-COMP

Some of the possible applications of EQ-COMP are:

- EQ-COMP can be used to predict phase equilibrium curves for pure hydrocarbons and supercritical properties so it can be used to design storage tanks for pure hydrocarbons.
- EQ-COMP can be used to predict the bubble point, hydrocarbon dew point and two phase properties for multicomponent hydrocarbon mixtures so it can be used to design flash chambers/ pressure vessels.
- EQ-COMP can predict cricondentherm, cricondenbar, critical point, retrograde condensation region etc. very accurately so it can be used for oil well simulation studies during oil well planning.
- EQ-COMP predicts cricondentherm very accurately using Peng-Robinson cubic equation of state so it can be used to fix the temperature at which the natural gas should be supplied to the power plants and this temperature specification is mentioned in Natural gas contracts for natural gas based power plants and cogen plants.
- EQ-COMP can predict various phase equilibrium properties for hydrocarbon mixtures so it can also be used to simulate planetary atmospheres like that of Titan, the moon of Saturn which contains mixture of Nitrogen and Methane in varying proportions.
- EQ-COMP can accurately find out various VLE properties at low as well as high pressures and can further post-process the data generated by running various modules of EQ-COMP number of times to generate Concentration diagrams, Temperature-Concentration diagrams and Enthalpy-Concentration diagrams for any binary mixture comprising of non-polar or mildly polar hydrocarbons at any pressure so it can be used directly for designing distillation columns for binary mixtures.

APPLICATIONS OF EQ-COMP

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- EQ-COMP can calculate enthalpy change from standard conditions, entropy change from standard conditions, gibbs free energy change from standard conditions, heat capacity at constant pressure (Cp), heat capacity at constant volume (Cv), heat capacity ratio (Cp/Cv) and Sonic speed at desired pressure values and corresponding bubble point and dew point temperature values of hydrocarbon mixture. Also it can calculate the above values for any hydrocarbon mixture throughout the phase envelope at increments of 0.4 bars. This enables the calculation of enthalpy changes, entropy changes and gibbs energy changes between saturated vapour and saturated liquid apart from heat capacity, heat capacity ratio and sonic speed values for saturated vapour and saturated liquid for any hydrocarbon mixture. These values have extensive usage in engineering calculations involving hydrocarbons.
- EQ-COMP can perform binary and multi-component distillation column design using rigorous stage by stage calculation.
- EQ-COMP can predict gas hydrate equilibrium curve and properties of gas hydrates formed for any mixture of non-polar or mildly polar hydrocarbons with at least one hydrate former.

These are some of the possible practical applications of EQ-COMP. Apart from these, EQ-COMP can be extensively used in various other natural gas processing, petrochemical and refinery design applications and in research studies in various research laps wherever accurate prediction of vapour liquid equilibrium properties for pure hydrocarbons or hydrocarbon mixtures is required.

DISTILLATION COLUMN DESIGN USING EQ-COMP

For multi-component distillation, separate detailed tray by tray calculations performed iteratively may be required for optimized design of the distillation column but simpler calculation procedures exist for binary distillation. Distillation columns for binary mixtures can be designed by very simple McCabe-Thiele method and slightly more complex and more accurate Ponchon-Savarit method. Both these methods require Concentration diagrams (x-y plot) and Temperature-Concentration diagrams (T-x-y plot) at the operating pressure of the distillation column. Ponchon-Savarit method requires enthalpy-concentration diagram in addition to these two diagrams.

EQ-COMP can be used to design multi-component distillation columns by calculating VLE properties at each of the tray conditions separately step by step. EQ-COMP can accurately find out various VLE properties at low as well as high pressures and can further post-process the data generated by running various modules of EQ-COMP number of times to generate Concentration diagrams (x-y plot), Temperature-Concentration diagrams (T-x-y plots) and Enthalpy-Concentration diagram (H-x-y plots) for any binary mixture comprising of non-polar or mildly polar hydrocarbons at any pressure. These diagrams can be used in McCabe-Thiele method or Ponchon-Savarit method to find out various design parameters like theoretical number of trays, feed tray location, reflux ratio etc. for distillation columns for binary mixtures.

