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Mathematical simulation of low-temperature gas separation

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Abstract

The relevance of this work is due to the need to increase the quality of the natural gas treatment. The aim of the work was to study separation process with a software package that simulates changes in the technological performance of the low-temperature separation installation in real time for the study of the effect of operating conditions changes on separate devices and technological system as a whole. As a method of research, a method of mathematical modeling of chemical processes has been selected. As an example, we developed the three-stage separator computer model. Thus, the study used a program module for calculating on a three-stage separator - one of the most important elements of low-temperature separation installation - considering the effect of control system parameters (control valves for gas and liquids) and the generally accepted principles of separation of three-phase mixture (Stokes' law, the laws of phase equilibrium, etc.).

Keywords: low-temperature separation; natural gas; mathematical simulation; dynamic behavior.

1. Introduction

Nowadays it is a time of actively developing industrial countries, such as People`s Republic of China and others. Thus, there is much tension around the issue of the energy consumption question. This is caused by one simple reason: economic growth is impossible without a well-developed industrial basement, which in its turn requests large amounts of energy produced mainly by the burning of fossil fuels.

It is widely known that oil reserves are not infinite and it is one of the irreplaceable resources. At least this statement is somehow true regarding the nowadays level of technical development worldwide. Furthermore, nobody knows exactly, when the "moment of truth' will come, i.e. the day or some other period that whole oil on the Earth would be produced, treated and its product burned.

Coal is not also unlimited. Also, its heating value is not so big too, comparing to oil. Emissions of pollutants which appear after coal burning threw out to the atmosphere increase the amount of greenhouse gasses in the atmosphere which causes harmful effect on the environment. This is especially critical for densely populated territories such as Europe. Besides, it is a source of expectable and righteous discontentment of the nature-protection organization, for example, Greenpeace.

At the current level of technological development, the widespread introduction of alternative fuels is not seen for realization in the near future. Nevertheless, this topic seems promising taking in account, as it stated above, unrelenting demand for energy and the gradual consumption of the non-renewable resource.

Therefore, gas seems as the most suitable solution of supposed energetic crisis.

As a science gas processing formed relatively recently. Its tremendous up-growth began in the second part of 20th century.

Nowadays there are about 390 billion cubic meters of gas on the natural resources market. Main proved reserves are held by 12 countries with a total share of plunder about 76 percent from worldwide. The USA, Russia, and Iraq have the biggest ones. Also, there are some other large accumulations in UAE, Qatar, Algeria and some other Middle-East countries [1].

Russia still holds the leading positions in the world with reservoirs and production of natural gas. The country remains to be the biggest exporter of natural gas. In total, about 200 billion cubic meters are sent abroad every year. From this amount about the quarter is exported to the former Soviet Union and other to the far-abroad countries primarily to Europe [2].

In our days there are a lot of ways of gas treating and recovery developed. However, this particular work is focused on low-temperature separation. The main idea is about extracting of liquid hydrocarbons with the means of multiple-stage or single-stage separation. This is performed with fluid dynamic separation of liquid and gaseous phases in equilibrium in conditions of low temperature. The range of temperatures covers from 5-10 down to 25-30 degrees below zero [3-4].

Meanings of computer mathematic simulations with special software seem like an adequate way to research this process. Such simulation systems offer different ways to calculate various thermodynamic, physical and chemical parameters, for example, enthalpy, entropy, density, phase equilibrium coefficient, etc. Also, Soave-Redlich and Peng-Robinson constitutive equations are used to describe oil and gas treatment processes. Up to date there are large amount of different simulation software, for example, Aspen HYSYS, Pro II, Cape-Open to Cape-Open [5].

Thus, the development of modern processes of natural gas processing and operation of existing plants is difficult without the use of simulation programs, which have high accuracy process data description parameters. Also, the program allows the study of these processes without the huge time and material costs. What is especially important because of the inaccessibility of deposits and rigidity of surrounding environment, which is typical for the northern fields, as well as transport difficulties, in particular through the pipeline, stretching for several thousand kilometers.

