Modeling the Phase Composition of Gas Condensate in Pipelines

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Abstract. Gas condensate fields demonstrate a number of thermodynamic characteristics to be considered when they are developed, as well as when gas condensate is transported and processed. A complicated phase behavior of the gas condensate system, as well as the dependence of the extracted raw materials on the phase state of the deposit other conditions being equal, is a key aspect. Therefore, when designing gas condensate lines the crucial task is to select the most appropriate methods of calculating thermophysical properties and phase equilibrium of the transported gas condensate. The paper describes a physical-mathematical model of a gas-liquid flow in the gas condensate line. It was developed based on balance equations of conservation of mass, impulse and energy of the transported medium within the framework of a quasi-1D approach. Constitutive relationships are given separately, and practical recommendations on how to apply the research results are provided as well.

1. Introduction
Transportation of raw hydrocarbons (RH) is one of the most energy intensive industry sectors. From the literature it is known that energy costs to pump a unit mass of RH in the form of gas2-3 times exceed energy costs to pump a unit mass of RH in the form of liquid. As far as energy conservation during RH transportation is concerned, an important task is development and application of a method to calculate gas-liquid hydrocarbons flow and heat and mass transfer in process and trunk pipelines during their design and operation.

2. Methods, results and discussion
Methods of calculating thermophysical properties (TPP) and phase equilibria are reviewed in quite a lot of scientific publications and reference books [1, 2, 3, etc.]. However, when it comes to such complex systems as oil, gas condensate, natural gas and their by-products, using even the known techniques is a difficult task. It should also be taken into account that large part of calculation methods is designed for individual hydrocarbons and mixtures of known composition, that is why using them to calculate TPP of complex mixtures of unknown composition is not always possible or can even results in additional, hard-to-estimate errors [1].

To calculate the thermophysical properties of the gas-liquid mixture in the pipeline a method of control volumes is used [2, 4]. The internal volume of the pipeline is divided into a finite number of sufficiently small areas – control volumes $V_i$, limited by the inner surface of the pipeline and cross sections $S_1$ and $S_2$, located at a distance $\Delta z$ from each other. With regard to the control volume, the following balance equations are used: of mass, momentum and total energy. Main balance equations of mass, impulse and energy conservation in case of a quasi-1D flow are written as suggested by A.B. Shabarov [2, 4, 5 et al].

The law of conservation of mass of gas-liquid mixture phases in case of applying a quasi-1D approach is:

$$\rho_{2_i} v_i S_{2_i} = \rho_{1_i} v_{1_i} S_{1_i} - \rho'_{i} v'_i S'_{i} + \sum_{j \neq i} J_{p_j} V - \frac{\partial \rho_i}{\partial t} V.$$  (1)
This equation takes into account the flow through the lateral surface, which is characteristic of loss calculations, flows during controlled input and output of the mass in branched pipeline systems and mass exchange between phases.

The mechanical energy balance equation is written as a common form of Bernoulli’s equation. For a model with a total phase pressure \( p_i = g, l \):

\[
\alpha g_i \frac{v_i^2}{2} + \frac{\alpha P_{lg}}{\rho_g} + g z_i = \alpha g_i \frac{v_i^2}{2} + \frac{\alpha P_{lg}}{\rho_g} + g z_i + l_{mg} - l_{mg} + l_i + l_g
\]

\[
\alpha l_i \frac{v_i^2}{2} + \frac{\alpha P_{lg}}{\rho_l} + g z_i = \alpha l_i \frac{v_i^2}{2} + \frac{\alpha P_{lg}}{\rho_l} + g z_i + l_{ml} - l_{ml} + l_i + l_g
\]

