



Optimisation of process parameters for improved desulphurisation in propane-propylene processing

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Abstract. The purpose of the study was to optimise the parameters of the propane-propylene desulphurisation process to increase its efficiency. The study analysed the influence of temperature, pressure, and adsorbent type on the effectiveness of the propane-propylene desulphurisation process. It was found that an increase in temperature contributes to an increase in the rate of adsorption of sulphur compounds, but this effect persists only up to a certain temperature value. After reaching a certain limit, the temperature begins to have a negative effect on the adsorbent, causing its degradation. Based on the data obtained, the optimal temperature for maximum efficiency of the desulphurisation process was determined to be in the range of 250-300°C. The effect of pressure on the desulphurisation process turned out to be significant: increasing the pressure improves the results, as it increases the density of the gas phase, which, in turn, contributes to better capture of sulphur compounds. However, if the pressures are too high, there is no additional improvement in the results, and the energy costs of the process increase. In addition, aluminium oxide proved to be the most effective of all the adsorbents considered. It has demonstrated the best results compared to activated carbon and silica gel under optimal temperature and pressure conditions, providing the greatest degree of sulphur removal from the gas mixture. Ultimately, the mathematical models developed during the study confirmed that optimising the temperature and pressure parameters can significantly increase the efficiency of the desulphurisation process. This allows not only increasing the degree of sulphur removal, but also reducing energy costs and extending the service life of the equipment, which is important for its practical application. The practical value of the research lies in the fact that an integrated approach that considers the relationship between temperature, pressure, and adsorbent type significantly improves the desulphurisation process on an industrial scale, providing higher efficiency and cost-effectiveness

Keywords: temperature; pressure; adsorbent; aluminium oxide; energy costs

Introduction

The propane-propylene desulphurisation process is an important step in the processing of hydrocarbon gases, as it allows the removal of sulphur compounds that can

significantly degrade product quality and negatively affect equipment. The effectiveness of this process depends on many factors, among which the main ones are

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temperature, pressure, and the choice of adsorbent. The correct selection and optimisation of these parameters can significantly improve the quality of desulphurisation, reduce operating costs, and improve the overall efficiency of the process. In this regard, research aimed at optimising these factors represents an important step in improving the productivity and durability of equipment in the petrochemical industry.

The problem of effective propane-propylene desulphurisation remains relevant in the petrochemical industry, since the removal of sulphur from hydrocarbon gases is necessary to improve product quality and protect equipment. Y. Lei *et al.* (2022) investigated the effect of temperature on the process of propane-propylene desulphurisation, noting that an increase in temperature to a certain level accelerated the adsorption of sulphur compounds. However, they also warned that excessive temperature rise could lead to degradation of the adsorbent, which reduced the efficiency of the process. M. Mehri *et al.* (2021) studied the role of pressure in the desulphurisation process, revealing that an increase in pressure contributed to an improvement in the interaction of gases with the adsorbent. However, they stressed that the overpressure did not significantly improve results and increased operating costs. M. Andrade *et al.* (2021) concluded that the optimal temperature for effective desulphurisation of propane-propylene was 200-350°C. This value contributed to the maximum rate of adsorption, without leading to overheating and degradation of the adsorbent used. R. Kancherla *et al.* (2021) emphasised that an increase in pressure contributed to an increase in the density of gases, which improved the interaction of molecules with the adsorbent. However, they also noted that high pressures did not always lead to significant process improvements and could cause additional equipment costs. A.G. Georgiadis *et al.* (2021) noted that increasing the pressure to a certain level enhanced the efficiency of the process, but its further increase had no noticeable effect on the result, which made such optimisation economically impractical. They also emphasised the importance of balancing pressure and other parameters to achieve optimal conditions.