2. THE ESSENCE AND THE THEORY OF LOW-TEMPERATURE SEPARATION PROCESS

2.1. Gas and gas condensate low-temperature separation technology

The use of low-temperature separation is caused due to the presence of water vapor in hydrocarbon gasses. As it is known, gas hydrates are formed under the following conditions: the presence hydrating agent, i.e. natural gas with moisture, and also in conditions of low temperature and high pressure of gas. Therefore, for further transportation through a pipeline presence of water may lead to hydrate formation in pipes. In addition, it could not be excluded the probability of ordinary ice appearing in the line. All of those mentioned above could lead to complete or partial blockage of the pipe - the formation of the so-called "plugs." Furthermore, hydrates are formed, break operation of control valves are responsible for maintaining the necessary pressure. Thus, the low-temperature separation is the most efficient process to prevent similar cases dehydrating gas and freeing from heavier compounds.

In processes requiring a drying and degreasing gas, the low-temperature separation process is indispensable for the following reasons. First of all, it is versatility. Also it is a high yield of the final product as the main parameter. Moreover, one that is not unimportant - free cooling achievable by the use of energy enclosed in themselves gas streams that are at high pressure.

The factors that determine the technological regime of low-temperature separation process are thermodynamic characteristics of developed deposits, the composition of the gas and associated condensate, and one that plays an important role - requirements for regulatory agencies to fishery products.

The scheme of low-temperature separation is presented in the Fig. 1. The gas enters the first stage separator, where performs the pre-separation of the liquid, which stood out in the riser and loop.

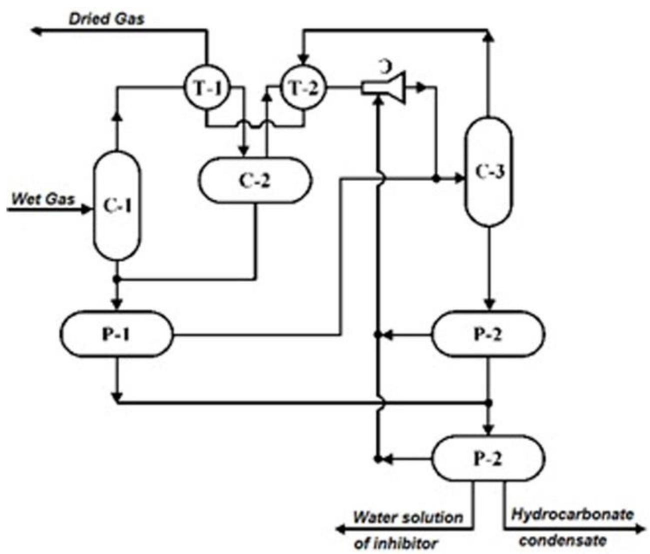

Figure 1. Low-temperature separation scheme

From there initially separated liquid is discharged into lagoons. Then the gas enters the gas heat exchanger, where the cooling process is finished the counter flow of separated gas. These steps may be repeated several times so that the gas passes separator circuit through the second, third, etc. stage-separators divided by heat exchangers. After the final heat exchanger, the gas passes through the nozzle, where the pressure is reduced to a maximum condensing pressure and temperature, due to the throttling effect being reduced. However, the turbine expansion units can be attached to a more rational use of energy, instead of the union formation. Due to the change of thermodynamic properties condensate and moisture drop in the low- temperature separator.

From there they enter the collector-condensate, and then - to the condensate stabilization unit. The pressure of the last stage of separation is determined by the pressure in the pipeline and the temperature control conditions of moisture and release of heavy hydrocarbons. One should also take into account that due to the development of the well gas pressure will inevitably fall. In this case, the refrigeration unit is switched to the circuit to maintain the desired separation temperature which is not possible due to the formation energy fall. It is also possible to prevent the formation of hydrates in pipes in the low-temperature separation system providing inhibitor input into the gas flow.

Thus, based on the description of the technological scheme, it can be concluded that the low-temperature separation process can be implemented under any climatic conditions. Also the other advantages of this separation method includes: becomes critical content of the gas non-hydrocarbon components, a high degree of condensate recovery-about 97% in some cases, the possibility of reaching the dew point at which no loss of moisture and heavier hydrocarbons in the pipes for transportation of gas, low capital and operating costs.

2.2. Physical and chemical processes of low-temperature gas separation

It is needed to describe three following processes to consider the process of low-temperature separation:

- Separation
- Heat exchange
- Throttling [6]

For the separation process, the main assumption is the achievement of phase equilibrium in the system. Thus, laws of phase equilibrium become applicable for systems [7].