where \( z_i \) = \( z_l - g_z, + g_z \), \( l_{m} = f_{d} \) – specific work of external forces, J/kg, excluding work to overcome gravity; \( l_{i} = \left( \frac{\alpha g}{g} - f_{d} \right) \frac{v_i^2}{2} \) – work expended when moving each of the phases to overcome the forces of friction and local resistance, \( l_i = \frac{\partial v_i}{\partial t} \) – specific work of inertial forces; \( l_{j} = -\frac{\partial S}{\partial v} \) – work of forces associated with the exchange of an impulse during input and output of the mass through the lateral surface; \( l_j = \sum l_{j} \) – specific work of interfacial forces which at small \( J \) comes down to the work of shear stresses at the phase boundary, \( \alpha \) – Coriolis coefficients taking into account the uneven distribution of the phase velocity along the radius of the pipe, \( \rho = \frac{2 \rho_g \rho_l}{\rho_g + \rho_l} \) – the average density in the section \( 1-2 \); \( P = P_{i} = P \). The work of shear stresses at the phase boundary \( P_{j} \) may be presented as \( P_{j} = \tau_{\pi} S \), where \( \tau_{\pi} \) – the shear stress at the fluid and gas boundary, \( S \) – the interface area of the selected volume.

The integral of internal energy conservation for a single-temperature mixture \( T_i = T \) is written as:

\[
\sum_{m=1}^{N} G_i \left( c_i T_i + U_{g0} \right) = \sum_{m=1}^{N} G_i \left( c_i T_i + U_{g0} \right) + \sum_{m=1}^{N} G_i \left( c_i T_i + U_{g0} \right) + \frac{\partial}{\partial t} \left( \sum_{i=1}^{N} \rho_i v_i \right) + \frac{\partial}{\partial t} \left( \sum_{i=1}^{N} \rho_i v_i \right) + V + Q_{m} + N_p
\]

where \( G_i = -\rho_i v_i^{(n)} \) – the input flow through the lateral surface; \( Q_{m} \) – external thermal power; \( N_p = f_d G \) – friction power; \( N_p = f_d G \) – a constant found from the normalization conditions during phase transitions \( l \leftrightarrow g \) [4].

**Closing relations of the physical-mathematical model of the gas-liquid mixture flow in the condensate line**

The dependence of the gas condensate mixture density on pressure and temperature.

Given the condensate line’s upstream initial conditions (the mass flow rate of a component – \( G_i \), the true density of the gas condensate – \( \rho_{sm,0} \), temperature – \( T_{0} \), pressure – \( P_{0} \), mass fractions of a component — \( N_{m,i} \)) let us find the density of a group of hydrocarbons hexane+ at the inlet of the rated pipeline section by:

\[
\rho_{C6+} = \frac{N_{m,i}}{\rho_{sm,0} \sum_{m=1}^{N} N_{m,i}}
\]

where \( \mu_i \) – the molar volume of other components calculated for both gas and liquid by a single Peng-Robinson equation of state [6].

Having determined the density of a group of hydrocarbons hexane+ by(5) we find the boiling temperature \( T_{bC6+} \), molar weight \( M_{C6+} \), critical pressure and temperature \( T_{cC6+} \), \( p_{cC6+} \) and...
acentricity factor $\omega_{C6+}$ using techniques from [1]. Using these data, mass fractions $z_i$ of the RH components are calculated. Therefore, a group of hydrocarbons hexane+ is included in the gas condensate mixture as a single pseudo-component. Having calculated the density of the mixture by substituting values for individual components and a pseudo-component $\rho_{sm}=661.7$ kg/m$^3$ in the equation of state and comparing its value to the given $\rho_{sm0}=662.0$ kg/m$^3$, we prove the adequacy of this approach, as relative deviation of the calculated $\rho_{sm}$ value from the given one is -0.05%.

