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Justification for the Choice of a Modeling Scheme for the Hydrocarbon Preparation Process for Transportation Using Supersonic Separation

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A study was conducted to select a modeling scheme for the process of preparing hydrocarbons for transportation by supersonic separation. Modeling was performed in the HYSYS environment, which allowed obtaining optimal parameters for effective removal of moisture and heavy hydrocarbons. The influence of pressure and temperature changes on the efficiency of heavy hydrocarbon extraction was analyzed. The most effective modeling scheme was selected, which provides high prediction accuracy. The results obtained can be used for further optimization of gas purification technological processes and their adaptation to industrial applications.

Keywords: supersonic separation, natural gas, modeling, associated formation water, hydrocarbon preparation.

Обґрунтування вибору схеми моделювання процесу підготовки вуглеводнів до транспортування методом надзвукової сепарації

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Проведено аналіз методів підготовки вуглеводнів до транспортування та обґрунтовано вибір схеми моделювання процесу надзвукової сепарації. Ця технологія дозволяє ефективно видаляти вологу, важкі вуглеводні та CO₂, що значно покращує якість газу та зменшує негативний вплив на довкілля. Виконано чисельне моделювання в програмному середовищі HYSYS, яке дозволило отримати оптимальні параметри процесу. Досліджено вплив ключових факторів, таких як тиск, температура та швидкість потоку, на ефективність сепарації. Отримано залежності, що демонструють, що збільшення тиску до 12,5 МПа підвищує ефективність процесу, однак подальше його зростання не дає значного покращення. Проведено порівняльний аналіз двох схем моделювання, в результаті якого досягнуто вибору оптимальної моделі, що забезпечує високу точність прогнозування та мінімізує обчислювальні витрати. Визначено, що запропонована схема дозволяє найбільш точно відтворити фізичні процеси, які відбуваються в надзвуковому сепараторі, включаючи розширення потоку, фазовий перехід, розділення рідкої та газової фаз і дифузію. Проаналізовано обмеження сучасних моделей, зокрема їхню чутливість до рівноважних припущень. Встановлено, що для підвищення точності прогнозів необхідні подальші удосконалення методів моделювання, оскільки реальний процес є нерівноважним. Досягнуто висновку, що використання надзвукового сепаратора може значно підвищити ефективність підготовки природного газу та забезпечити додаткове вилучення конденсату. Отримані результати можуть бути використані для подальшої оптимізації технологічних процесів очищення газу та їхньої адаптації до промислового застосування.

Ключові слова: надзвукова сепарація, природний газ, моделювання, супутньо-пластова вода, підготовка вуглеводнів

Introduction

Efficient hydrocarbon feedstock preparation is a crucial stage in the technological processes of the oil and gas industry. One of the promising methods for enhancing the separation efficiency of gas-liquid mixtures is supersonic separation, which provides high-speed and selective removal of undesirable impurities such as moisture, condensate, and solid particles.

The successful implementation of supersonic separation requires a thorough selection and justification of the modeling scheme, taking into account the thermodynamic and hydrodynamic characteristics of the flow, phase state changes of the components, and the influence of key parameters such as pressure, temperature, and gas flow velocity.

Despite the significant potential of supersonic separation technology, its practical application is often limited by the complexity of process modeling and the lack of standardized approaches to predicting separation efficiency under different operating conditions. The choice of a grounded modeling scheme is essential for optimizing equipment design, improving energy efficiency, and ensuring the stability of the separation process. Therefore, this study aims to address these challenges by providing a justification for selecting an appropriate modeling scheme for hydrocarbon feedstock preparation using supersonic separation.

Review of the research sources and publications

The study of hydrocarbon preparation processes involving supersonic separation technology is rapidly evolving, as reflected in modern scientific publications. The main focus is on modeling this process, optimizing the design of supersonic separators, and integrating them into real technological chains.

In study [1], a Unit Operation Extension (UOE) was

developed for use in the HYSYS environment, enabling effective modeling of supersonic separation processes. Specifically, the study examined in detail the processes of dehydration, heavy hydrocarbon fraction removal, and decarbonization in high-carbon-content natural gas.