Based on the assumptions made, it is necessary to determine the equilibrium constants for the Peng-Robinson equation:

$$P = \frac{RT}{V-b} - \frac{a\alpha}{V^2-2bV-b^2} \quad (1)$$

Thus, using this equation, phase behavior could be predicted for a mixture of natural hydrocarbon in the case of foreknowing its composition and properties of its components.

Description of the heat transfer process is to deal with the thermal balance. Mathematically, this is expressed by the basic heat transfer equation [8-9]:

$$Q = K \cdot F \cdot \Delta t_{\text{cp}} \cdot \tau \quad (2)$$

However, for a more detailed and approximate to the real conditions description of the process, it is necessary to determine the K coefficient, which takes into account various parameters such as the construction of the heat exchanger, flow state, changing the state of aggregation (condensation), contaminated walls, etc.

Also throttling process plays an important role for this technology when gas maintained at a constant pressure, occupied the volume of the last separator, then exits the vessel and enters another low-temperature separator volume with another constant pressure in it. This process is also called the process of Joule-Thomson.

In mathematical form, throttling is characterized by a coefficient of Joule-Thomson: the temperature change when the pressure drops by 0,1MPa. The integral form is represented as:

$$T_2 - T_1 = \int_{P_1}^{P_2} \frac{T\left(\frac{\partial V}{\partial T}\right)_P - V}{C_p} dP \tag{3}$$

Thus, the throttling process is one of the main methods of obtaining low temperatures. In fact, the throttling is performed by slowly pushing the gas from one vessel to another system via thin capillaries, or in this case, the expansion turbine nozzle of relatively small diameter.

2.3. Formation of gas hydrates

Gas hydrates formation in pipelines-one of the main problems in the preparation of gas and its transportation. Substances of this type are deposited on the inner walls of the pipeline, which leads to partial or complete occlusion line, which leads, in its turn, to an emergency stop on a plant. Thus, time is lost during which production capacities idle and that inevitably leads to a drop in income as a whole. Therefore, oil and gas companies spend significant amounts on research in the field of prevention and fight against this phenomenon and reducing thus the operating costs.

Hydrocarbon gas hydrates are similar in appearance to the ice or snow and are unstable hydrocarbon compounds with water. Structurally, they are one or more molecules of gas (methane, propane, *etc.*) surrounded by an ordered structure of water molecules. The main conditions that define the formation of gas hydrates are temperature, gas composition, pressure and saturation of the gas with water vapor.

For the first time, gas hydrates were called cause complications in the operation of gas pipelines by E. Hammerschmidt, American scientist, who found that these crystals can accumulate inside the pipes, causing a blockage.

Often hydrate formation takes place in the winter season when the gas flow in the pipeline cools down considerably. Often hydrate formation takes place in the winter season, when the gas flow in the pipeline cools down considerably. This phenomenon affects all lines except where the dew point is below the minimum operating temperature.

Technological factors affecting the formation of hydrates include:

- insufficiently thorough purge pipeline before the start;
- lack of condensate and purge pipes in low areas of the pipeline, or irregular removal of accumulating fluid;
- insufficient gas cleaning before putting it in the gas pipeline.

As the water flow and hydrating agent incomes, a "plug" forms under appropriate conditions on the section of the pipeline. Simultaneously, water vapors are released from the gas which decreases the elasticity of the water vapor, thereby accelerating the process of local formation of a hydrate blockage.

To hydrate natural gas formation and decomposition conditions are not always the same. The pressure at which the hydrates are decomposed significantly below the pressure at which they are formed under the same temperature. This difference can be explained due to the reduction of pressure of water vapor over the form hydrates.

2.4. Dynamic model of low-temperature separation

2.4.1. Dynamic model design

At the basement of the development of a dynamic model lay the equations of material and heat balance for each of the devices in the circuit.

For a single unit material balance is as follows:

$$F = L + P \qquad (4)$$

In turn, for each component:

$$Fx_{Fi} = Ly_{Li} + Gx_{Pi} \qquad (5)$$

This equation allows calculating following parameters:

- Phase state
- Liquid level
- Pressure [10]

It uses the laws on the basis of which it is possible to calculate separated phases composition. Such as, for example, the law Raoult-Dalton [11-12]:

$$x_{Gi} = k_i y_{Li} \qquad (6)$$

here k_i is phase equilibrium constant.