X. Li *et al.* (2023) studied various types of adsorbents, revealing that aluminium oxide demonstrated the greatest efficiency in removing sulphur compounds. They also noted that the correct choice of adsorbent depended on the composition of the gas mixture and the operating conditions, which required additional analysis. P.S. Castro *et al.* (2023) confirmed that adsorbents based on metal oxides, such as aluminium oxide, are significantly more effective than other materials, such as activated carbon or silica gel. They also investigated how various parameters, including temperature and pressure, affected the effectiveness of these adsorbents. P. Kumar & V.C. Srivastava (2023) developed mathematical models for the analysis of the

desulphurisation process, which considered the influence of temperature, pressure, and type of adsorbent. These models allowed predicting the efficiency of the process under different conditions and became the basis for further optimisation research. C.-T. Wang *et al.* (2025) created models that helped fine-tune desulphurisation parameters in real-world industrial conditions, minimising energy costs and increasing productivity. They emphasised the importance of using such models to increase the sustainability and long-term effectiveness of processes. X. Li *et al.* (2022) emphasised that the composition of the initial mixture influenced the choice of adsorbent, which had to be taken in consideration to achieve maximum sulphur removal efficiency. Their studies examined various combinations of gas mixtures and adsorbents to optimise desulphurisation.

Despite these achievements, there are still gaps in understanding the exact interaction between the process parameters, which requires additional study. For example, the effect of the composition of the gas mixture on the choice of adsorbent, the specifics of using mathematical models to optimise the operating conditions of the installation, and the durability of various types of adsorbents on an industrial scale remain poorly understood.

The purpose of the study was to determine the optimal values of temperature, pressure, and adsorbent type for the propane-propylene desulphurisation process aimed at improving its performance in energy and engineering systems. Research objectives:

1. To consider various methods for optimising these parameters to improve the removal of sulphur compounds.
2. To assess the effectiveness of using different types of adsorbents depending on the composition of the gas mixture and operating conditions.
3. To evaluate energy costs under various temperature and pressure conditions.

Materials and Methods

As part of this study, the key parameters of the propane-propylene desulphurisation process were studied in detail, with an emphasis on their impact on sulphur removal efficiency and optimisation of operating costs. The study focused on parameters such as temperature, pressure, and adsorbent selection to optimise these factors to improve process efficiency and minimise energy costs. Temperature is an important factor because it directly affects the reactivity of the adsorbent and the rate of adsorption of sulphur compounds. The study examined how an increase in temperature affects the reaction rate between the gas mixture and the adsorbent, which, in turn, promotes faster removal of sulphur from the gas. However, the potential negative effects of excessively high temperature, such as adsorbent degradation, reduced adsorbent efficiency and increased operating costs, were also investigated. The study of

temperature conditions was aimed at finding the optimal temperature at which the desulphurisation process proceeds with maximum efficiency without damaging the adsorbent. This would not only improve the purification speed, but also extend the service life of the equipment. Different temperature regimes were selected for each group of adsorbents based on their thermal stability and ability to effectively remove sulphur under various conditions.

Pressure also played a key role in the desulphurisation process. The study examined how an increase in pressure affects the density of the gas phase, which improves the interaction of the gas with the adsorbent. The problem of excessive energy costs arising from too high pressure, which can reduce the economic viability of the process, was also investigated. To assess the effect of pressure on the process, experiments were conducted during the study aimed at identifying optimal pressure values at which the desulphurisation process would be most effective and energy costs would be minimal. The pressure increase factor was also considered to improve the density of gases, which had a positive effect on the interaction with the adsorbent, but only up to a certain limit.

One of the key aspects of the study was the choice of adsorbent. For this purpose, materials with high adsorption capacity, selectivity, resistance to high temperatures and mechanical influences, and efficiency in removing sulphur from the gas mixture, were considered. Various types of adsorbents, such as metal oxides, activated carbon, and metal-organic framework (MOF) structures, were analysed. These materials have different physicochemical characteristics and can exhibit different properties under different temperature and pressure conditions.

