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RESEARCH ARTICLE

An Integrated Technique for Natural Gas Numerical PVT Modelling: Case Study of Retrograde Condensate Gas with Python Programming

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ABSTRACT

After the discovery of a gas field, PVT analyses are performed in laboratory to understand the behavior of the reservoir fluid when pressure, temperature, or volume changes. Thereafter, physical or numerical representations of the fluid, called PVT fluid models, are designed to simulate the real fluid behavior when pressure, volume or temperature conditions change. This study aims to propose an integrated technique for natural gas numerical PVT modelling that will help petroleum engineers in determining the mol fractions and compositions of the vapor and liquid phases of hydrocarbon systems as function of pressure and temperature, as well as their trends in some pressure and temperature conditions. A case study has been performed on a historical retrograde condensate gas. The results show that over the production, when the reservoir pressure declines, the gas becomes much dryer and will therefore free less condensate into the reservoir. During its motion from the reservoir to the well head, the liquid phase mol fraction becomes lower so that the condensate-to-gas ratio (CGR) will be low. At pressures under 1000 psia, the decline rate of liquid phase mol fraction becomes higher. At the standard temperature, the more is pressure applied to the gas, the more the liquid phase proportion is. As a result, in the gas storage tanks, the more the gas is compressed, the more the condensate (liquid phase) deposit will be noticed. While transporting the gas through pipeline, the higher the pressure undergone by the gas, the more is the amount of condensate to be counted in pipelines. Moreover, at the standard temperature, the condensate proportion unit variation as function of pressure unit variation is higher when the pressure is under 20 bar.

Keywords: Natural gas, PVT modelling, Python programming, Retrograde condensate gas.

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1. INTRODUCTION

1.1. *Why Natural Gas?*

Crude oil and natural gas have been the major energy sources since the end of the nineteenth-century middle. In fact, the ratio of world oil and gas energy consumption to the overall energy consumption has risen from 27% in 1950 to 58% in 2019 [1]. Natural gas and its byproducts are used for energy production in different sectors (transport, electricity production, industrial engine powering, cooking, household heating, etc.).

In [2], it is underlined that natural gas combustion releases greenhouse gases (carbon dioxide (CO_2)), Nitrous oxide (N_2O), and methane (CH_4) in the atmosphere, and this contributes to the climate change. To prevent disasters due to climate change, [3] recognized that the impacts of climate change will be much lower at the temperature increase of 1.5 °C as compared with 2 °C and resolved to pursue efforts to limit the temperature increase to 1.5 °C. This act [3] also recognizes that limiting global warming to 1.5 °C requires rapid, deep, and sustained reductions in global greenhouse gas emissions, including reducing global carbon dioxide emissions by 45% by 2030 relative to the 2010 level and to net zero around mid-century, as well as deep reductions in other greenhouse gases. To achieve this goal, the international community is relying

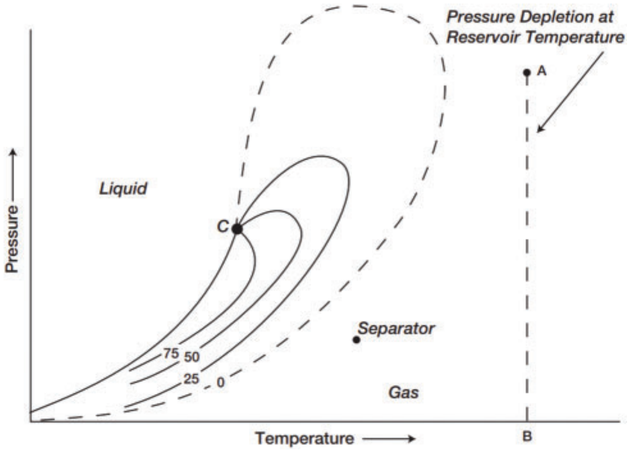


Fig. 1. Phase diagram of a dry gas [8].

on green energy whose majority is composed of renewable energy sources. Besides this, one can keep using natural gas until a quite move to renewable energy since natural gas is the cleanest fossil energy. Indeed, [2] shows that natural gas has a CO_2 emission factor of 53.06 kg CO_2 per mmBtu while coal and coke's CO_2 emission factors range between 93.28 kg and 113.67 kg CO_2 per mmBtu and from 61.71 kg to 102.41 kg CO_2 per mmBtu for crude oil and its byproduct oils.

Despite the obligation of the world to move to green energy, set at Paris Conference of Parties (COP21) in 2015, natural gas consumption continues rising till 2022. In fact, according to [4], [5], natural gas consumption has maintained a rising trend from 3,558.6 billion cubic meters in 2016, 4,034.9 billion cubic meters in 2021.

1.2. *What is a Natural Gas?*

The natural gas is a complex mixture of hydrocarbons with other compounds such as non-hydrocarbon gases (CO_2, N_2, H_2S, etc.), water and metal impurities such as the steal (Fe), nickel (Ni), vanadium (V), found in gaseous form in an underground reservoir [3], [6], [7]. It is mainly composed of lighter hydrocarbons (C1-C4) and is also called methane (CH_4). A reservoir is referred to as gas reservoir if the reservoir temperature is greater than the critical temperature of the reservoir fluid [8], [9]. A reservoir is an underground porous and permeable rock containing a natural, individual, and separated accumulation of hydrocarbons limited by a rock barrier and often an aquifer barrier characterized by a unique pressure system [7].

1.3. *Types of Natural Gas*

As spotlighted by [3], [8]–[13], there are four main types of gases: dry gas, wet gas, near-critical gas-condensate, and retrograde gas-condensate. A dry gas is predominantly composed of methane and non-hydrocarbons such as nitrogen and carbon dioxide [10]. The hydrocarbon mixture exists as a gas both in the reservoir and in the surface facilities [12]. Fig. 1 is a phase diagram of a dry gas reservoir. Usually, a system having a gas-oil ratio (GOR) greater than 100,000 scf/STB is considered to be a dry gas [9].

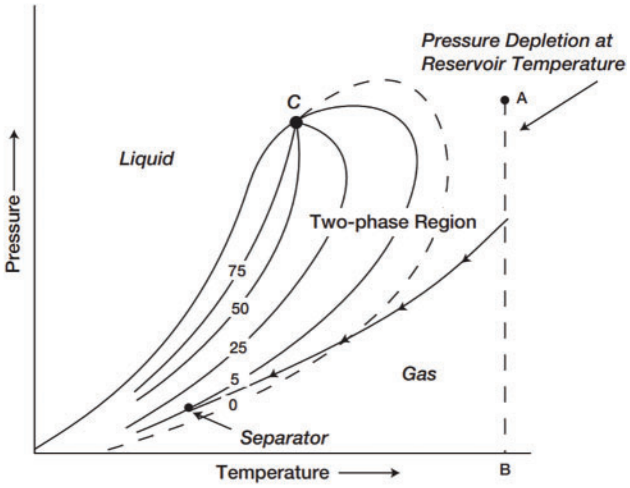


Fig. 2. Phase diagram of wet gas [8].