To further drawing model must enter distillate ratio. This ratio of the separated liquid portion to the total flow at the inlet of the apparatus [13-14]:

$$\varepsilon = \frac{L}{F} \qquad (7)$$

While solving these equations material balance becomes:

$$Fx_{Fi} = \varepsilon F k_i x_{Gi} + (1-\varepsilon)Fx_{Gi} \qquad (8)$$

Expressing x_{Pi} and normalizing sum of the components to 1:

$$\sum x_{Gi} = \sum \frac{X_{Fi}}{1+\varepsilon(k_i+1)} = 1 \qquad (9)$$

Thus, it becomes possible to calculate liquid level in apparatus, on the assumption of equations (4) and (7):

$$L = F(1-\varepsilon) \qquad (10)$$

Using the ideal gas equation pressure in the system could be found:

$$P = \frac{GRT}{V} \qquad (11)$$

2.4.2. Simulation of low-temperature separation process

As a working simulation environment the language of object-oriented programming Delphi was selected. The model is characterized by the following features:

- A visual representation of the process;
- Ability to change all of the input parameters;
- Change the data in real time;
- Low requirements to computing power of a PC;
- Availability [15-17].

An important advantage of the model is the simplicity of its interface, as it could be seen in the Fig.2. This allows even inexperienced users to learn how to work in this environment with high efficiency in a short time.

Every element of the process schematically displayed. Each of them is fixed field of inter-related variables, such as temperature, pressure or flow rate allow you to change the operating mode and get the result in real time. As the example, there is the first-stage separator is given in the Fig.3.

The starting point for any work with this software is to load data from Excel-file then calculations could be started.

Thus, introduced model offers to research a system with following parameters:

- Change of the basic technological parameters in the apparatus depending on the dew point under perturbation of the system;
- Change of the basic technological parameters in the apparatus depending on the flow rate under a perturbation in the system;
- Change of the basic technological parameters in the apparatus depending on the pressure at the perturbations in the system;
- Change of the basic technological parameters in the apparatus according to the temperature under perturbation of the system;

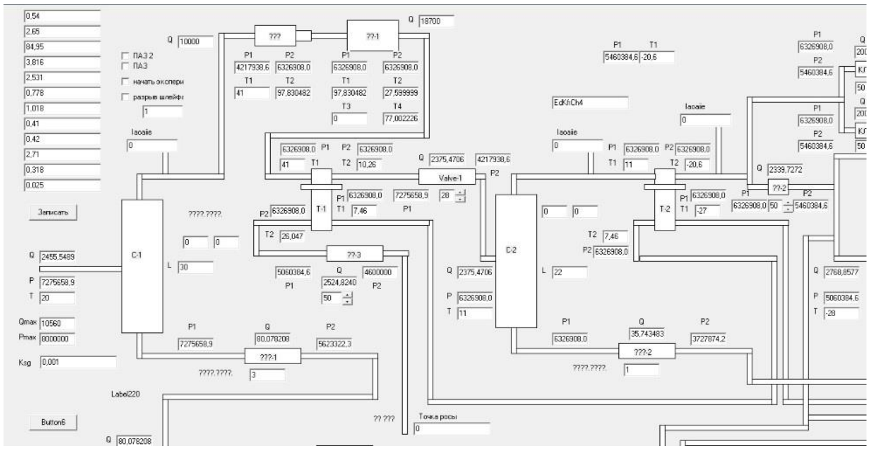

Figure 2. Simulation environment

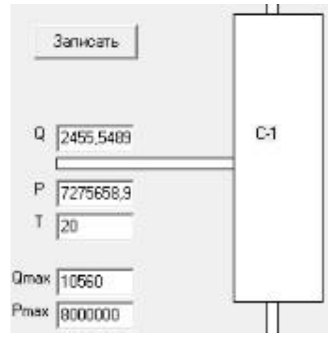

Figure 3. First-stage separator and its inlet parameters

2.4.3. Changing the basic technological parameters in the apparatus before the second stage separator

The main way to change process parameters in the model is represented by changing the degree of opening and closing the valve. Fig.4 shows an example of such a valve.