CALCULATION MODULES OF EQ-COMP

Various calculation modules of EQ-COMP along with the results generated by them are given below:

- Bubble point temperature module: It calculates the bubble point temperature/s, equilibrium constants (K values) and compositions at a given pressure. In addition it calculates liquid and vapor compressibility factor values, molecular weights and densities at bubble point. Also it gives Equilibrium temperature, compositions, K values and compressibility factor values at pressure values throughout the bubble point curve at increments of 0.4 bars.
- Hydrocarbon dew point temperature module: It calculates the dew point temperature and compositions at a given pressure. In addition it calculates liquid and vapor compressibility factor values, molecular weights and densities at dew point. Also it gives Equilibrium temperature, compositions, K values and compressibility factor values at pressure values throughout the hydrocarbon dew point curve at increments of 0.4 bars.
- Bubble point pressure module: It calculates the bubble point pressure and compositions at a given temperature. In addition it calculates liquid and vapor compressibility factor values, molecular weights and densities at bubble point. Also it gives Equilibrium temperature, compositions, K values and compressibility factor values at pressure values throughout the bubble point curve at increments of 0.4 bars.

CALCULATION MODULES OF EQ-COMP

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- Hydrocarbon dew point pressure module: It calculates the dew point pressure and compositions at a given temperature. In addition it calculates liquid and vapor compressibility factor values, molecular weights and densities at dew point. Also it gives Equilibrium temperature, compositions, K values and compressibility factor values at pressure values throughout the hydrocarbon dew point curve at increments of 0.4 bars.
- Two phase composition module: It calculates the two-phase compositions along with liquid and vapor compressibility factor values, molecular weights and densities at given conditions and at bubble point temperatures and dew point temperatures for the given pressure conditions. Also it gives Equilibrium temperature, compositions, K values and compressibility factor values at pressure values throughout the phase envelope including bubble point curve and hydrocarbon dew point curve at increments of 0.4 bars.
- Phase envelope module: It gives temperature and pressure values for the complete phase envelope along with plot of phase envelope. It also provides critical point temperature and pressure values and bubble point and dew point compositions and properties at critical point. Also it gives equilibrium temperature, compositions, K values and compressibility factor values at pressure values throughout the phase envelope including bubble point curve and hydrocarbon dew point curve at increments of 0.4 bars.

CALCULATION MODULES OF EQ-COMP

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- Water dew point temperature module: It calculates the water dew point temperature value at given pressure. Also it gives water dew poin temperature, compositions, K values and compressibility factor values at pressure values throughout the water dew point curve at increments of 0.4 bars along with plot of water dew point curve.
- Liquid compressibility factor calculation module: It calculates liquid compressibility factor values for the provided range of temperatures and pressures with provided increments in temperatures and pressures
- Vapor compressibility factor calculation module: It calculates vapor compressibility factor values for the provided range of temperatures and pressures with provided increments in temperatures and pressures
- Binary VLE calculation module: It calculates bubble point temperature and dew point temperature at desired pressure and phase envelope data for binary mixtures of same compounds with 9 different compositions starting from 0 % of one compound to 100 % of that compound with increments of 12.5 %. It calculates liquid and vapor compressibility factors, liquid and vapor densities and liquid and vapor molecular weights on 15 points on concentration diagram (x-y plot) Further it generates concentration diagram (x-y plot), concentration diagram (x-y plot) data, temperature-concentration diagram (T-x-y plot), Temperature-concentration diagram (T-x-y plot) data, Enthalpy-concentration diagram (H-x-y plot), Enthalpy-concentration diagram (H-x-y plot) data and critical point locus curve for the binary mixtures.

CALCULATION MODULES OF EQ-COMP

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- Thermodynamic properties calculation module: It calculates enthalpy change from standard conditions, entropy change from standard conditions, gibbs free energy change from standard conditions, heat capacity at constant pressure (Cp), heat capacity at constant volume (Cv), heat capacity ratio (Cp/Cv) and Sonic speed at desired pressure values and correspomding bubble point and dew point temperature values of hydrocarbon mixture. In addition it calculates temperature, enthalpy change from standard conditions, entropy change from standard conditions, gibbs free energy change from standard conditions, heat capacity at constant pressure (Cp), heat capacity at constant volume (Cv), heat capacity ratio (Cp/Cv) and Sonic speed at pressure values throughout the bubble point and dew point curve at increments of 0.4 bars.
- Multi-component distillation column calculation module: It calculates stages in rectification and stripping section of a distillation column, minimum reflux using Underwood method, q value of feed, liquid and vapour compositions for various stages and temperature in various stages for any binary or multicomponent mixture of non-polar or mildly polar hydrocarbon or inorganic gases using rigourous stage by stage calculation.
- Hydrate dissociation curve calculation module: It calculates gas hydrate equilibrium curve for any mixtures of non-polar or mildly polar hydrocarbons and inorganic gases with atleast one hydrate former along with types of hydrate formed, liquid-vapour-hydrate equilibrium composition and fractional filing of large and small hydrate cavities for pressures between 0.4 bars to 800 bars with increments of 0.4 bars.