A wet gas is mainly composed of methane and other light components, with its phase envelope located entirely over a temperature range below that of the reservoir [10], [13]. A typical phase diagram of a wet gas is shown in Fig. 2, where the reservoir temperature is above the cricondentherm of the hydrocarbon mixture. According to [12], because the reservoir temperature exceeds the cricondentherm of the hydrocarbon system, the reservoir fluid always remains in the vapor phase region as the reservoir is depleted isothermally along the vertical line AB. However, as the produced gas flows to the surface, the pressure and temperature of the gas decline. If the gas enters the two-phase region, a liquid phase condenses out of the gas and is produced from the surface separators. Wet gases are characterized by GOR between 60,000 and 100,000 scf/STB, and stock-tank oil gravity above 60° API [9].

If the reservoir temperature is near the critical temperature, as shown in Fig. 3, the hydrocarbon mixture is classified as a near-critical gas condensate [9]. The volumetric behavior of this category of natural gas is described through the isothermal pressure declines as shown by the vertical line 1–3 in Fig. 3. The volumetric behavior of this category of natural gas is described through the isothermal pressure declines, which characterizes a rapid liquid buildup immediately occurring below the dew point [12]. This can be justified by the fact that several quality lines are crossed very rapidly by the isothermal reduction in pressure. At the point where the liquid ceases to build up and begins to shrink again, the reservoir goes from the retrograde region to a normal vaporization region [9].

If the reservoir temperature lies between the critical temperature and cricondentherm of the reservoir fluid, the reservoir is classified as a retrograde condensate gas [12]. Most known retrograde condensate gas reservoirs range 3000 to 6000 psia and 200 to 400 °F [13]. The gas will droup-out liquid by retrograde condensation in the reservoir when the pressure falls below the dew point, from point 1 to point 2 in Fig. 4 [10]. Further condensation from the produced gas also occurs at separator conditions due to cooling. This hydrocarbon systems are characterized by GOR between 8,000 and 70,000 scf/STB (increases with time due to the liquid dropout and the loss of heavy

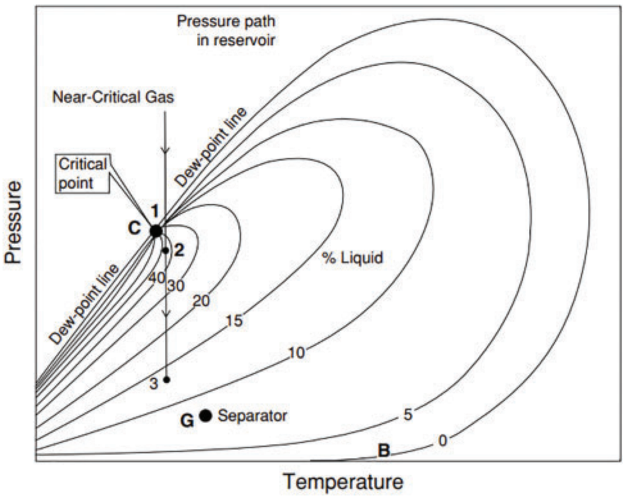


Fig. 3. Typical phase diagram of a near-critical gas condensate system [8].

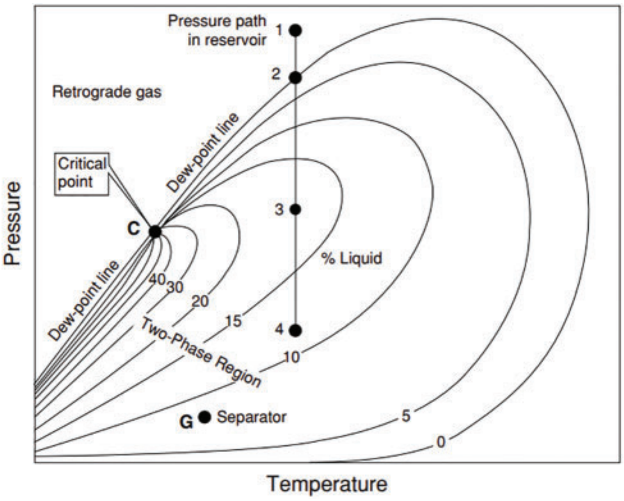


Fig. 4. Typical phase diagram for a retrograde condensate gas [8].

components in the liquid) and a condensate gravity above 50° API [9], [14].

1.4. *What is a PVT Analysis, and Why is PVT Analyses?*

For the proper management of petroleum reservoirs, the main challenges of reservoir and petroleum engineers are to answer the following questions [6]: How large are the reserves? What will the primary recovery be? What kind of crude will be produced, and what will the market pay for it? Does the crude contain unwanted compounds that will destroy tubing or plug the well? For offshore wells, will the crude oil solidify at ocean-bottom temperatures, thereby stopping production? Will gas or condensate be produced at the surface? These questions can be answered through the reservoir fluid phase behavior and volumetric analysis [10] called pressure-volume-temperature (PVT) analysis. It is a series of analyses performed in laboratory whose results tell the behavior of the reservoir fluid when pressure and volume, pressure and temperature or temperature and volume change [15]. The main experiments used for natural condensate gas PVT analysis are gas chromatography tests, flash differential and expansion, constant mass expansion, dew point test, and constant volume depletion [6], [16], [17].

As underlined by [10], most reservoirs are produced by depletion, in which the reservoir pressure declines as fluids are recovered, and the reservoir temperature stays practically constant in most recovery methods. The main variable that determines the behaviour of fluids under reservoir conditions during depletion is, therefore, the reservoir pressure. The fluid behavior changes when it passes from the reservoir to the surface (wellhead, separators, stock tank, and pipeline) conditions. These justify why the fluid pressure-temperature behavior analysis is important for field management. Moreover, PVT analysis can help to establish how much gasoline, kerosene, fuel oil, heavy oil, and bitumen come from refining a barrel of crude and how much gaseous compounds (methane, ethane, propane, and butane), natural gas liquid (C5+), and liquefied petroleum gases are derived from processing a cubic meter of natural gas [6].

1.5. *What is a PVT Model, and Why PVT Modelling?*

A fluid PVT model is a physical or numerical representation of the fluid that can simulate the real fluid behavior when pressure, volume, or temperature conditions change [15]. A numerical fluid PVT model is a set of mathematical functions of pressure, volume, or temperature that can return physiochemical (also called PVT) properties of the fluid for pressure, volume, or temperature conditions change standing in specific ranges [17]. For natural gas, the compositional phase behavior model is used for PVT modelling. This model can predict all PVT properties using only the composition of the original reservoir fluid [10]. For wet or retrograde condensate gases, the modelled properties are generally the fluid system apparent molecular weight, density, specific gravity, isothermal compressibility, formation volume factor, viscosity, coefficient deviation factor, and phase proportion of the gas and the condensate, the deviation factor, condensate-to-gas ratio and the dew point of the gas as well as the bubble point of the condensate [15].