A similar approach was applied in study [2], where an HYSYS model was developed to simulate the operation of a supersonic separation module. This research proposed a design solution that ensures stable nozzle performance even under varying inlet pressure or gas composition. In particular, it was demonstrated that the system can maintain the dew point with a deviation of no more than ± 2.5 °C from the established criteria, even with inlet pressure variations of $\pm 18\%$. The impact of natural gas composition changes was also analyzed, confirming the system's high stability under such fluctuations. The computational scheme of the supersonic separation process is presented in figure 1.

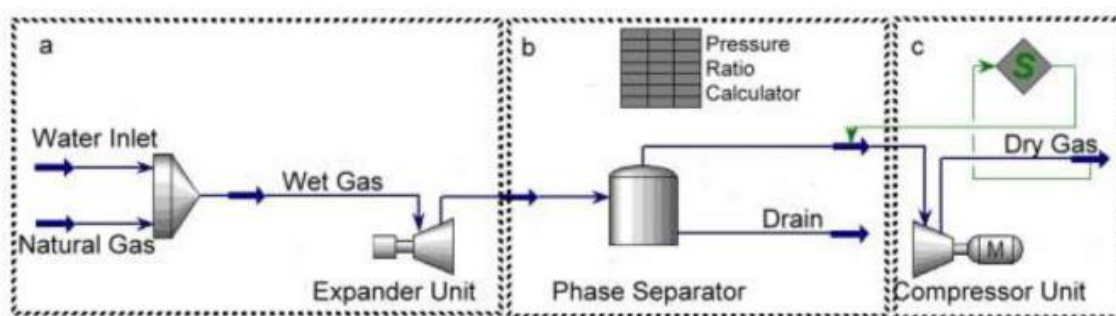


Figure 1 – Calculation scheme

In addition to its use in natural gas dehydration and heavy hydrocarbon removal, supersonic technology has significant potential for industrial application. One of its important applications is decarbonization, i.e. the extraction and utilization of CO₂ from gas mixtures with a high carbon concentration, such as natural gas or exhaust gases from internal combustion engines. Effective reduction of CO₂ emissions using this technology opens up opportunities not only to reduce environmental risks, but also to provide economic benefits through further storage and use of carbon dioxide. Research activities in the field of supersonic separation cover numerous aspects: experimental studies of flow properties, mechanisms of intraphase transition condensation, as well as structural features of devices. In particular, eddy flows [3], diffusion recovery processes [4], dehydration efficiency of separation tubes [5] and optimization of nozzle designs using CFD (computational fluid dynamics) [6] have been studied.

Other examples include the study of methods for modeling such processes using software such as UniSim Design [7] and HYSYS [8], which allow for increased accuracy in estimating the efficiency of separation tubes at the design stage. In [9], a one-dimensional model of a supersonic tube was proposed, which significantly reduces the computational complexity during the initial design.

Definition of unsolved aspects of the problem

Although substantial advancements have been made in this field, a range of persistent challenges continues to demand attention. One notable issue is the heavy reliance of the technology on accurate modeling to achieve optimal performance. Currently, there is an absence of a clearly established or universally accepted computational framework capable of adequately representing the complexities involved in the supersonic separation process. This gap highlights the pressing need for more focused and in-depth research efforts to address these limitations and enhance our understanding in this area.

Problem statement

The operation of the separation equipment can be simulated using modern software. However, since the 3S separator is a non-standard separation equipment, it is necessary to substantiate the model of the supersonic separation process by comparing the simulation results for different model variants.

Basic material and results

The literature review examined various schemes used for simulation. Two main schemes for simulating the 3S separator process were selected for comparison (Fig. 2, 3).