BENEFITS OF EQ-COMP IN COMPARISON WITH OTHER SIMILAR SOFTWARES

- A conventional simulation software though an extension of EQ-COMP cost may cost close to a 100,000 USD with various limitations to number of users and time validity of licence. EQ-COMP is the basis of some main modules of these simulation softwares. Services of EQ-COMP can be availed at an extremly low cost on per calculation basis.
- EQ-COMP is offered on software as a service (SAAS) model where ready results of the queries are provided to the customer as a service. This way the customer would not have to arrange for infrastructure like a standalone high-end computer with suitable backend softwares programs for running and safeguarding the software. Also the customer would not have to learn how to operate the software as ready results of the queries would be provided to him through e-mail. The only requirement for availing the services of EQ-COMP is a valid official e-mail address to send and receive queries for which any internet enabled computer can be used. This way the results can be obtained by the Engineer/ Scientist even when he is not in his office during off hours or while on site when he can not use his office resources.
- A conventional simulation softwares has number of modules meant for different industries, all of which may not be required by one client. EQ-COMP has been specifically designed for hydrocarbon industry complying specific requirements which can be foreseen before paying for the services of EQ-COMP.
- EQ-COMP can give almost any result involving hydrocarbon VLE most accurately using the preferred Peng-Robinson equation of state making it truly world-class as far as final results of the software are concerned.

LIMITATIONS OF EQ-COMP

- The results of EQ-COMP are based on standard chemical engineering equations. These results may not completely match with experimental results. So while asking for or using the results it should be kept in mind that these are just theoretical calculations calculated using modern computers as calculating them otherwise may not be possible or may be very difficult.
- As EQ-COMP uses MS Excel for calculations so the results would not be calculated online but be calculated on a standalone PC based on the data entered into the form on the website www.eq-comp.com and sent to our office in New Delhi, INDIA through e-mail by submitting it on the website. Because of time difference between the country from where enquiry is send and India, the enquiry may take upto 24 hours to clear. The final result will be sent through e-mail to the user in the form of an MS Excel attachment.
- EQ-COMP, though world-class as far as final output is concerned, is a solo effort using very basic infrastructure and basic software tools like MS-excel. MS-excel is not designed for such extensive calculations and plenty of inherent limitations of MS-excel have been overcome in development of EQ-COMP. Still some areas of improvements and shortcomings may exist in EQ-COMP which have yet remained unnoticed The same may be conveyed at info@eq-comp.com.