1.6. *Objective of the Study*

This study aims to propose an integrated technique for natural gas numerical PVT modelling that will help petroleum engineers in determining the mol fractions and compositions of the vapor and liquid phases of hydrocarbon systems as functions of pressure and temperature, as well as their trends in some pressure and temperature conditions.

1.7. *Case Study*

A case study will be performed for a hypothetical retrograde condensate gas. Python codes will be written for different PVT properties to compute from the numerical model.

2. MATERIALS AND METHODS

2.1. *Materials*

The main materials used are the results of the PVT analysis performed on the hypothetical condensate gas sample. These PVT analysis results are summarized in Table I.

TABLE I: CASE STUDY GAS PVT ANALYSIS RESULTS [13]

Components	Molar mass, lb/lb-mol	Mol fraction	Pc, psia	Tc, °R	ω
CO_2	44.010	0.009	1071	547.9	0.225
N_2	28.010	0.003	493	227.6	0.040
C1	16.040	0.535	667.8	343.37	0.0104
C2	30.100	0.115	707.8	550.09	0.0986
C3	44.100	0.088	616.3	666.01	0.1524
i-C4	58.100	0.023	529.1	734.98	0.1848
n-C4	58.100	0.023	550.7	765.65	0.2010
i-C5	72.200	0.015	490.4	829.1	0.2223
n-C5	72.200	0.015	488.6	845.7	0.2539
C6	86.200	0.015	436.9	913.7	0.3007
C7+	4452	0.159	320.3	1139.4	0.5069

Apart from these data, MS Excel and Jupyter Notebook (through Anaconda) have been used for data processing and programming, respectively.

2.2. *Methods*

Several numerical or empirical PVT modelling techniques exist for natural gases modelling, most of them being forms of the compositional model. Composition model formulae or algorithms are based on the number of hydrocarbons components to be considered. The model proposed by the current study is a seven-item (or nine-item) model. The items are the hydrocarbon components C1, C2, C3, C4, C5, C6 and C7+ or C1, C2, C3, iC4, nC4, iC5, nC5, C6 and C7+ when the different forms of butane and pentane (iso and normal) have been separated in the chromatography process. One can see that the number of these components are seven or nine when the different forms of butane and pentane are separated.

The proposed technique will set formulae and algorithms for the determination of the following PVT properties and the PVT properties curves plotting:

- the mol fractions of the vapor and liquid phases ($n_v(p, T)$ and $n_L(p, T)$),
- the composition of each phase of the gas ($y_i(p, T)$ and $x_i(p, T)$.

2.2.1. *PVT Properties Determination*

The formulae and algorithms proposed for the PVT properties determination are as follows.

To determine the mol fraction of the vapor and liquid phases ($n_v(p, T)$ and $n_L(p, T)$) and the composition $y_i(p, T)$ of vapor phase and $x_i(p, T)$ of liquid phase, it is needed to perform flash calculations by solving Rachford-Rice equation with an iterative method of Newton-Raphson.

Equation (1), the Rachford-Rice equation, is written as follows [12]:

$$f\,(n_v) = \sum_{i=1}^{m} \frac{z_i(K_i - 1)}{1 + n_v(K_i - 1)} = 0 \qquad (1)$$

where z_i the mol fraction of the component i of the mixture, $K_i = y_i/x_i$ the equilibrium ratio of i (y_i and x_i the respective mol fractions of i in the vapor and liquid phases), n_v the mol fraction of the vapor phase.

The algorithm proposed in the current study for the determination of the mol fractions of the vapor and liquid phases ($n_v(p, T)$ and $n_L(p, T)$, respectively) and the composition $y_i(p, T)$ of vapor phase and $x_i(p, T)$ of liquid phase, is as follows:

Algorithm 1: Algorithm for Solving Rachford-Rice Equation

- **Step 1:** For each component i, compute the equilibrium ratio $K_i = y_i/x_i$ with:

  –Wilson's correlation (2) for hydrocarbon components (C1 to C6) at low pressure (less than 1000 psia),

  –Whitson and Torp's correlation (3) for hydrocarbon components (C1 to C6) at pressure above 1000 psia,

  –Katz and Hachmuth's rule (5) for C_{7+} fraction,

  –Lohrenze, Clark, and Francis' correlation ((6) to (8)) for non-hydrocarbon components (CO_2, H_2S and N_2):

$$K_i = \frac{P_{ci}}{P} exp\left[5.37(1 + w_i)\left(1 - \frac{T_{ci}}{T}\right)\right] \qquad (2)$$

$$K_i = \left(\frac{P_{ci}}{P_k}\right)^{A-1} \frac{P_{ci}}{P} exp \left[5.37(1 + w_i)\left(1 - \frac{T_{ci}}{T}\right)\right] \qquad (3)$$

where $A = 1 - \left(\frac{p}{P_k}\right)^{0.7}$, P_k the convergence pressure, in psig, given by the Standing formula of (4); where p is the system pressure in psig, T the system temperature in °R, P_{ci} the critical pressure of the component i, in psig, T_{ci} the critical temperature of the component i, in °R and w_i the acentric factor of component i.

$$p_k = 60M_{aC7+} - 4200 \qquad (4)$$

$$K_{C_{7+}} = 0.15\,K_{C_7} \qquad (5)$$

$$\ln\left(K_{H_2S}\right) = \left(1 - \frac{p}{P_k}\right)^{0.8}$$

$$\begin{bmatrix} 6.3992127 + \dfrac{1399.2204}{T} - \\ \ln(p)\left(0.76885112 + \dfrac{18.215052}{T}\right) - \\ \dfrac{1112446.2}{T^2} \end{bmatrix} \tag{6}$$

$$\ln\left(K_{N_2}\right) = \left(1 - \frac{p}{P_k}\right)^{0.4} \begin{bmatrix} 11.294748 + \dfrac{1184.2409}{T} - \\ 0.90459907 \ln(p) \end{bmatrix} \tag{7}$$

$$\ln\left(K_{CO_2}\right) = \left(1 - \frac{p}{P_k}\right)^{0.6} \begin{bmatrix} 7.0201913 + \dfrac{152.7291}{T} - \\ \ln(p)\left(1.8896974 + \dfrac{1719.2956}{T}\right) - \\ \dfrac{644740.69}{T^2} \end{bmatrix} \tag{8}$$

where P_k the convergence pressure, in *psig*, p is the system pressure in psig and T the system temperature in °R.

- **Step 2:** Attribute a value $n_v^{(0)}$, between 0 and 1, to n_v. One can use the relationship of (9) for a good value attribution to n_v. Here, $n = 0$ is the iteration order.

$$n_v^{(0)} = \frac{A}{A+B} \tag{9}$$

where

$$A = \sum\nolimits_{i=1}^{N} \left[z_i\left(K_i - 1\right)\right] \tag{10}$$

$$B = \sum\nolimits_{i=1}^{N} \left[z_i\left(\frac{1}{K_i} - 1\right)\right] \tag{11}$$

where N is the number of components in the hydrocarbon mixture, z_i the mol fraction of the component i of the mixture and $K_i = y_i/x_i$ the equilibrium ratio of i.