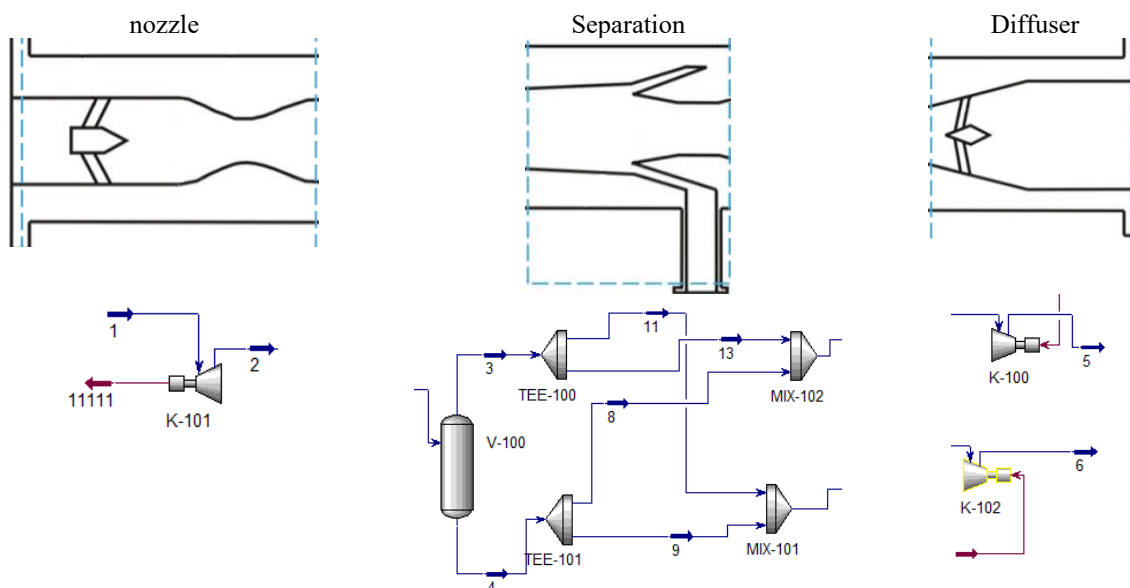


Figure 2 – Equivalent circuit of a supersonic separator in HYSYS (option 1)

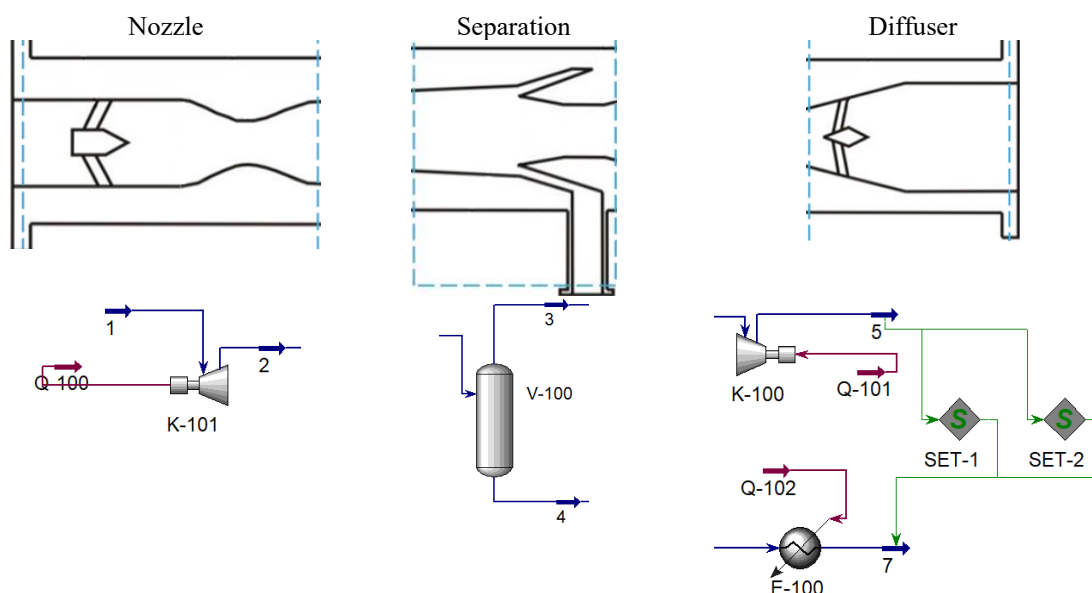


Figure 3 – Equivalent circuit of a supersonic separator in HYSYS (option 2)

The functional stages of liquefaction, separation and diffusion in a supersonic gas separator require replacement by equivalent processes and simplification in the HYSYS software used for modeling.