When the valve is opened by 75 per cent the following picture on the pressure, temperature, the yield of methane and phase equilibrium constant for methane is observed as it is shown in the Fig.5-8.

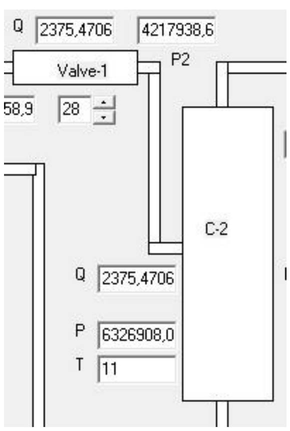

Figure 4. Valve before second-stage separator

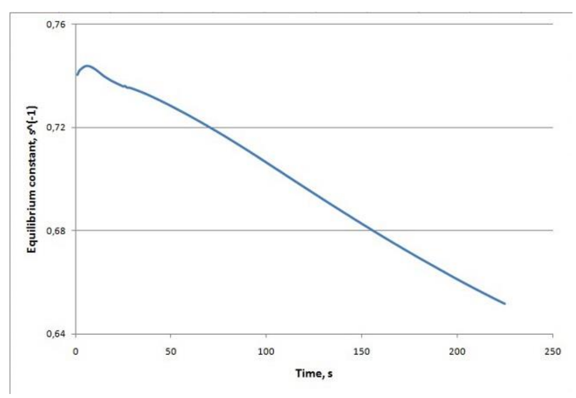

Figure 5. Methane phase equilibrium constant changing during certain time

As it could be seen from the graph of the methane phase equilibrium constant, the value passes the minimum point and then increases linearly. This is due to the overall stabilization of the system and the transition to a steady state.

The charts of pressure and temperature confirm thermodynamic stabilization mode in the apparatus and the separator outlet to the stationary regime.

A somewhat different situation is observed in the half-closed valve.

As it could be seen from the graph in the Fig.9, the value of phase equilibrium constants in these conditions passes through a maximum, after which there is a sharp decline, which is smoothed over time, meaning the transition to a steady state.

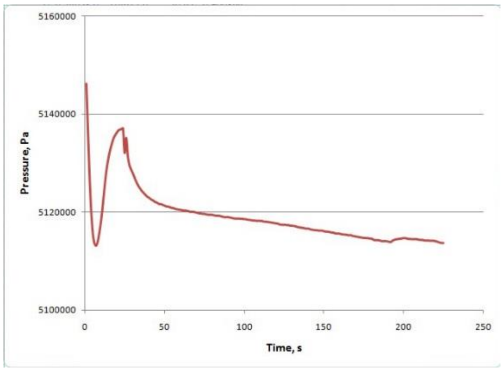

Figure 6. Pressure stabilization in second stage separator during certain time

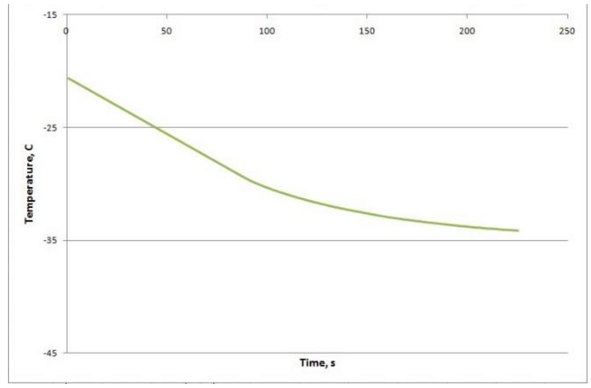

Figure 7. Temperature stabilization in second stage separator during certain time