- **Step 3:** Compute the function $f\left(n_v\right)$ as given by (1) with the value of n_v obtained in step 1.

If the absolute value of $f\left(n_v\right)$ is smaller than a preset tolerance *eps*, then $n_v^{(0)}$ is the desired solution of (1).

If the absolute value of $f\left(n_v\right)$ is greater than the preset tolerance, then update n_v with (12):

$$n_v^{(n+1)} = n_v^{(n)} - \frac{f\left[n_v^{(n)}\right]}{f'\left[n_v^{(n)}\right]} \tag{12}$$

where n the iteration order and $f'\left(n_v\right)$ the derivative of $f\left(n_v\right)$ defined as follows (13):

$$f'\left(n_v\right) = -\sum_{i=1}^{m} \left\{\frac{z_i\left(K_i - 1\right)^2}{\left[1 + n_v\left(K_i - 1\right)^2\right]}\right\} \tag{13}$$

This procedure is repeated with the new value of $n_v^{(n)}$ until convergence is achieved, that is, when $\left|f\left(n_v\right)\right| \leq eps$ or $\left|f\left(n_v^{(n+1)}\right) - f\left(n_v^{(n)}\right)\right| \leq eps$.

The common tolerance used is 10^{-6}.

The last computed $n_v^{(n)}$ satisfying the convergence condition is the researched n_v.

- **Step 4:** Calculate n_L with (14):

$$n_L = 1 - n_v \tag{14}$$

- **Step 5:** Calculate the composition of the liquid phase x_i by applying (15):

$$x_i = \frac{z_i}{n_L + n_v K_i} = \frac{z_i}{1 + n_v(K_i - 1)} \tag{15}$$

- **Step 6:** Calculate the composition of the vapor phase y_i by applying (16):

$$y_i = x_i K_i = \frac{z_i K_i}{1 + n_v(K_i - 1)} \tag{16}$$

As one can see in (2) and (3), the pseudo critical pressure and temperature P_{pc} and T_{pc} of C_{7+} and the other components will be required. There are computed with (17) and (18) [7], [15], [18]:

$$T_{pc} = \sum_{i=1}^{m} y_i T_{ci} \tag{17}$$

$$P_{pc} = \sum_{i=1}^{m} y_i p_{ci} \tag{18}$$

where T_{ci} the critical temperature of component I in °R, P_{ci} the critical pressure of component I in psia, T the temperature in °R and p the pressure in psia.

When the gas contains non-hydrocarbon components (CO_2, H_2S and N_2), the adjusted pseudo critical properties T'_{pc} and P'_{pc} are used [18].

Several adjustment techniques are developed. The one to use is the adjustment method of Witchert and Aziz. The formulae of Witchert and Aziz are given by (19) and (20) [13]:

$$T'_{pc} = T_{pc} - \in \tag{19}$$

$$p'_{pc} = \frac{p_{pc} T'_{pc}}{T_{pc} + B\left(1 - B\right) \in} \tag{20}$$

where:

$$\in = 120\left(A^{0.9} - A^{1.6}\right) + 15\left(B^{0.5} - A^{4.0}\right) \tag{21}$$

$$A = y_{H_2S} + y_{CO_2} \tag{22}$$

$$B = y_{H_2S} \tag{23}$$

where T_{pc} and T'_{pc} are in °R, P_{pc} and P'_{pc} in psia and $\in$ the adjustment factor, y_{H_2S} and y_{CO_2} the mol fraction of H_2S, and CO_2 in the vapor phase.

2.2.2. Hydrocarbon System PVT Properties Trends Determination

In practice, PVT properties curves help engineers to know the trend of these properties as function of one of the explicative variables (pressure and temperature) or both (when they depend on the two variables) and for quick analyses thereof. Since this study set down techniques for different PVT parameters determination, it is going to propose ways to plot in two dimensions (2D), parameters variations as function of pressure or temperature. When the PVT property of interest depends on pressure and temperature, the 2D curve can be gotten for a specific (fixed) pressure or temperature.

The following is algorithm for plotting a PVT parameter as function of temperature. The process is the same for a parameter curve as function of pressure.

Algorithm 2: Algorithm for PVT Property Curve Plotting

Let I be the PVT parameter of interest.

- **Step 1:** If I depends on pressure and temperature, that is $I = I(p, T)$, let's note $I_{p_0}(T) = I(p_0, T)$ the function of that parameter for the pressure p_0 for which the curve of I is needed.
- **Step 2:** Set a temperature range $[T_{min}; T_{max}]$ to be used for computation of the parameter I.
- **Step 3:** Choose the number M of the parameter I required for the curve plotting.
- **Step 4:** Determine the temperature step dT. It is given by (24):

$$dT = \frac{T_{max} - T_{min}}{M} \tag{24}$$

- **Step 5:** Determine the sets of temperatures to be used, $S_T = \{T_1, T_2, \ldots, T_M\}$. Here $T_1 = T_{min}$ and $T_M = T_{max}$. T_i is computed with (25), for $2 \le i \le M - 1$.

$$T_i = T_1 + (i - 1)\,dT \tag{25}$$

- **Step 6:** For each temperature T_i of $S_T = \{T_1, T_2, \ldots, T_M\}$, compute the value $I_i = I_{p_0}(T_i) = I(p_0, T_i)$ of the parameter I.
- **Step 7:** Form the set of the parameter I points, $A = \{A_1 = (T_1, I_1); A_2 = (T_2, I_2); \ldots; A_M = (T_M, I_M)\}$ using the computed I_i and the corresponding temperatures.
- **Step 8:** Plot the curve of the parameter I using the A_i points $(1 \le i \le M)$. The curve is obtained by linking the consecutive A_i points with straight line segments.

3. RESULTS AND DISCUSSION

3.1. Python Codes

The case study has been performed with Python programming on Jupiter Notebook through Anaconda. Three (03) Python functions have been written. These are:

- K (Component, P, T) for hydrocarbon systems components equilibrium ratio Ki computation as a function of component, pressure and temperature,
- RRSolver_Nv (P, T) for hydrocarbon systems vapor and liquid mol fractions computation as a function of pressure and temperature,
- RRSolver_XY (P, T) for vapor and liquid phases compositions computation as a function of pressure and temperature.

The codes of these functions are those of Figs. 5 to 7.