Particular attention should be paid to the fact that the two separated liquid streams in a real supersonic separator are not completely pure gas or liquid. Therefore, it is necessary to simulate the procedure of redistribution and recombination of these streams in certain proportions in order to reproduce the real efficiency of the supersonic separator as accurately as possible. Subsequently, two redistributed streams are obtained at the output. Based on the principles of operation of the supersonic separator and the functionality of the modules in HYSYS, the following scheme can be considered an optimal equivalent model.

In the first section (nozzle), the compressed gas expands adiabatically, as a result of which the flow velocity reaches supersonic values, and the temperature and pressure decrease sharply. This promotes phase transition and condensation in the target components. The role of this stage is played by the expansion module, which forms the effect of cooling and liquefaction of important components. In the second stage, the formed high-energy gas-liquid flow is directed to the separation section, where the droplets are separated through the side outlet. The equivalence of this phase is ensured by a modular combination of a separator, tees and mixers. After the separation of the two-phase mixture, the dry gas is directed to the diffusion segment, where its speed decreases, and the pressure and temperature increase. In the simulation, this process is reproduced using a compressor module, ensuring the restoration of

the physical parameters of the gas at the end of the diffusion section.

In the process of modeling supersonic separation in HYSYS, several assumptions are introduced to simplify the calculations and more accurately reflect the results.

For physical properties, the Peng-Robinson equation of state (PR EOS) is used, which is suitable for gas preparation. A stable flow regime within the supersonic separator is taken into account as a basic assumption.

The separator throughput is set to 100 kg/h, which exceeds the minimum critical value for stable operation.

For the treatment of humid air, the flow distribution coefficients in the gas-phase and liquid-phase tees are set to $0.7 + 0.3$ and $0.32 + 0.68$, respectively. In the case of natural gas, these figures change to $0.75 + 0.25$ and $0.002 + 0.998$.

The flow within the entire separator is assumed to be adiabatic. For equivalent modeling, the adiabatic efficiency of the compressor and expander is set to 99%.

The construction of the equivalent module is aimed at minimizing energy losses due to the impact of shock waves and secondary gasification of condensate.

The pressure and temperature at the outlet of the nozzles are considered critical parameters that have a direct impact on the quality of component separation. Thus, the proposed model in HYSYS allows for a fairly accu-

rate reproduction of the functional stages of a supersonic gas separator and provides the necessary flexibility for laboratory or industrial applications. [5].

The modeling working environment is equipped with all the necessary components to solve the task. It includes raw material components, material and energy flows, technological equipment, process control and regulation tools, as well as logical operations and utilities. The Peng–Robinson equation of state was chosen as the thermodynamic method in the modeling. For the correct implementation of the 3S separator device model using standard tools, it is necessary to reflect three key physical processes occurring in the device: – expansion of the gas input flow with its subsequent cooling; – separation of the resulting gas condensate flow into gas and gas-liquid fractions; – compression of the separated gas flow after separation.

It is also necessary to make a reservation that the software environment gives the most accurate results when modeling equilibrium processes. Since the process occurring in the supersonic separator is non-equilibrium, this method of modeling is considered as a first approximation to the actually occurring processes. To justify the choice of the model type, a study was conducted for weathering gas. The study was conducted for both models. Model options 1, 2 (Fig. 4,5).