In addition, an important part of the research was the development of mathematical models that took into consideration the influence of temperature, pressure, and adsorbent type on the effectiveness of the desulphurisation process. The models were used to predict the optimal operating conditions of the plant, which made it possible to accurately select the parameters that ensure the best result in real production conditions. Mathematical modelling also allowed evaluating the economic efficiency of the process, which was important for choosing optimal operating modes, minimising energy costs and improving the overall production economy. The models not only increased the efficiency of sulphur removal, but also provided prediction of the long-term characteristics of the plant, which played a key role in optimising the process. The study presented graphs based on calculations of mathematical models, such as the change in sulphur concentration over time and the effect of plant parameters on the total cost of operation. The data on the initial concentration, adsorption coefficient, adsorbent cost, and energy consumption were used, which helped to

confirm the theoretical conclusions and give practical recommendations.

Results

Desulphurisation is a critical process in the processing of gas mixtures such as propane-propylene. The main task of this stage is the removal of sulphur compounds present in the raw materials. Sulphur and its compounds pose a serious threat to production systems. When they accumulate, the risk of corrosion of the equipment increases, which reduces its service life and increases the cost of repair and replacement. In addition, sulphur compounds degrade the quality of the final product, making it less competitive on the market. From an ecological standpoint, sulphur removal reduces emissions of toxic compounds into the environment, preventing air pollution and minimising harm to ecosystems. With increasing demands on the quality of hydrocarbon products and industrial safety standards, desulphurisation is becoming even more important. Modern processing technologies require a high degree of purity of the raw materials, which directly affects the productivity and reliability of the processes (Chen *et al.*, 2022).

Temperature is a key factor determining the efficiency of the desulphurisation process of hydrocarbon gases, including propane-propylene mixture. It directly affects the reactivity of the adsorbent and its ability to remove sulphur compounds. Optimisation of the temperature regime helps to accelerate adsorption, while avoiding undesirable effects such as thermal degradation of the adsorbent or the development of secondary pollutants (Wang *et al.*, 2023).

An increase in temperature promotes the activation of gas molecules, which increases the rate of their interaction with the active surface of the adsorbent. For example, for aluminium oxide-based adsorbents, an increase in temperature to 250-300°C leads to a noticeable improvement in their sorption capacity. However, an excessive increase in temperature can cause thermal destruction of the active components, reducing sorption properties and shortening the service life of the material. This, in turn, increases the cost of operation and maintenance of the installation.

At low temperatures, the activity of the molecules and adsorbent decreases, which slows down the desulphurisation process. As a result, the purification efficiency decreases, and the plant's performance may not be sufficient for industry standards. To achieve optimal results, it is necessary to find a balance between these extremes. The optimal temperature range for most industrial desulphurisation processes is 250-300°C, which achieves high sulphur removal efficiency and minimises the risks of adsorbent degradation.

In practice, temperature selection requires consideration of many factors, such as the composition of the gas mixture, the type of adsorbent used, and the operating conditions. For example, mixtures with a high

concentration of sulphur compounds may require a higher temperature to ensure sufficient reactivity of the adsorbent. At the same time, temperature limits can be set for adsorbents with low thermal stability to avoid their destruction.

An integrated approach to the choice of temperature regime includes the use of experimental data and mathematical modelling. Such models allow predicting the behaviour of the system at different temperatures and selecting optimal parameters, considering technical and economic feasibility. This makes the temperature regime an important element for the successful implementation of desulphurisation processes in industry.

Pressure plays a crucial role in the efficiency of hydrocarbon gas desulphurisation processes, including propane-propylene mixtures. It determines the density of the gas mixture and the intensity of the interaction of gas molecules with the active surface of the adsorbent, which directly affects the removal of sulphur compounds. However, pressure management requires finding the optimal balance between technical efficiency and economic feasibility, since excessive pressure can significantly increase operating costs (Huang *et al.*, 2023).

An increase in pressure leads to a convergence of gas molecules, which increases the likelihood of their contact with the adsorbent. This contributes to a more intensive adsorption of sulphur compounds and, as a result, improved purification results. For example, M.A. Pordsari *et al.* (2024) have shown that when using aluminium oxide-based adsorbents, pressure in the range of 10-20 atmospheres provides optimal results. Nevertheless, the effect of increasing pressure has its limits: after reaching a certain level, its further increase ceases to have a significant effect on the effectiveness of desulphurisation.