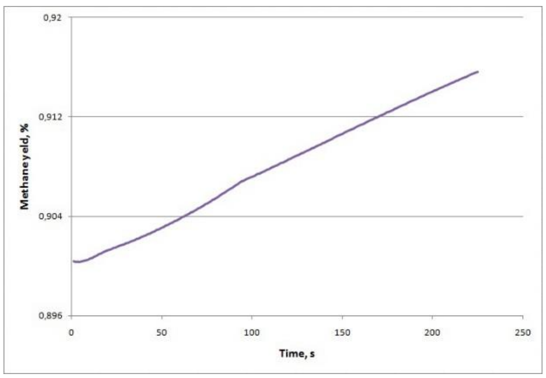

Figure 8. Methane yield in these thermodynamic conditions

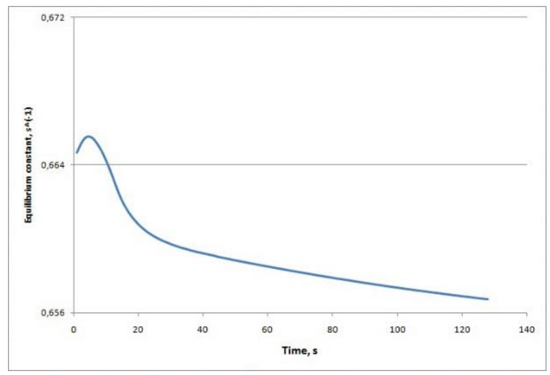

Figure 9. Methane phase equilibrium constant changing during certain time with half-opened valve

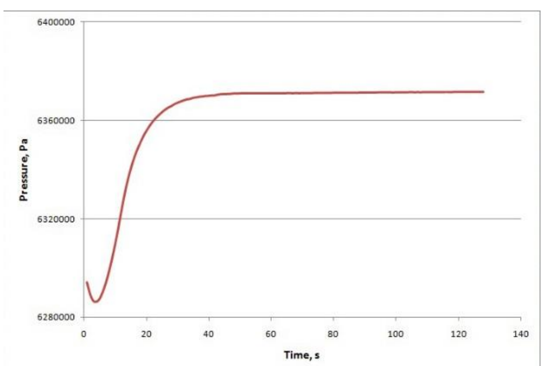

Figure 10. Pressure stabilization in second stage separator during certain time with half-opened valve

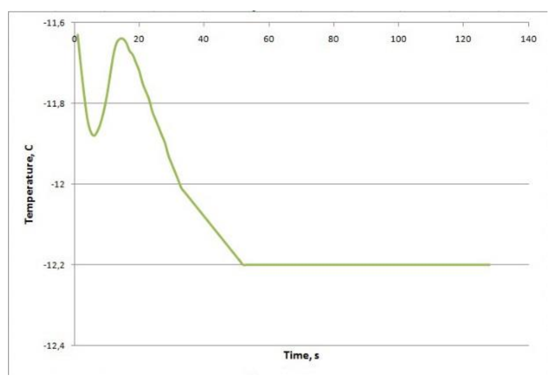

Figure 11. Temperature stabilization in second stage separator during certain time with half-opened valve

Data on the pressure and temperature in this mode of the half-opened valve confirms the assertion made above, which could be seen in the Fig.10-11.

As can be seen in the graph of pressure change over time, this value passes through a minimum and then increases sharply, and finally stabilized.

Much more interesting is the establishment of the temperature regime in the machine. Passing through the so-called "pit" temperature rising again, passing through a maximum value and then decreases until it stabilizes. This may be due to the inertia of the whole system. First, the gas is cooled, as expected, under the action of the throttling effect. However, then there is a parasitic effect, when the flow of purified gas used as a cooling agent may not effecttively cool the raw gas, thereby heating agent. However, after reaching a certain maximum, the system has stabilized, continuing drop in temperature. The most notable difference from the preceding case is falling, and not the temperature increase, which is likely due to the throttling effect appeared, whereby gas is passing through the narrower section "quenched."