3.2. Trends of the Retrograde Condensate Gas Vapor and Liquid Phases Mol Fractions and Compositions

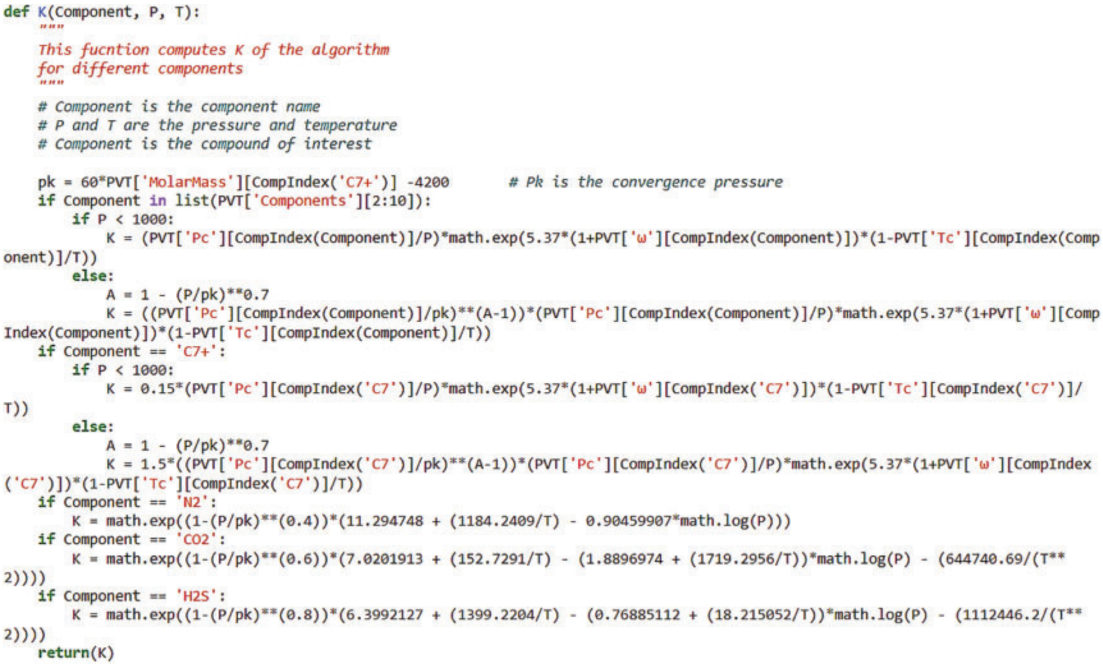
The different algorithms described in the methodology section have been applied to determine the retrograde condensate gas liquid and vapor phases mol fractions and their compositions trends at the reservoir temperature (270 °F) and the standard temperature (60 °F).

Their trends at the reservoir temperature will help to simulate the gas behavior in the reservoir over the production. At the surface temperature, the gas behavior in the storage facilities in compressed form or in pipelines over its transportation can be simulated. The results are as follows.

3.2.1. Vapor and Liquid Phases Mol Fractions Trends

At the reservoir temperature, the vapor mol fraction has a decreasing trend (Fig. 8a) and the liquid mol fraction has an increasing trend (Fig. 8b) when the reservoir pressure increases. This means that while the reservoir pressure raises, the mol proportion of the gas vapor phase will drop in favor of its liquid phase. As a result, over the production, when the reservoir pressure declines, the gas becomes much dryer and will therefore free less condensate into the reservoir (Fig. 8a). During its motion from the reservoir to the well head, the liquid phase mol fraction becomes lower so that the condensate-to-gas ratio (CGR) will be low (Fig. 8b). At pressures under 1000 psia, the decline rate of liquid phase mol fraction becomes higher (Fig. 8b). Then, the lower the well head pressure (WHP) under 1000 psia, the lesser the amount of produced condensate.

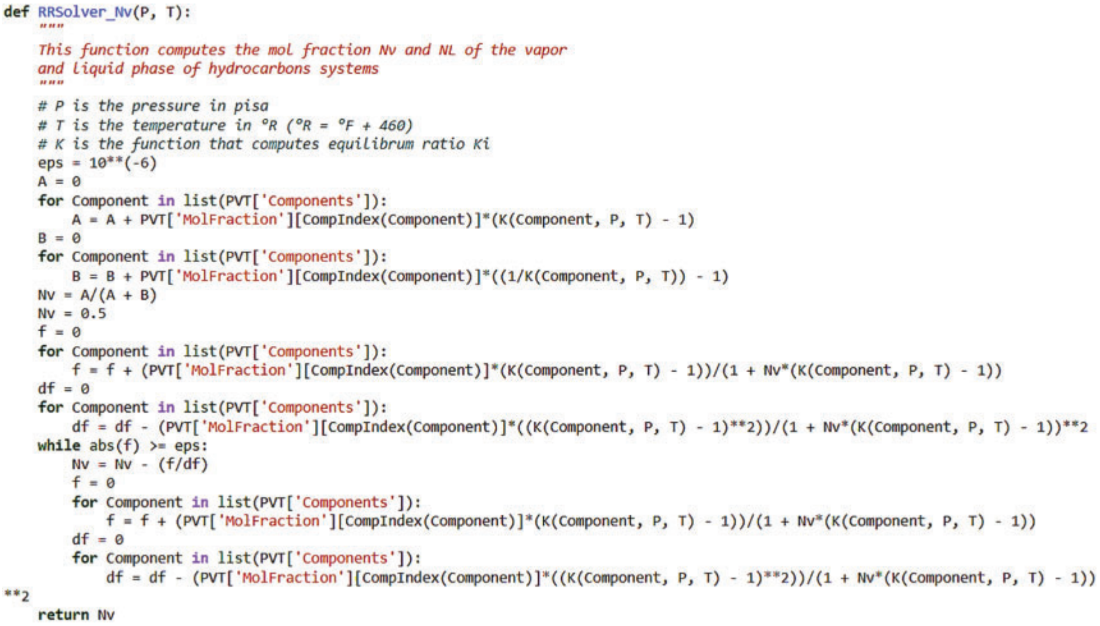
At the standard temperature, the vapor and liquid phases mol fractions have decreasing and increasing trends, respectively (Figs. 9a and 9b). Therefore, the more is pressure applied to the gas, the more the liquid phase proportion is (Fig. 9b) and less the vapor phase is (Fig. 9a). In practice, the fact derived from this gas behavior is as follows. In the gas stockage tanks, the more the gas is compressed, the more condensate (liquid phase) deposit will be noticed. While transporting the gas through pipeline, the higher the pressure undergone by the gas, the more is the amount of condensate to be counted in pipelines. The condensate proportion unit variation as function of pressure unit variation is higher when the pressure is under 20 bar (Fig. 9b).



```
def K(Component, P, T):
    """
    This fucntion computes K of the algorithm
    for different components
    """
    # Component is the component name
    # P and T are the pressure and temperature
    # Component is the compound of interest

    pk = 60*PVT['MolarMass'][CompIndex('C7+')] -4200       # Pk is the convergence pressure
    if Component in list(PVT['Components'][2:10]):
        if P < 1000:
            K = (PVT['Pc'][CompIndex(Component)]/P)*math.exp(5.37*(1+PVT['ω'][CompIndex(Component)])*(1-PVT['Tc'][CompIndex(Comp
onent)]/T))
        else:
            A = 1 - (P/pk)**0.7
            K = ((PVT['Pc'][CompIndex(Component)]/pk)**(A-1))*(PVT['Pc'][CompIndex(Component)]/P)*math.exp(5.37*(1+PVT['ω'][Comp
Index(Component)])*(1-PVT['Tc'][CompIndex(Component)]/T))
    if Component == 'C7+':
        if P < 1000:
            K = 0.15*(PVT['Pc'][CompIndex('C7')]/P)*math.exp(5.37*(1+PVT['ω'][CompIndex('C7')])*(1-PVT['Tc'][CompIndex('C7')]/
T))
        else:
            A = 1 - (P/pk)**0.7
            K = 1.5*((PVT['Pc'][CompIndex('C7')]/pk)**(A-1))*(PVT['Pc'][CompIndex('C7')]/P)*math.exp(5.37*(1+PVT['ω'][CompIndex
('C7')])*(1-PVT['Tc'][CompIndex('C7')]/T))
    if Component == 'N2':
        K = math.exp((1-(P/pk)**(0.4))*(11.294748 + (1184.2409/T) - 0.90459907*math.log(P)))
    if Component == 'CO2':
        K = math.exp((1-(P/pk)**(0.6))*(7.0201913 + (152.7291/T) - (1.8896974 + (1719.2956/T))*math.log(P) - (644740.69/(T**
2))))
    if Component == 'H2S':
        K = math.exp((1-(P/pk)**(0.8))*(6.3992127 + (1399.2204/T) - (0.76885112 + (18.215052/T))*math.log(P) - (1112446.2/(T**
2))))
    return(K)
```

