Application of REFPROP software package for examinations automation of phase states of multicomponent hydrocarbon systems

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Abstract. This article is concerned with the automation of the experimental examinations of the phase states of multicomponent hydrocarbon systems. Experimental examinations of the mixtures of natural gas and gas condensate from the gas-condensate field on the PVT-installation have been performed to determine if the composition of the hydrocarbon mixtures influence the regularities of their phase changes. The comparison of the calculations by means of the REFPROP software package with the experimental data of Russian and foreign authors show that this software program can be used for automatization of the estimated calculations of the phase balances in the range of low temperatures as well as for controlling of the critical parameters of hydrocarbon mixtures. The authors demonstrate the possibility of the REFPROP software package application for choice automation of the hydrocarbon mixture composition for transportation in the low-temperature pipelines in the chosen range of temperatures and pressures.

1. Introduction
At the present time, the calculating experiment during scientific research realization is one of the key directions of tasks study of multicomponent hydrocarbon phase state examination. Nevertheless, it is rational to use different software programs and software application packages for scientific and technical tasks solution to achieve better understanding of physical effects, high price or impossibility of physical or natural experiment realization [1].

A large number of researchers are busy with development of calculation methods and with creation of software programs and software application packages for scientific and technical tasks solution. There are software application packages for thermal-physical properties (TPP) calculation (for pressure, temperature and other combinations of parameters) and for phase balances (PB) calculation of pure substances and multicomponent mixtures of hydrocarbon. The most powerful software application packages of universal purposes are SimulisThermodynamics (ProSim), MultiFlash (Infochem – KBC), VMGThermo (VMG), PVTSim (Calsep), PPDS (NEL) and others.

The license specialized thermodynamical library of TPP and PB REFPROP is used in our researches for automation of experimental examinations and tests (examination of multicomponent hydrocarbon phase states).
2. Application of REFPROP software packages for phase states calculation of multicomponent hydrocarbon systems at different temperatures and pressures

For calculation it is necessary to examine the phase state of multicomponent hydrocarbon systems for preparation and transportation of multicomponent hydrocarbon mixtures from gas condensate fields in pipelines [2]. Phase diagrams and critical parameters of gas and gas condensate mixtures in different proportions allow one to determine the necessary mixture for transportation in single-phase liquid state in the specified range of temperatures and pressures, to forecast phase behavior of the liquified hydrocarbon at different temperatures and pressures with the aim of the following transportation in the low-temperature pipeline.

The efficiency of multicomponent hydrocarbon mixtures transportation from gas condensate fields depends on the correct choice of transportation parameters: pressure P and temperature T for providing the single-phase liquid state of the pumped product. In connection with that, it is necessary to examine the phase state and the state behavior of liquified hydrocarbon mixtures, and critical parameters (critical pressure and critical temperature). For low-temperature pipelines, it is important to maintain single-phase state of the stream along the whole length of the pipeline [3, 4].

Calculating experiments (with usage of different software application packages) and experimental researches [5, 6], in our case on PVT installations (installations for examinations of phase balances of hydrocarbon systems), take an important place during study of the phase state and the phase behavior of hydrocarbon mixtures.

The REFPROP software program has been bought for phase equilibrium examination of multicomponent hydrocarbon systems at different temperatures and pressures. The REFPROP library was developed by the American National Institute of Standards and Technologies and it is considered as a world-wide standard applied for high precise calculations of the physical properties of pure products and mixtures for cooling agents, hydrocarbon and components of natural gas [7, 8]. Thermodynamic properties and their derivatives as well as transporting properties (viscosity, heat conductivity, surface tension as well as dielectric constant, higher and lower heating value) can be calculated. According to the results, the software program allows one to generate and to look through the calculation results in a tabulated form with different values of the initial parameters, to schedule graphs of TPP variance and phase diagrams in different coordinates.

It follows from the work [9] that software programs don’t always give an opportunity to make an accurate analysis of the phase states at close-to-critical temperatures and pressures, especially with regard to negative temperatures. For this purpose let’s make an assessment of calculations accuracy by means of the REFPROP software program for the range of pressures and temperatures at which it is possible to transfer hydrocarbon mixtures in single-phase liquid state; let’s compare experimental and calculated data. In the authors’ work [10], the graphs showing P – T diagrams (pressure – temperature) for two-component, three-component and multicomponent mixtures of hydrocarbon of different proportions are compared, the results of the comparative analysis of design and experimental data of the phase state diagrams are shown. As well as in the work [10] for assessment of the REFPROP software application package acceptability, the authors have given the table with the list of examined binary, ternary, multicomponent hydrocarbon mixtures including natural gas mixtures with design and experimental data at different temperatures and pressures as well as deviations.

Processing of Russian and foreign authors’ experimental data and comparison of these data with design data by means of the REFPROP software program has shown that the deviation is not more than 5%. This means that it is possible to use the REFPROP software application package for examination of the phase states mixtures of natural gas and gas condensate from the gas condensate fields in the range of different temperatures and pressures.
The authors also performed laboratory tests to know different factors’ (for example, composition of hydrocarbon mixtures) influence on the consistency of hydrocarbon mixtures phase changes. The experimental examinations of the phase state of natural gas and gas condensate mixtures were performed in the branch office of «Gazprom VNIIGAS» Ltd. in Ukhta together with the personnel of the department of the Research Center of oil-and-gas layered systems and process simulation under the direction of A.N. Volkov. During laboratory examinations, the following parameters were measured: critical temperature and critical pressure in case of change of the gas condensate mixture composition (natural gas and gas condensate proportion). In figures 1 and 2 there is a phase diagram for the mixtures in proportion 83:17 and 90:10 (mass % gas separation).