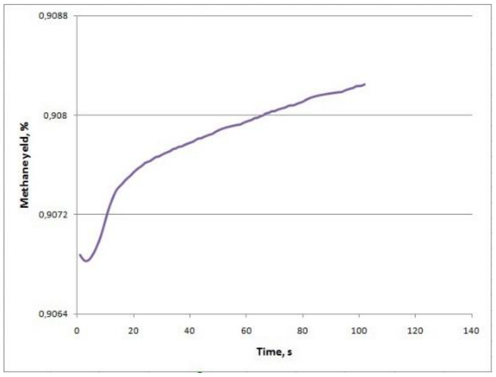

Figure 12. Methane yield in thermodynamic conditions of half-opened valve

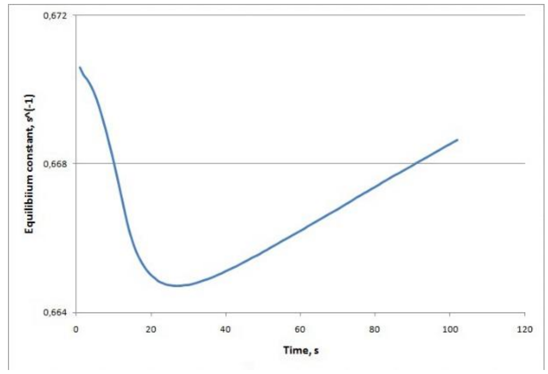

Figure 13. Methane phase equilibrium constant changing during certain time with quarter-opened valve

Another parameter to change its behavior is the yield of methane. If in the previous case, it dropped, passing through a maximum, then in case of the half-closed valve this rate increases, passing the contrary, through a minimum point, which can also be explained by appeared throttling effect.

Fig.13 shows that when the valve is opened for a quarter the methane phase equilibrium constant changes relatively quiet. It is an almost linear graph with a small peak in the beginning.

Fig.14-15 show behavior of pressure and temperature in this mode. The schedule of change of pressure in many respects similar to the temperature behavior of the half-open gate. That can also be explained by the effect of the inertia of the system.

The opposite situation occurs with changes in temperature in this mode: the graph smoothly becomes a horizontal line, when the temperature is stabilized.

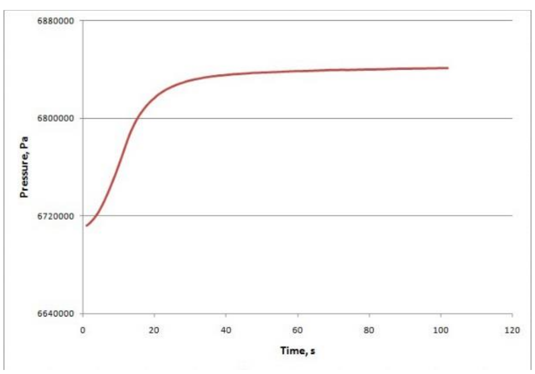

Figure 14. Pressure stabilization in second stage separator during certain time with quarter-opened valve

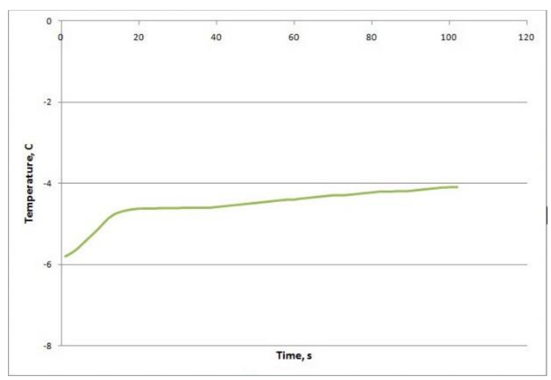

Figure 15. Temperature stabilization in second stage separator during certain time with quarter-opened valve

Also, in this case, the yield of methane grows smoothly. The graph in the Fig.16 is almost linear.

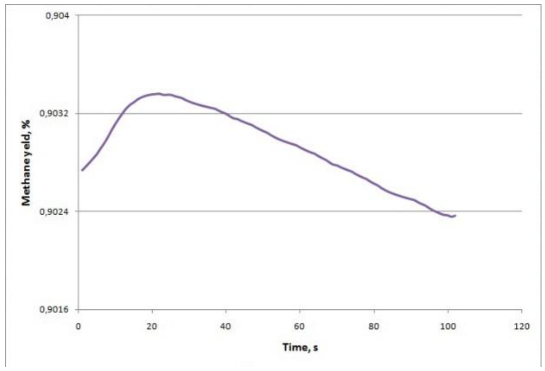

Figure 16. Methane yield in thermodynamic conditions of quarter-opened valve

3. Conclusions

As it was stated in the beginning, developing the adequate mathematical model is one of the important tasks of the gas producing industry. In nowadays business struggle it is necessary to save as much money as it is possible.

Thus, the process of preparation of natural gas has been studied for low-temperature separation technology. The developed simulation model is capable of displaying the dynamic transients in a dynamic mode. This is proven with a demonstration of changes in the main parameters of the system when making over its main regulatory impacts.

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