Fig. 5. Python code for K (Component, P, T) function.



```
def RRSolver_Nv(P, T):
    """
    This function computes the mol fraction Nv and NL of the vapor
    and liquid phase of hydrocarbons systems
    """
    # P is the pressure in pisa
    # T is the temperature in °R (°R = °F + 460)
    # K is the function that computes equilibrum ratio Ki
    eps = 10**(-6)
    A = 0
    for Component in list(PVT['Components']):
        A = A + PVT['MolFraction'][CompIndex(Component)]*(K(Component, P, T) - 1)
    B = 0
    for Component in list(PVT['Components']):
        B = B + PVT['MolFraction'][CompIndex(Component)]*((1/K(Component, P, T)) - 1)
    Nv = A/(A + B)
    Nv = 0.5
    f = 0
    for Component in list(PVT['Components']):
        f = f + (PVT['MolFraction'][CompIndex(Component)]*(K(Component, P, T) - 1))/(1 + Nv*(K(Component, P, T) - 1))
    df = 0
    for Component in list(PVT['Components']):
        df = df - (PVT['MolFraction'][CompIndex(Component)]*((K(Component, P, T) - 1)**2))/(1 + Nv*(K(Component, P, T) - 1))**2
    while abs(f) >= eps:
        Nv = Nv - (f/df)
        f = 0
        for Component in list(PVT['Components']):
            f = f + (PVT['MolFraction'][CompIndex(Component)]*(K(Component, P, T) - 1))/(1 + Nv*(K(Component, P, T) - 1))
        df = 0
        for Component in list(PVT['Components']):
            df = df - (PVT['MolFraction'][CompIndex(Component)]*((K(Component, P, T) - 1)**2))/(1 + Nv*(K(Component, P, T) - 1))
**2
    return Nv
```

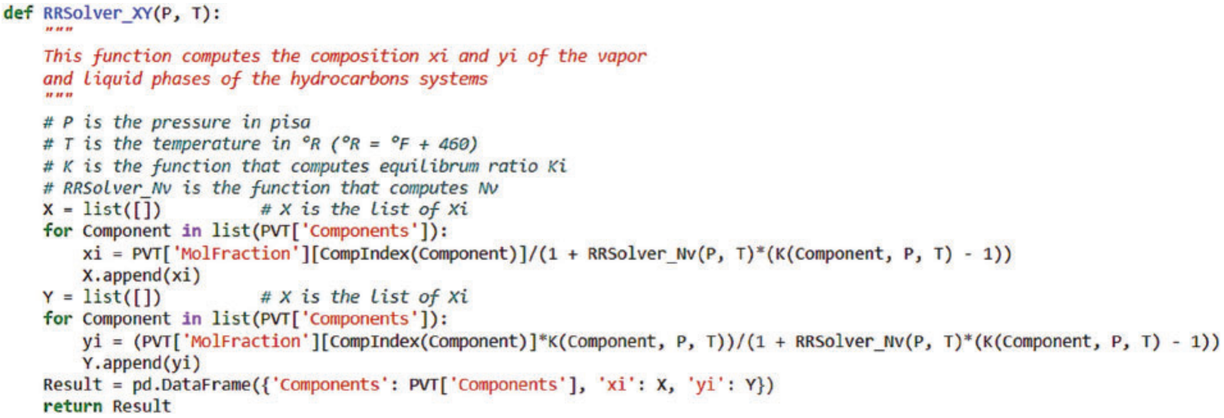
Fig. 6. Python code for RRSolver_Nv (P, T) function.

3.2.2. *Gas Vapor and Liquid Phases Compositions*

At the reservoir temperature, the hydrocarbon system vapor phase is mainly composed of methane (Fig. 10a), followed by ethane and propane (Fig. 10b). When the system pressure decreases, the mol fraction of methane decreases (Fig. 10a) and those of ethane and propane increase (Fig. 10b). As far as the hydrocarbon system liquid phase is concerned, it is mainly composed of heptane-plus (Fig. 11a), followed by propane and methane (Fig. 11b). When the system pressure decreases, the mol fraction of heptane-plus increases (Fig. 11a), while those of propane and methane decrease (Fig. 11b).

At the standard temperature, the hydrocarbon system vapor phase is mainly composed of methane (Fig. 12a), followed by ethane and propane (Fig. 12b). When the system pressure increases, the mol fractions of methane and ethane increase (Fig. 12a and 12b) while the one of propane decreases (Fig. 12b). The hydrocarbon system liquid phase, it is mainly composed of heptane-plus (Fig. 13a), followed by hexane, pentane, and propane (Fig. 13b). When the system pressure increases, the mol fraction of heptane-plus decreases (Fig. 13a) while those of hexane, pentane and propane increase (Fig. 11b).

These vapor and liquid phases composition trends come and confirm the gas behavior determined on the basis of the vapor phase and liquid phase mol fraction trends. Indeed, the vapor phase and methane mol fractions go in the same direction; that is, the vapor phase mol fraction increases when the one methane raises and vice versa. In the same way, the more the liquid phase mol fraction, the



```
def RRSolver_XY(P, T):
    """
    This function computes the composition xi and yi of the vapor
    and liquid phases of the hydrocarbons systems
    """
    # P is the pressure in pisa
    # T is the temperature in °R (°R = °F + 460)
    # K is the function that computes equilibrum ratio Ki
    # RRSolver_Nv is the function that computes Nv
    X = list([])          # X is the list of Xi
    for Component in list(PVT['Components']):
        xi = PVT['MolFraction'][CompIndex(Component)]/(1 + RRSolver_Nv(P, T)*(K(Component, P, T) - 1))
        X.append(xi)
    Y = list([])          # X is the list of Xi
    for Component in list(PVT['Components']):
        yi = (PVT['MolFraction'][CompIndex(Component)]*K(Component, P, T))/(1 + RRSolver_Nv(P, T)*(K(Component, P, T) - 1))
        Y.append(yi)
    Result = pd.DataFrame({'Components': PVT['Components'], 'xi': X, 'yi': Y})
    return Result
```

Fig. 7. Python code for RRSolver_XY (P, T) function.