*The viscosity of the gas condensate mixture.*

The viscosity of individual hydrocarbons is calculated using a database from [3]. The viscosity of a group of hydrocarbons hexane+ is determined using techniques from [1]. The viscosity of the entire mixture was calculated at temperature of 20°C and pressure of 1 atm by the formula:

$$\mu_{sm} = \frac{\sum_{i=1}^{N} z_i \sqrt[M_i]{\mu_{ind_i}}}{\sum_{i=1}^{N} z_i \sqrt[M_i]{M_i}}$$

(6)

Recalculation of viscosity on thermobaric conditions in different sections of the pipeline was carried out according to the formula:

$$\mu_{sm} = 10^{\log_{10}(\mu_{sm0})+1.450310^{-3}\left(10^{-0.101325}\left(5.2054\mu_{sm0}^{0.278}+0.0239\right)^{-3}\right)}.$$  

(7)

*The isobaric heat capacity of the gas condensate mixture.*

The isobaric heat capacity of the individual components in the mixture is calculated using a database from [3]. The isobaric heat capacity of a group of hydrocarbons hexane+ is determined using the Watson-Nelson formula. The heat capacity of the entire mixture was calculated according to the additivity rule:

$$C_{p_{sm}} = \sum_{i=1}^{N} z_i \frac{C_{p_i}}{M_i}$$

(8)

*The thermal conductivity of the gas condensate mixture.*

The thermal conductivity of the gas condensate mixture was calculated using a database and recommendations from [3], and the molar volumes of the mixture components were calculated using a single Peng-Robinson equation of state.

*The soil heat transfer.*

The soil heat transfer is found by [7]:

$$\alpha_{gr} = \begin{cases} 
\frac{2 \cdot \lambda_{gr}}{D \cdot \ln \left(\frac{2 \cdot H}{D} + \sqrt{\left(\frac{2 \cdot H}{D}\right)^2 - 1}\right)}, & \text{if } \frac{H}{D} > 3 (\text{Forchheim} - \text{Vlasov}) \\
\frac{2 \cdot \lambda_{gr}}{D \cdot \ln \left(\frac{H_{pr}}{D} + \frac{1}{Nu_{gr}}\right)}, & \text{if } \frac{H}{D} < 3 (\text{Arson} - \text{Kutateladze})
\end{cases}$$

(9)

Where $H$ – the depth of the pipeline occurrence in the soil, $m$, $H_{pr}$ is found by:

$$H_{pr} = H + H_e, \quad H_e = H_m \frac{\lambda_{gr}}{\lambda_{sn}};$$

(10)

and also $\lambda_{sn}$ and $\lambda_{gr}$ – the thermal conductivity coefficients for snow and soil.
$\lambda_{sn} = 0.465 \frac{W}{m \cdot K}$, $\lambda_{gr} = 1.4 \frac{W}{m \cdot K}$.

$Nu_{gr}$ – the Nusselt number for soil:

$$Nu_{gr} = \frac{\alpha_{vcd} \cdot D}{\lambda_{gr}}.$$  \hspace{1cm} (11)

where $\alpha_{vcd}$ – the heat exchange coefficient for air:

$$\alpha_{vcd} = 11.6 \frac{W}{m^2 \cdot K}$$

The equation of state for the components of the gas condensate system.
In this paper, a single cubic Peng-Robinson equation of state (PR) was used as a phase state equation. This equation is of a Van-der-Waals type. It is commonly used to solve the tasks of designing, developing and operating hydrocarbon fields, as well as when simulating chemical processes. It is a simple form of a four-coefficient equation of state:

$$p = \frac{RT}{\nu-b} - \frac{a}{(\nu+c)(\nu+d)}.$$  \hspace{1cm} (12)

Where $b, c, d$ – coefficients, constant for a given substance; the coefficient $a$ depends on temperature ($a = a(\varphi(T))$, where $a$ - a constant, $\varphi$ – a function of temperature equal to one at the critical temperature).