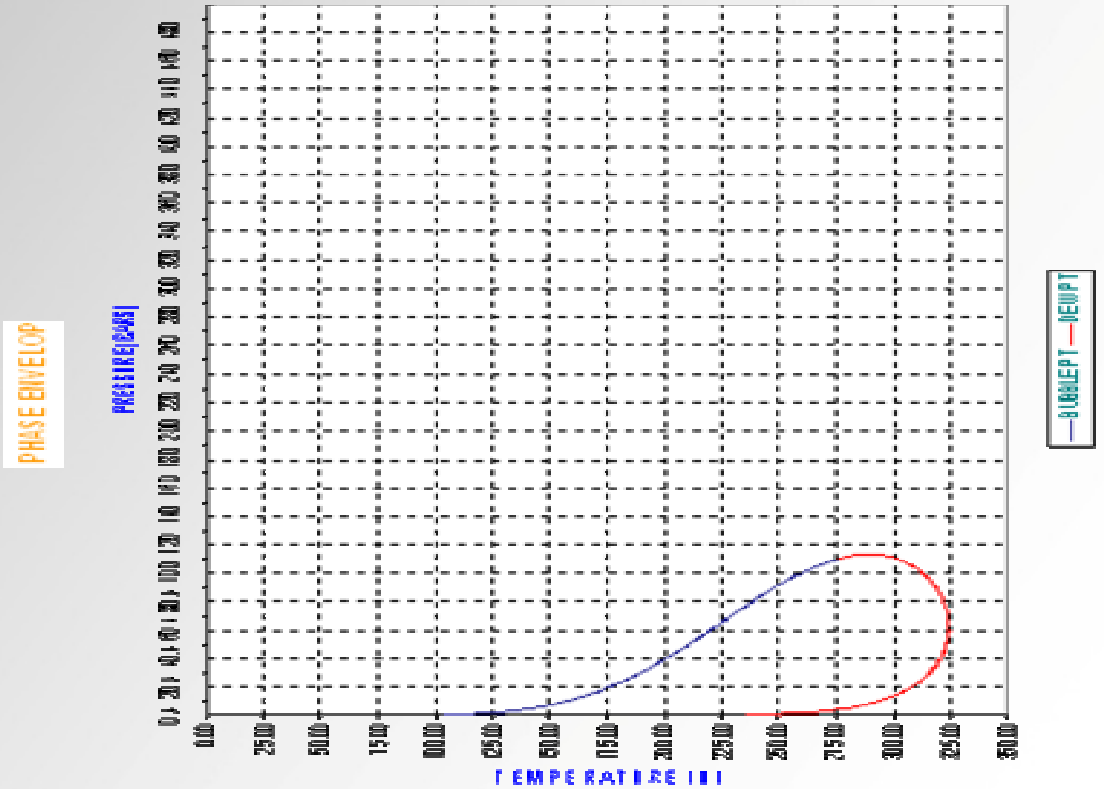
DESIGNER'S/DEVELOPER'S PROFILE

EQ-COMP is the result of more than 10 years of continuous research in the field of vapour-liquid equilibrium and involves extensive software development effort to optimize and automate the calculations. It has been designed and developed by Mr. Amit Katyal who is a Bachelor in Chemical Engineering from the prestigious Indian Institute of Technology, Delhi, INDIA. He has a total experience of more than 20 years in hydrocarbon sector in diverse segments like research, operations, technical services and marketing. Apart from EQ-COMP he has also developed HYD-PREDIC, LIQ-PROP, BUBBLE-SIM and MIX-CP softwares and gas hydrates based water desalination technology and horizontal distillation technology. His work is showcased at www.eq-comp.com website.

HOW TO AVAIL SERVICES OF EQ-COMP

EQ-COMP software is not available for purchase on license basis but is available for use as per SAAS (Software as a service) model. Services of EQ-COMP can be availed on per calculation basis. The calculations can be availed by registering your email on VLE Calculator page of the website, www.eq-comp.com, downloading the input MS excel file for the required calculation, paying for the calculation using the respective paypal button, filling the downloaded input MS excel file and sending it on info@eq-comp.com. The request for calculation results may take upto 24 hours to clear depending on the time difference between the Country of origin of the request and INDIA as the same would have to be fed into EQ-COMP application at our office in INDIA for getting the results which will then be sent to the registered e-mail as an MS Excel attachment.