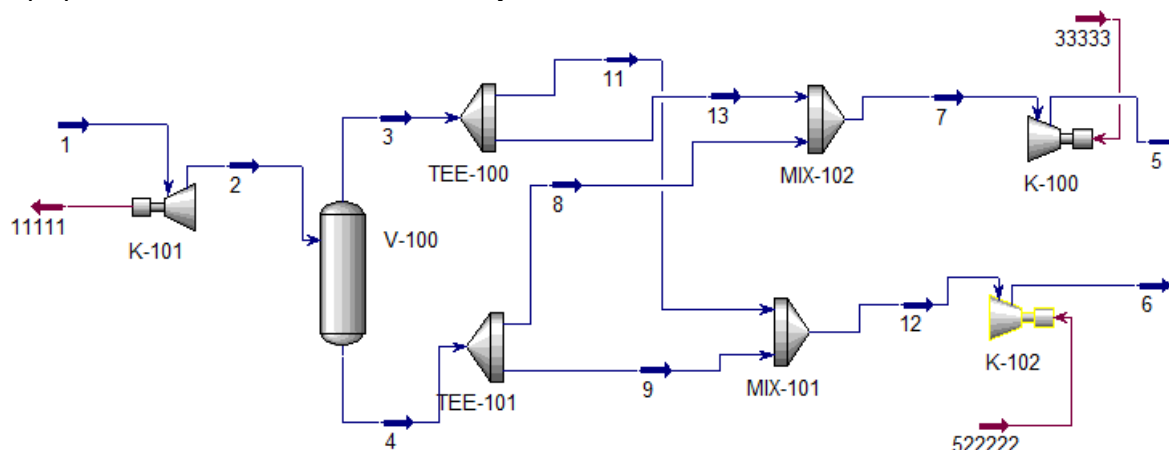


Figure 4– Option 1 of the separation process modeling

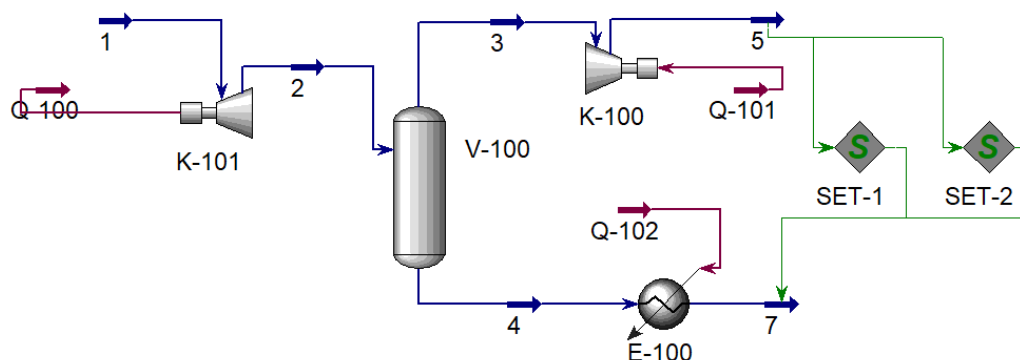


Figure 5 – Option 1 of the separation process modeling

The influence of pressure on the extraction of target components. For the raw material stream, the dependence of the extraction of the C3 + fraction (% wt.) into the condensed phase of the gas-liquid flow (gas– liquid

phase) on the pressure at the inlet to the 3S– separator in the range of 7–15 MPa in 1 MPa increments at a raw material temperature of +10 ° C was studied. The results of the studies for the two options are shown in the

figures 6-9. For options 1 and 2, the data obtained during the study on the dependence of the extraction of the C3 + fraction on the pressure of the raw material allow us to conclude that in the considered pressure range, the extraction of the target components increases non-linearly. At a pressure of 12.5 MPa, the content of the C3 + fractions practically does not change. This is confirmed by Fig. 8, in which the mass of condensate per year, starting from a pressure of 12.5 MPa, almost does not change. The dew point temperature for moisture and hydrocarbons of the extracted gas meets the re-

quirements of the Code of the Gas Transportation System of Ukraine. For all considered raw material flows, the deviation of the graphs from linearity is insignificant. It should also be noted that temperature, unlike pressure, has an anti-battery effect on the yield of the liquefied product. Therefore, it can be stated that both schemes show convergent results, since the nature of the distribution is the same. Further use is possible for both option 1 and option 2. We choose scheme 1 for further modeling, since it has fewer components.