According to the results of the experimental examinations, the tests data have been marked on graphs P – T for different mixtures calculated by means of the REFPROP software application package. This allows appreciating the calculation accuracy of multicomponent mixtures in this software application package.

The comparison of the obtained results of the experimental examinations and the calculations by means of the REFPROP software application package shows the possibility of its application for the forecasting of phase states and for the examination of phase behavior of hydrocarbon natural mixtures from gas condensate fields.

![Figure 1](image1.png)

**Figure 1.** Pressure-temperature diagram for gas separation and wet condensate mixture in proportion of 83:17 mass % of gas separation:
- calculated data, ◆ - experimental data.

![Figure 2](image2.png)

**Figure 2.** Pressure-temperature diagram for gas separation and wet condensate mixture in proportion of 90:10 mass % of gas separation:
- calculated data, ◆ - experimental data.

Consequently approved calculation accuracy allows using the REFPROP software application package for automation of the phase states examination of the multicomponent hydrocarbon mixtures from the gas condensate fields of Yamal Peninsula in the area of low temperatures.
3. Phase states examination of liquefied hydrocarbon mixtures from the South-Tambey gas-condensate field of Yamal Peninsula by means of REPROP software application package

Examinations were performed using the example of the South-Tambey gas-condensate field of Yamal Peninsula which is the main resource base of the first plant SPG. The analysis of the phase states of liquefied hydrocarbon mixtures at low temperatures is performed to provide liquefied hydrocarbon mixtures transmission in low-temperature pipelines in single-phase liquid state. The composition of typical natural gas (according to the data of the REPROP software application package), gas and gas condensate from the South-Tambey field is given in [10]. Their composition and quantity depends on the place and conditions of recovering, that’s why they can be varied in the wide ranges.

In Table 1 there are critical parameters (critical pressure and critical temperature) of the gas and gas-condensate mixtures from the South-Tambey gas-condensate field in different proportions calculated by means of the REPROP software program, ver. 9.1. These parameters show that adding of 3 % gas condensate according to the mass of produced natural gas leads to that the mixture critical temperature rises from minus 73 °C for typical natural gas and from minus 50.8 °C for the gas from the South-Tambey field up to minus 39.6 °C (the critical pressure is 10.03 MPa). If 5 % is added, the mixture critical temperature rises up to minus 37.1 °C at critical pressure 10.45 MPa. If 7 % and 10 % of gas condensate is contained, the critical temperature equals minus 34.96 and minus 28.9 °C, and the critical pressure equals 10.81 and 11.72 MPa relatively.

| Components | Designation       | Mixture of gas and gas condensate, mass percent of gas |
|------------|-------------------|-------------------------------------------------------|
|            |                   | 100  | 97   | 95   | 93   | 90   |
| 1          | Critical temperature | °C   | -50.8 | -39.6 | -37.1 | -34.96 | -28.90 |
| 2          | Critical pressure  | MPa  | 8.7   | 10.03 | 10.45 | 10.81 | 11.72 |

In figure 3 there is a phase diagram P – T (pressure – temperature) of the mixture in proportion of 95 % mass natural gas and 5 % mass gas condensate constructed by means of the REPROP software program ver. 9.1. On this phase diagram of the multicomponent system, the cricondenbar and the cricondentherm correspond to the maximum ratings of pressure and temperature. For the mixture of ratio 95 % mass natural gas and 5 % mass gas condensate, the ratings of the cricondenbar, the cricondentherm and the critical point, which are obtained by means of the REPROP software program ver. 9.1, are given in Table 2. Consequently, in accordance with the set task, the mixture of multicomponent hydrocarbon at the chosen range of temperatures (minus 50 - minus 40 °C) and pressures (10 – 12 MPa) will be in the liquid phase.
Figure 3. The pressure-temperature (P-T) diagram of the mixture of gas and gas condensate in the proportion 95 and 5 % mass.

Table 2. The values of the cricondentherm, the cricondenbar and the critical point of the mixture of gas and gas condensate in the proportion 95 and 5 % mass

| Critical parameters | Temperature (K) | Temperature (°С) | Pressure (MPa) |
|---------------------|----------------|-----------------|---------------|
| 1 Critical point    | 236            | -37.1           | 10.45         |
| 2 Cricondentherm    | 336.85         | 63.7            | 7.3           |
| 3 Cricondenbar      | 290.44         | 17.3            | 14.75         |

Consequently, the quoted results of the phase state of the mixtures from the gas-condensate fields on Yamal Peninsula by the example of the South-Tambey field allow forecasting the behavior of liquefied hydrocarbon at different temperatures (including low temperatures) as well as determining the parameters for its following transportation in single-phase liquid state in the low-temperature pipelines.

4. Conclusion

The quoted results of the phase state of the mixtures from the gas-condensate fields on Yamal Peninsula by the example of the South-Tambey field, by means of the REFPROP software application package ver. 9.1, allow forecasting the behavior of liquefied hydrocarbon at low temperatures, controlling the critical parameters of the mixtures of natural gas and gas condensate as well as determining the parameters for its following transportation in the single-phase liquid state in the low-temperature pipelines.

It is possible to make the following conclusion: the method of the numerical experiment allow analyzing the phase state of the product pumped in the pipeline, as well as allow refusing a large number of laboratory tests. Besides the application of the mathematical apparatus during liquid movement simulation easily allows varying the given initial parameters for the purpose of finding optimal solution of the set task. Thus, the application of modern computer technologies for pipelined transportation of hydrocarbon allows simplifying and computerizing the performance of complicated experimental examinations and tests.

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