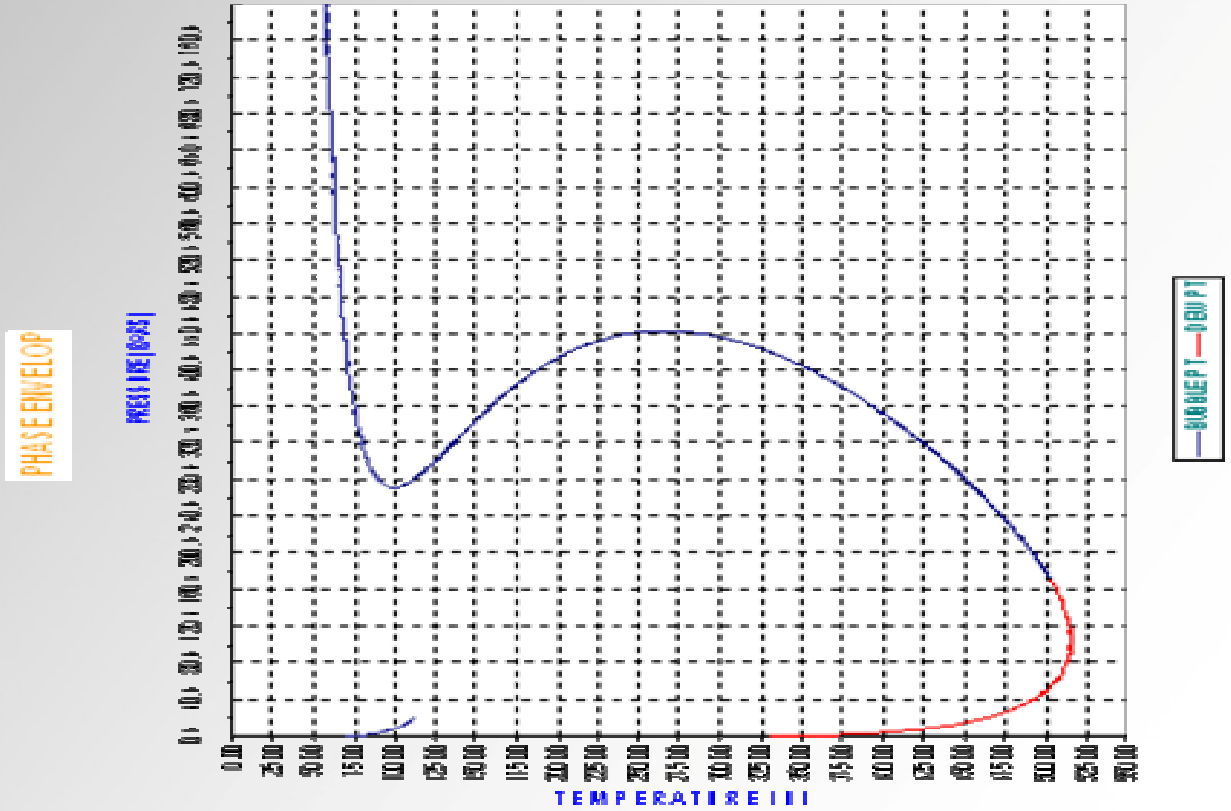
SAMPLE RESULTS FROM EQ-COMP



The phase envelop result for a standard natural gas composition calculated using EQ-COMP is given below:

Methane : 70 %, Ethane : 15 %, Propane : 8 %
i-Butane : 2 %, n-Butane : 2 %, n-Pentane : 1 %
2 Methyl Butane : 1 %, n-Hexane : 1 %