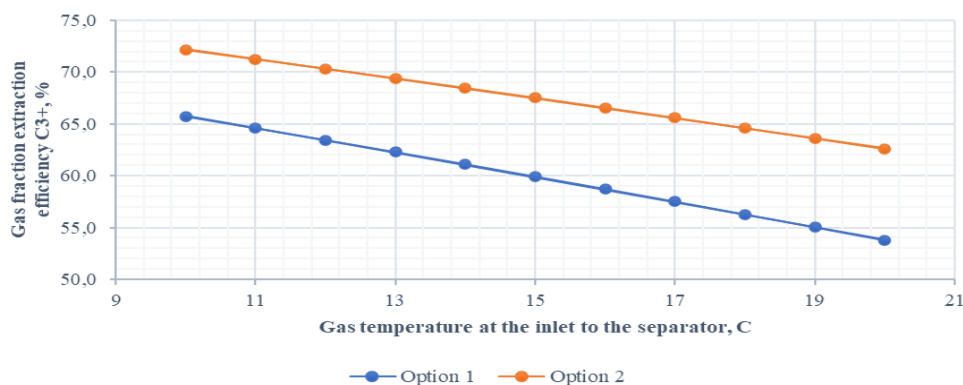


Figure 6 – Extraction of target components C3 + from the pressure at the inlet to the apparatus at P = 10 MPa

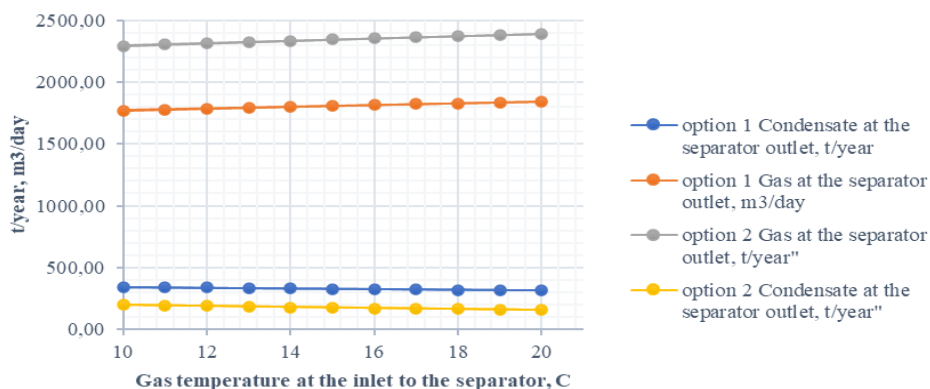


Figure 7 – Gas and condensate extraction at the pressure at the inlet to the apparatus at P = 10 MPa

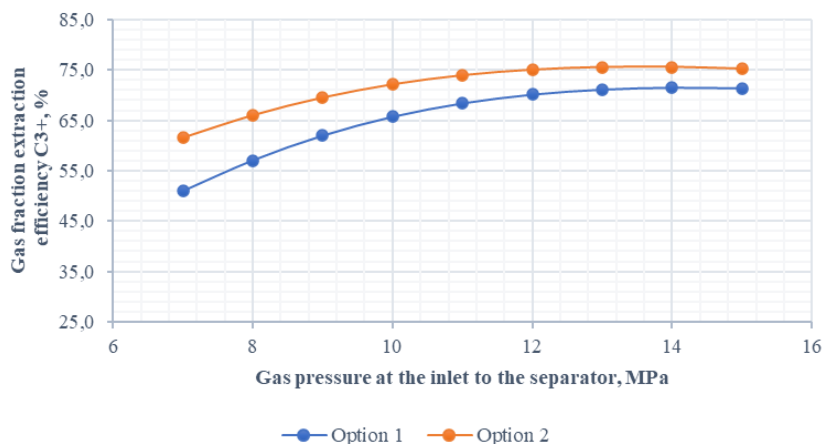


Figure 8 – Extraction of target components C3 + from the pressure at the inlet to the apparatus at Tc = 283 K