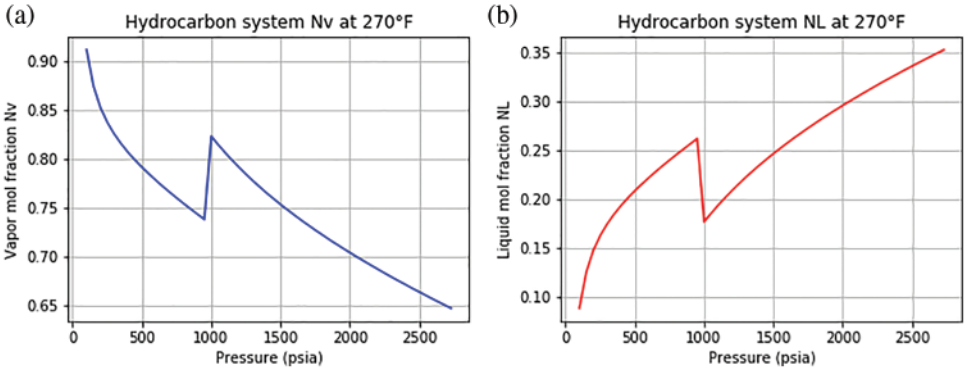


Fig. 8. Trend of hydrocarbon system: a) vapor phase mol fraction, b) liquid phase mol fraction at the reservoir temperature.

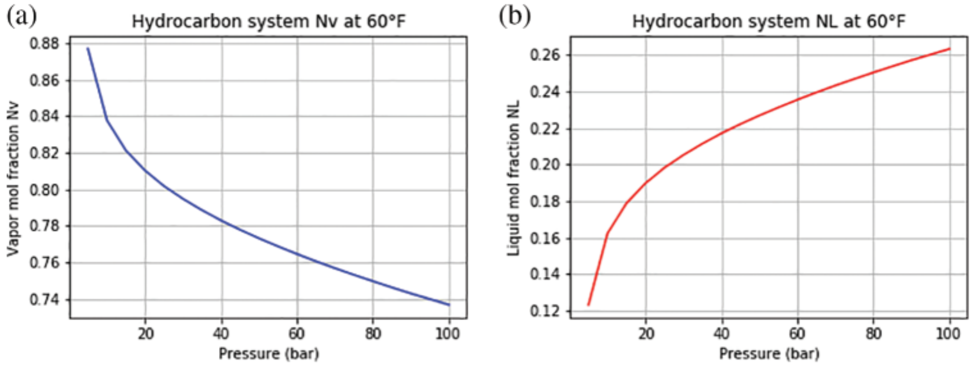


Fig. 9. Trend of hydrocarbon system: a) vapor phase mol fraction, b) liquid phase mol fraction at the standard temperature.

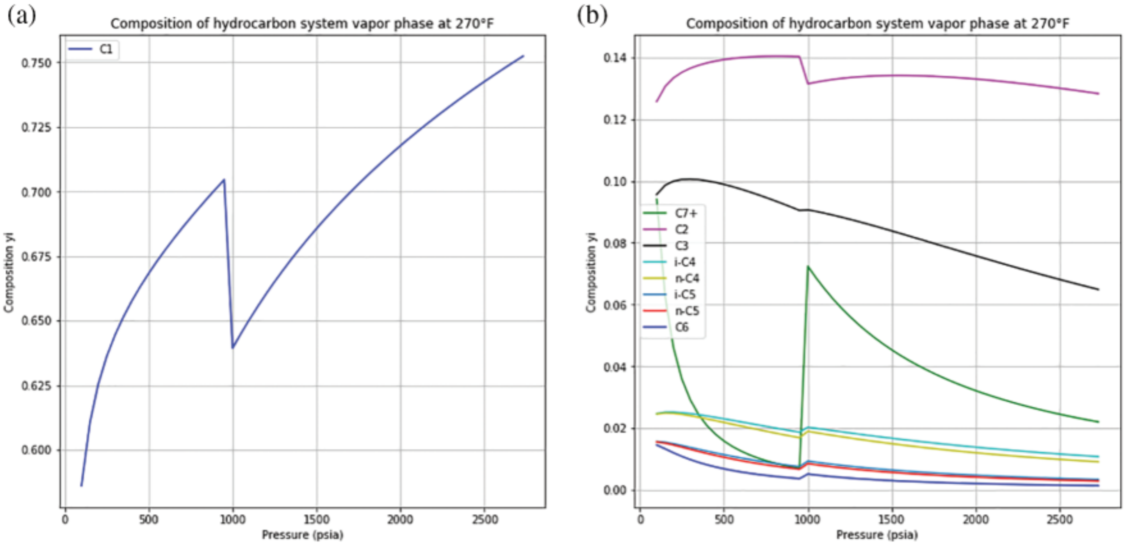


Fig. 10. Trend of hydrocarbon system: a) vapor phase composition in C1, b) vapor phase composition in C2 to C7+ at the reservoir temperature.

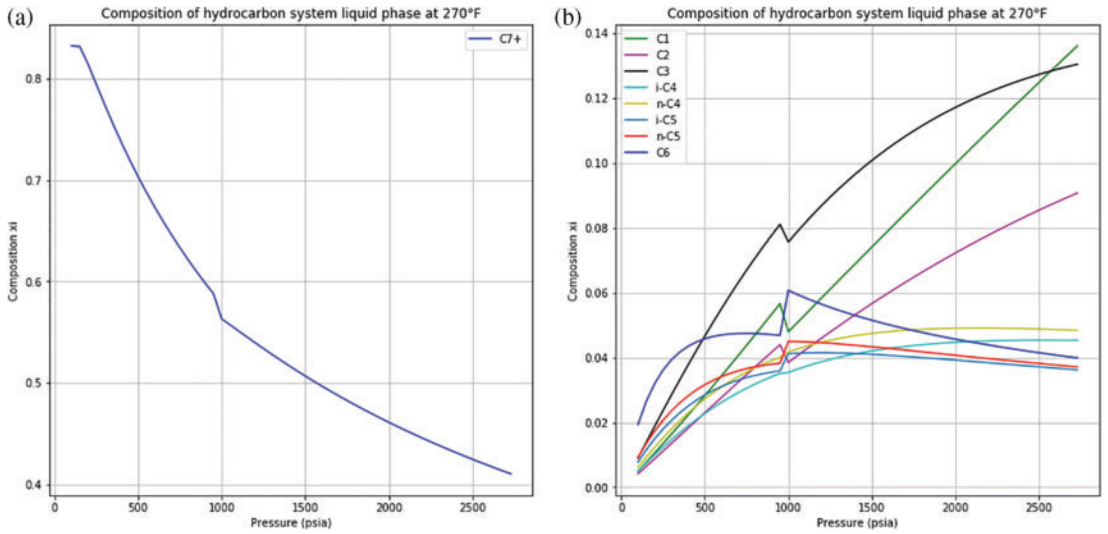


Fig. 11. Trend of hydrocarbon system: a) liquid phase composition in C7+ at the reservoir temperature, b) liquid phase composition in C1 to C6 at the reservoir temperature.