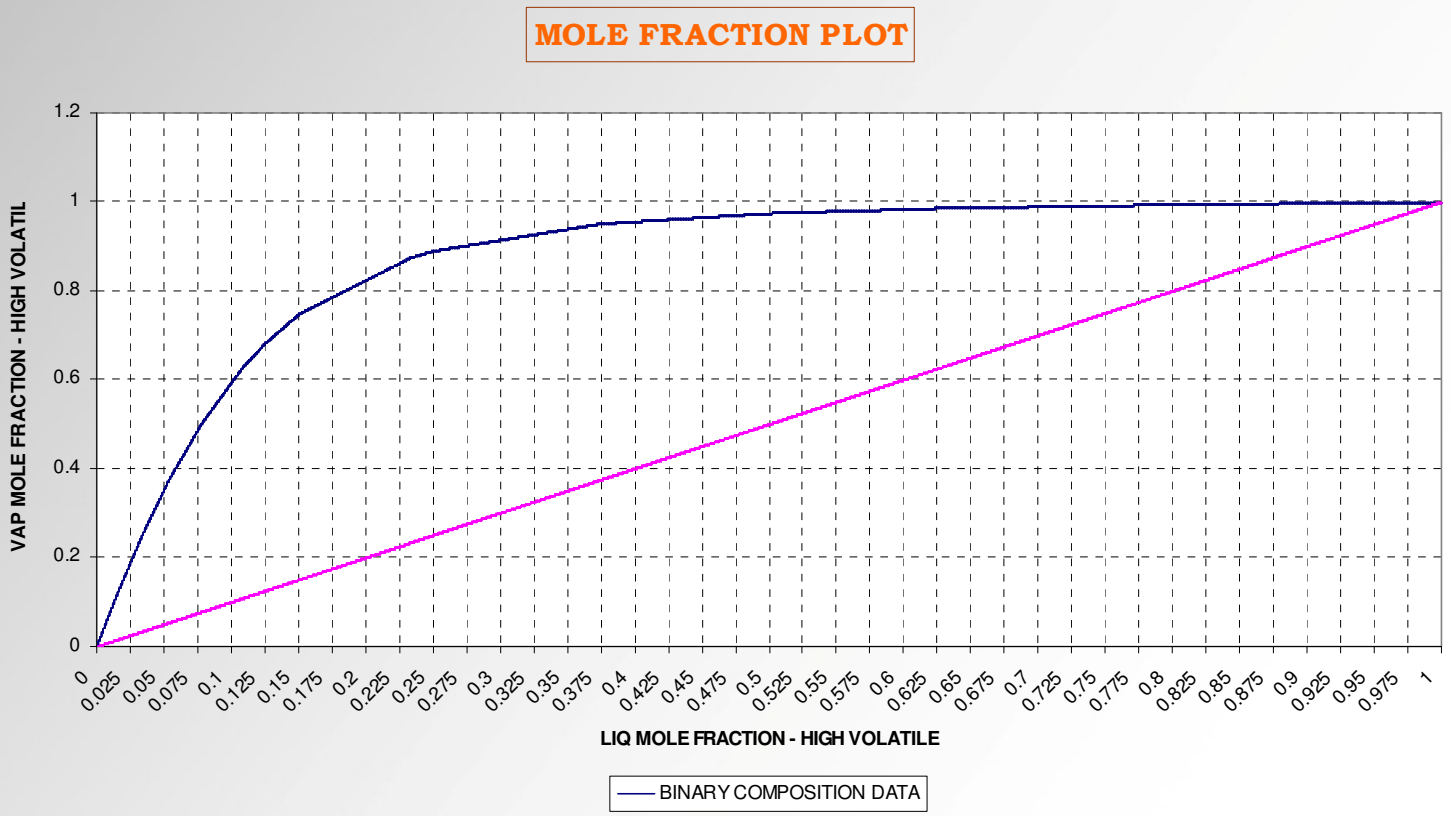
SAMPLE RESULTS FROM EQ-COMP



The phase envelop result for a non-standard composition with high proportion of non-condensables using EQ-COMP is given below:

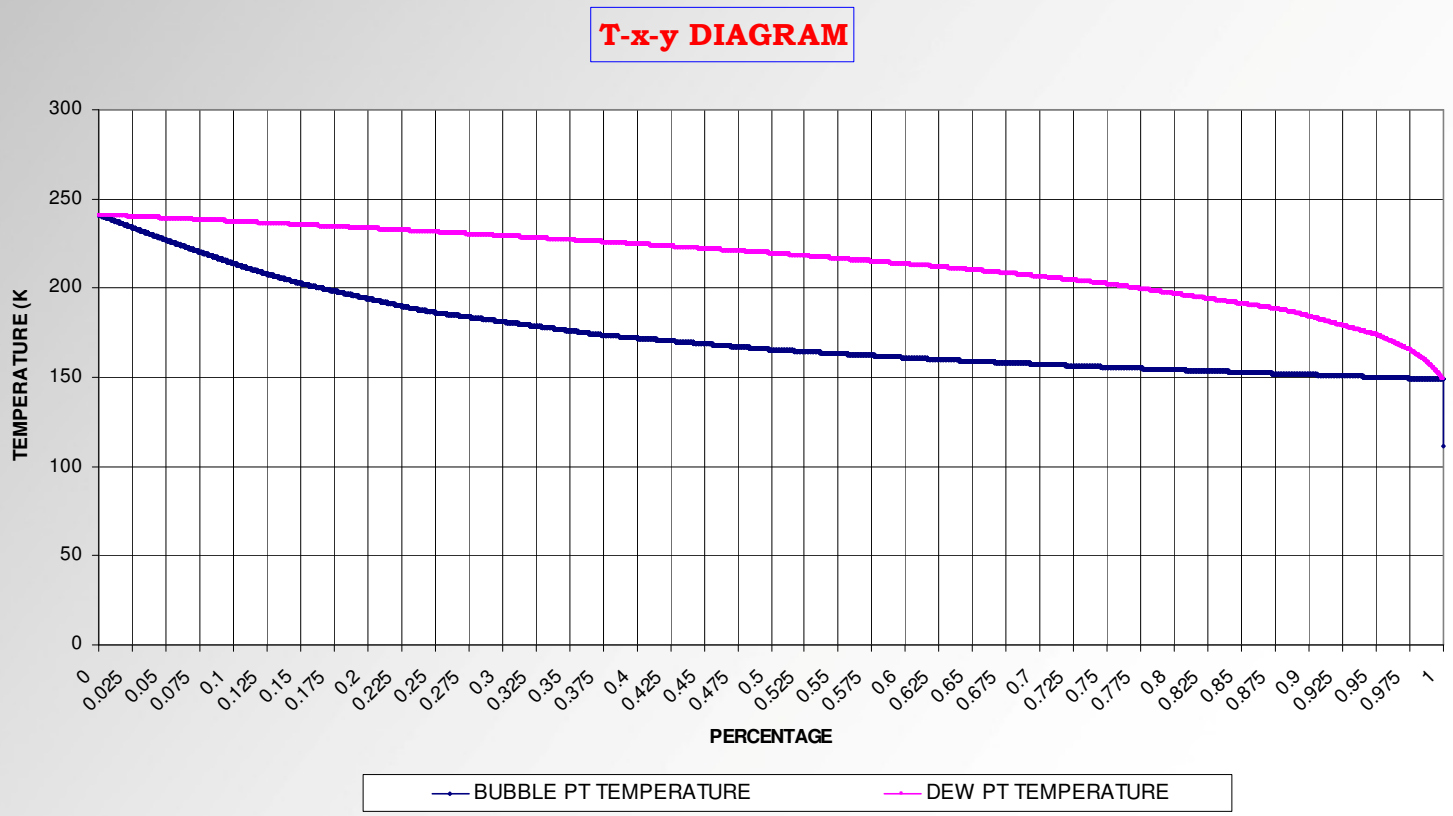
Methane : 10%, n-Hexane : 10%, n-Heptane : 10%
n-Octane : 20 %, Nitrogen : 50 %