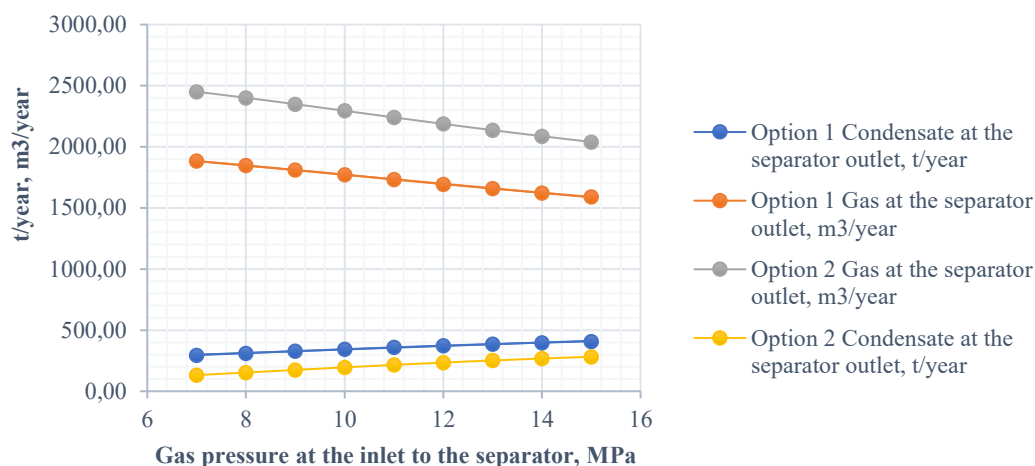


Figure 9 – Gas and condensate extraction at the pressure at the inlet to the apparatus at $T_c = 283\text{ K}$

The object of modeling was chosen as the hydrocarbon preparation system at the gas condensate field. It has a capacity for: gas – 2 million m^3/day , gas condensate – 150 t/day, formation water – 52 t/day.

The component composition of the gas is given in Table 1.

Table 1 – Component composition of hydrocarbons

Name and chemical formula		Component content, % vol.
Methane	CH_4	86,607
Ethane	C_2H_6	5,739
Propane	C_3H_8	1,253
i-Butane	iC_4H_{10}	0,154
n-Butane	nC_4H_{10}	0,198
neo-Pentane	$\text{neoC}_5\text{H}_{12}$	0,007
i-Pentane	iC_5H_{12}	0,063
n-Pentane	nC_5H_{12}	0,041
Hexane+higher	C_6H_{14+}	0,204
Oxygen	O_2	0,000
Nitrogen	N_2	0,240
Carbon dioxide	CO_2	4,494

The process of gas and condensate preparation at the installation for further transportation includes: gas collection at the unit of the input threads of the installation; gas separation at the input separators of the first stage, pre-cooling at recuperative heat exchangers (for gas from high-pressure wells) throttling and separation at low-pressure separators of the second stage, heating at recuperative heat exchangers (for gas from high-pressure wells) before feeding into the main gas pipeline; separation of gas condensate from associated formation water from condensate in the dehydrator 1; final separation of associated formation water from gas condensate in the dehydrator B-1; degassing of gas condensate in the degasser B-2; final degassing of condensate on the ladder and in condensate storage tanks.

Gas preparation is carried out on two technological

lines (high-pressure and low-pressure) with a total design capacity of 2 million m^3/day . Additionally, a measuring technological line with a capacity of 300-600 thousand m^3/day is provided for the performance study of wells.

The gas-water-condensate mixture from the production wells of the gas condensate field is supplied to the unit of the input threads of the installation using gas pipelines-loops, where the technological mode of operation of the “formation-well-loop” system is set using regulating fittings. Also, at the input string node, gas (wells) is distributed into high-pressure and low-pressure technological lines or to a measurement line for performance monitoring.

The gas obtained as a result of the technological process is sent to the commercial metering unit and then transported to the gas pipeline connecting to the main gas pipeline.

The condensate obtained after stabilization to atmospheric pressure and separated from the sub-product water is shipped from the condensate park tanks to tanker trucks.

The associated formation water, which was separated from the condensate as a result of the technological process, is sent via a bypass to the formation water storage tank. The results of the calculation using a supersonic separator are shown in Figure 10.

The figure shows the input parameters of the gas along 3 lines and shows the parameters of the prepared gas, winding gas, condensate and formation water.

The ventilation gas at the installation can be utilized immediately: from the separator of another stage it is directed to the low side of the ejector, from the degasser tank the condensate is sent to the compressor, also when necessary. It is possible to direct the ventilated gas from the separator to another stage and from the degasser tank to the condensate to the compressor or ejector.