The coefficient structure of the equation of state is determined as follows [3]:

$$a_c = \alpha R^2 T^2_c / p_c,$$

$$b = \beta RT_c / p_c,$$

$$c = \sigma RT_c / p_c,$$

$$d = \delta RT_c / p_c,$$

$$\alpha = \Omega_c 0.5^2$$

$$\beta = Z_c^* + 0.5^2$$

$$\sigma = -Z_c^* + 0.5^2$$

$$\delta = -Z_c^* + 0.5^2,$$  \hspace{1cm} (13)

Where

$$\sigma = -Z_c^* + 0.5^2,$$

$$\delta = -Z_c^* + 0.5^2.$$  \hspace{1cm} (14)

Here $Z_c$, $\Omega_c$–independent parameters of the equation of state. Their values together with $\varphi(T)$ completely determine the equation of state of a pure substance.

Determining the composition and quantitative relation of equilibrium vapor and liquid phases.

The distribution coefficient or equilibrium constant of the $i^{th}$ component of the hydrocarbon mixture $K_i$ is the relation of its molar fraction in a vapor phase $y_i$ to its molar fraction in a liquid phase $x_i$.

$$x_i = \frac{z_i}{V(K_i-1)+1},$$  \hspace{1cm} (15)

$$y_i = \frac{z_i K_i}{V(K_i-1)+1}.$$  \hspace{1cm} (16)

Equations (12) and (15) are called equations of phase concentrations of the mixture components. They allow us to determine the molar fractions of components in vapour and liquid phases of the
mixture composition $z_i$ at given values of distribution coefficients $K_i$ and molar fraction of the vapor phase $V$.

Calculating the actual volumetric gas content.

By definition, the actual volumetric gas content is equal to:

$$ \alpha_g = \frac{V_g}{V} = \frac{\frac{V_g}{V_{eq}}}{1 + \frac{V_g}{V_{liq}}} = \frac{1}{1 + \frac{V_g}{V_{liq}}} \cdot \frac{V_{eq}}{V_g}. $$

(17)

If gas and liquid volumes are found as a product of the molar volume of gas and liquid ($v_g, v_l$ – calculated by the equation of state given the known phase compositions) and the number of moles of the mixture in the vapor and liquid state, respectively ($N_g, N_l$),

$$ \alpha_g = \frac{1}{1 + \frac{v_l}{v_g} \frac{N_l}{N_g}} = \frac{1}{1 + \frac{v_l}{v_g} \left( \frac{1}{V} - 1 \right)} $$

(18)

Determining the two-phase gas-liquid medium flow in the condensate line.

At each calculation stage we checked the phase behavior of the gas condensate mixture by the temperature and pressure conditions in the given section of the condensate line. If the mixture was in a single-phase liquid state ($V \leq 0$ at equilibrium values of $K_i$), the system (2, 3) had only one equation, as $\alpha_g$ was assumed to be equal to zero, and $\alpha_l$ — equal to one. If at any calculation stage parameter $V$ was $0 < V < 1$, then by (15) and (16) equilibrium compositions of gas – $y_i$ and liquid – $x_i$ phases were calculated. After that, according to a single Peng-Robinson equation of state, we calculated the density, and then viscosity of the gas and liquid phases and the surface tension of the liquid phase. According to the known molar ratio between the gas and liquid, mass flow rates of RH in the form of gas - $G_g$ and liquid - $G_l$ were calculated. These values were used later to determine the flow regime of the gas-liquid mixture by a known procedure [5].

3. Summary

A physical-mathematical model of a hydrocarbon mixture (HCM) flow in the gas condensate line considering phase transitions and changes in the phase composition was developed. A numerical procedure for determining “liquid-gas” balance equations for each component of the mixture was proposed using a data base on thermophysical properties of the components, including a single Peng-Robinson equation of state. Based on the developed model a technique and calculation algorithm are composed to determine the phase composition in arbitrary pipeline sections and to find the valid values of mass concentration of light hydrocarbons in the inlet condensate line section on condition that a single-phase flow regime along the entire length of the pipeline is provided.

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