SAMPLE RESULTS FROM EQ-COMP



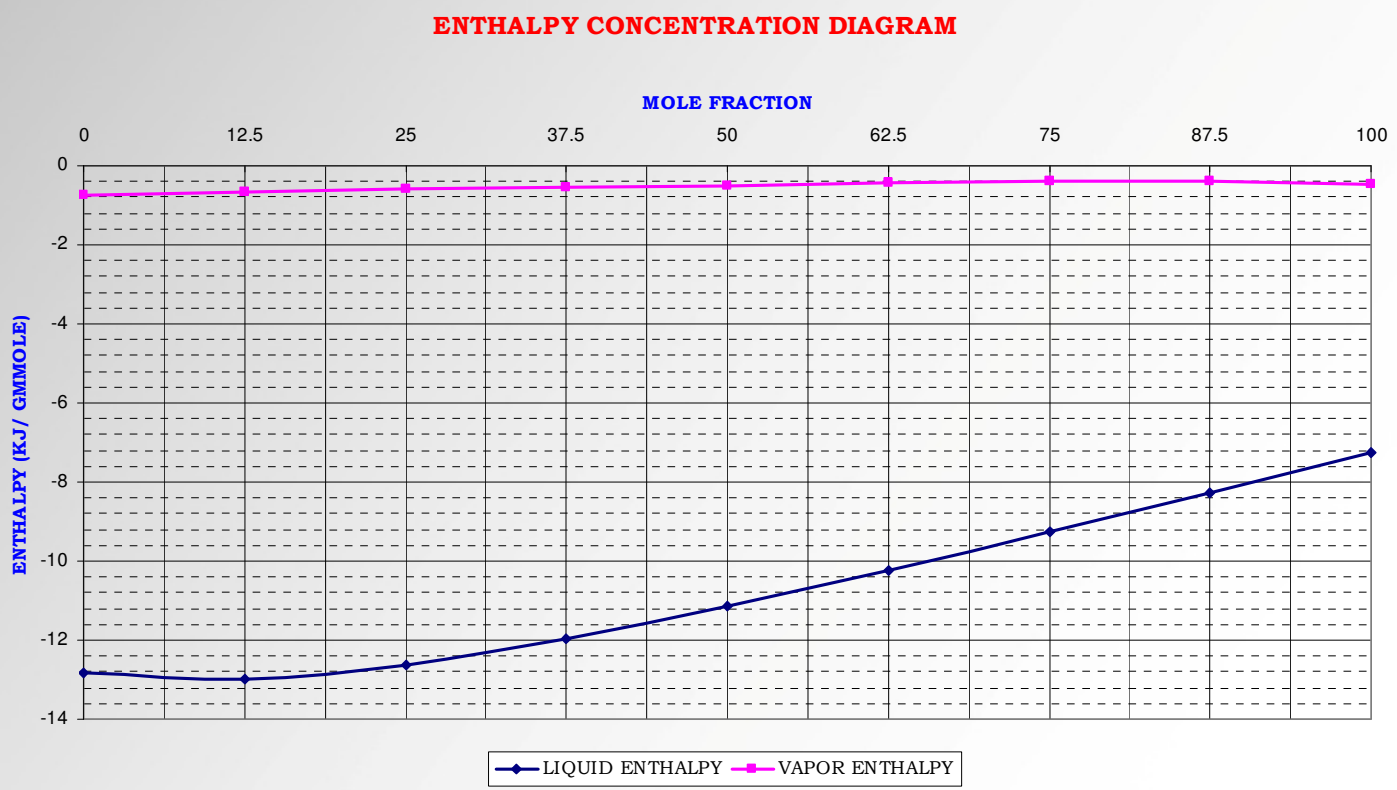
x-y plot for methane-ethane mixture at 10 bars pressure (generated by EQ-COMP)