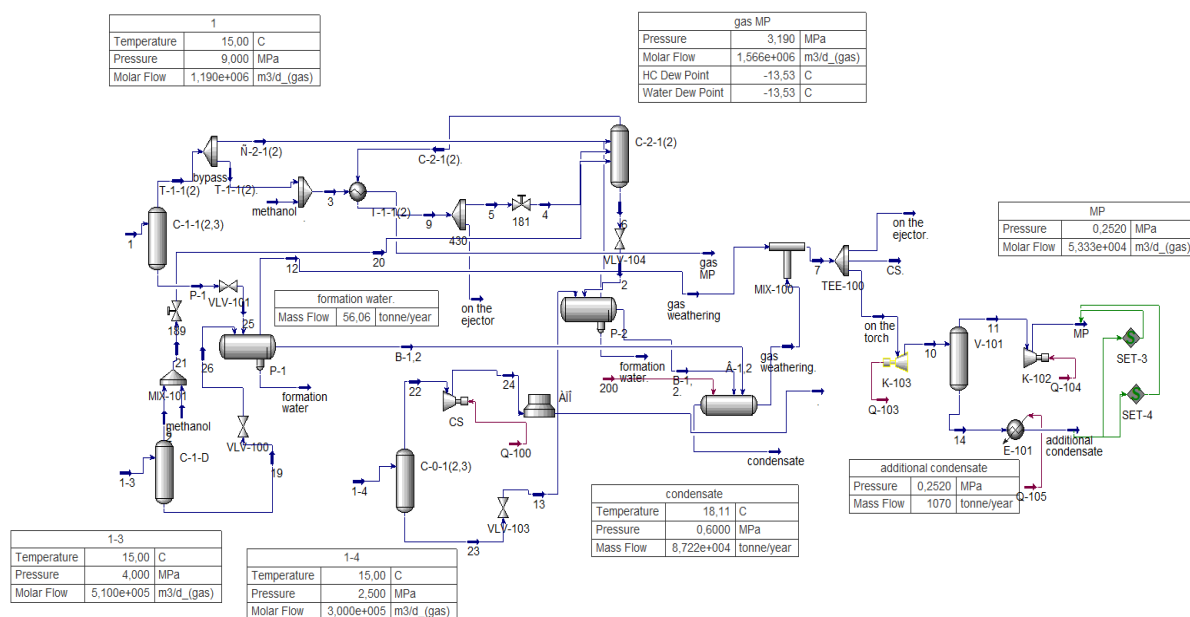


Figure 10 – Equivalent calculation scheme of a complex gas preparation installation

Also, when connecting to the compressor, it is possible to direct the gas supply to the power gas separator. Whenever there is a supply of gas, excess gas from the gas separator is discharged to the flare. It is advisable to install a supersonic separator at the installation, and if there is a presence of winding gas, direct it not to the torch, but to this separator. The results of modeling an improved scheme for the preparation of carbohydrates are shown in Figure 4.3. It can be seen that additional condensate of 1070 t/year was recovered, but not much was recovered, and gas can also be supplied to the supersonic separator, which is sent to the propane refrigeration unit of another gas treatment unit. After supersonic separation of the gas, this gas is determined by the dew point temperatures of the liquid and carbohydrates.

Conclusions

The simulation of the supersonic separation process was performed in the HYSYS environment, which allowed obtaining optimal parameters for the extraction

of heavy hydrocarbons from natural gas. The effect of pressure on the efficiency of the separation of target components was studied. Data were obtained that when the pressure was increased to 12.5 MPa, the efficiency of the process increases, however, a further increase in pressure does not provide significant advantages. A comparative analysis of two modeling schemes was carried out, as a result of which the optimal option was selected, which has fewer components and provides sufficient prediction accuracy.

The limitations of existing models were analyzed, in particular their sensitivity to equilibrium assumptions. Using the example of an existing gas preparation plant, it was proven that the use of a supersonic separator contributes to increasing the efficiency of natural gas preparation and additional condensate extraction. The results obtained can be used to further improve natural gas purification technologies and their adaptation to industrial application.

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