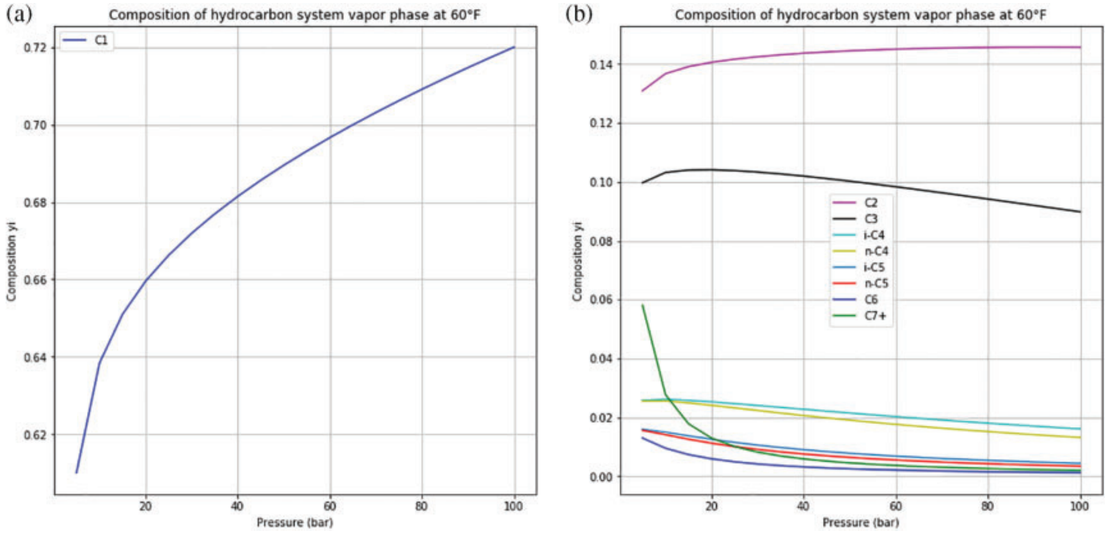


Fig. 12. Trend of hydrocarbon system: a) vapor phase composition in C1, b) vapor phase composition in C2 to C7+ at the standard temperature.

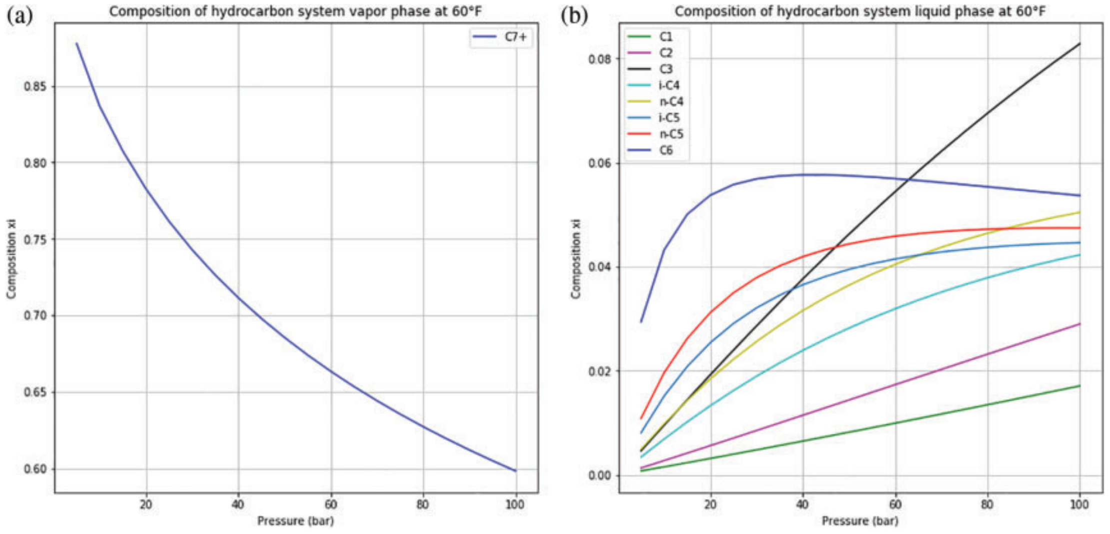


Fig. 13. Trend of hydrocarbon system: a) liquid phase composition in C7+, b) system liquid phase composition in C1 to C6 at the standard temperature.

higher C5+ mol fraction (and then C7+ mol fraction) and vice versa.

4. CONCLUSIONS AND RECOMMENDATION

Natural gas is a complex mixture of hydrocarbons with other compounds such as non-hydrocarbon gases, water, and metal impurities, and is mainly composed of lighter hydrocarbons (C1–C4). Despite the obligation of the world to move to green energy, natural gas consumption continue rising till 2022 since it is the cleanest fossil energy. Four main gas reservoirs exist, each one characterized by a phase behavior when pressure and temperature conditions change: dry gas, wet gas, near-critical gas condensate and retrograde condensate gas.

After the discovery of gas fields, a series of analyses (PVT analyses) are performed in the laboratory to understand the behavior of the reservoir fluid when pressure, temperature or volume changes. On the basis of PVT analyses, physical or numerical representations of the fluid, called PVT fluid models, are designed to simulate the real fluid behavior when pressure, volume or temperature conditions change. For instance, these models help engineers to know reservoir fluids behavior when they pass from the reservoir to the surface (wellhead, separators, stock tank and pipeline) conditions and the amount of each byproduct to obtain after the reservoir fluid processing.

This study proposed an integrated technique for natural gas numerical PVT modelling, that will help petroleum engineers to determine the mol fractions and the compositions of the vapor and liquid phases of hydrocarbon systems as function of pressure and temperature, as well as their trends in some pressure and temperature conditions.

A case study has been performed on a historical retrograde condensate gas. The results show that over the production, when the reservoir pressure declines, the gas becomes much dryer and will therefore free less condensate into the reservoir. During its motion from the reservoir to the well head, the liquid phase mol fraction becomes lower so that the condensate-to-gas ratio (CGR) will be low. At pressures under 1000 psia, the decline rate of liquid phase mol fraction becomes higher. At the standard temperature, the more is pressure applied to the gas, the more the liquid phase proportion is. As a result, in the gas storage facilities, the more the gas is compressed, the more condensate (liquid phase) deposit will be noticed. While transporting the gas through pipeline, the higher the pressure undergone by the gas, the more is the amount of condensate to be counted in pipelines. Moreover, at the standard temperature, the condensate proportion unit variation as function of pressure unit variation is higher when the pressure is under 20 bar.

We recommend the design of numerical models for the other hydrocarbon fluids (gas and crude oil) PVT properties that are not considered in the current study.

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CONFLICT OF INTEREST

There is no conflict of interest for this research work.

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