SAMPLE RESULTS FROM EQ-COMP



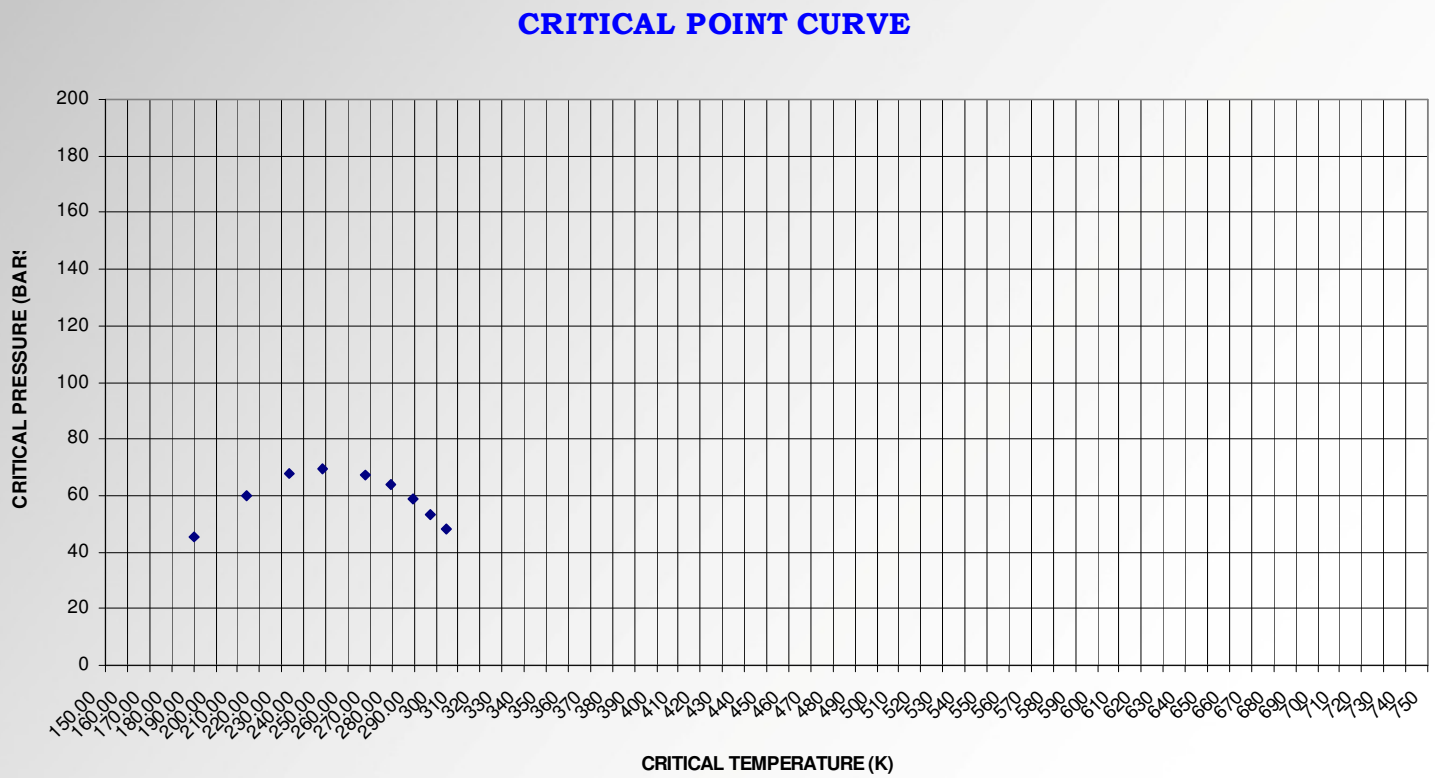
T-x-y plot for methane-ethane mixture at 10 bars pressure (generated by EQ-COMP)

SAMPLE RESULTS FROM EQ-COMP



H-x-y plot for methane-ethane mixture at 10 bars pressure (generated by EQ-COMP)

SAMPLE RESULTS FROM EQ-COMP



Critical point profile for methane-ethane mixture (generated by EQ-COMP)

THANKS

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