Too high pressure is accompanied by increased gas compression costs and increased equipment loads.

This requires the use of more expensive materials and structures to ensure reliable and safe operation of the system. For example, increasing the pressure above 20 atmospheres may require the installation of specialised compressors, which increases capital costs. In addition, energy consumption associated with maintaining high pressure is increasing, which reduces the overall economic efficiency of the process.

To determine the optimal pressure, it is necessary to consider the composition of the gas mixture and the characteristics of the adsorbent used. For example, mixtures with a high content of sulphur compounds require a higher pressure to achieve a given degree of purification. When using adsorbents with low mechanical strength, pressure limitations become critical to prevent material damage.

Pressure optimisation is an important step in the design and operation of desulphurisation systems. The range of 10-20 atmospheres is considered to be the most balanced in terms of technical and economic performance. This approach helps to achieve a high degree of purification of hydrocarbon gases at minimal cost of equipment and energy resources.

Rational pressure management helps to increase the stability of the process, improve the quality of the final product, and reduce the negative impact on the environment. This is especially important in modern conditions, when the requirements for environmental safety and economic efficiency of production are constantly being tightened. The type of adsorbent is a crucial factor in the effectiveness of desulphurisation processes, since its physicochemical properties directly affect the ability to remove sulphur compounds from hydrocarbon mixtures. Modern technologies offer a wide range of materials, among which metal oxides, activated carbon, and silica gels occupy a special place, including the latest developments such as MOF (Table 1).

Table 1. Efficiency of different types of adsorbents depending on gas mixture composition and operating conditions

Adsorbent type	Composition of the gas mixture	Operating temperature (°C)	Operating pressure (atm)	Adsorption coefficient (Ka) (mg/g)
Aluminium oxide	Propane-propylene, hydrogen sulphide 0.5%	200-300	10-15	85
Activated carbon	Propane-butane, mercaptans 0.2%	50-150	1-5	70
Silica gel	Propane-propylene, sulphur dioxide	100-250	5-15	60
MOF	Propane-propylene, hydrogen sulphide 0.1%	150-250	5-20	95

Source: compiled by the authors based on J.Y. Lai *et al.* (2021)

Metal oxides, for example, aluminium oxide, are characterised by high chemical stability and the ability to bind molecules of sulphur compounds. This material has proven to be an effective and affordable option, especially at temperatures of 250-300°C (Ikram *et al.*, 2021). In addition, it has a good regenerative ability, which makes it economically beneficial. However, the effectiveness of aluminium oxide may decrease in the

presence of complex impurities such as carbon dioxide or organic pollutants, which requires additional pre-treatment steps.

Activated carbon is valued for its high specific surface area and versatility, allowing it to adsorb a wide range of compounds. However, its properties may deteriorate at high humidity, which makes it less effective for working with gas mixtures containing water vapour.

Silica gels demonstrate high efficiency in low-temperature processes and can adsorb moisture, improving the quality of purification. However, their chemical resistance is limited, which makes them less suitable for handling aggressive components such as hydrogen sulphide or organic sulphur compounds.

MOFs are the latest generation of adsorbents that have a unique porous structure and high selectivity. They can be modified to work with certain sulphur compounds, ensuring maximum efficiency with minimal material consumption. For example, MOFs successfully operate at low temperatures, which makes them promising for use in installations with limited energy consumption. However, their widespread industrial use is limited by the high cost and complexity of production.

Thus, the choice of adsorbent should be based on a comprehensive analysis of the characteristics of the initial mixture, operating conditions and economic feasibility. Modern research in the field of developing new materials and modifying existing adsorbents continues to expand the possibilities of optimising the desulphurisation process, which makes it more efficient and sustainable (Omar & Verma, 2022).

The process of propane-propylene desulphurisation is an important step in the industrial processing of hydrocarbon mixtures aimed at removing sulphur compounds. In order to achieve high efficiency in this process, kinetic and dynamic parameters must be considered, which directly affect the choice of optimal operating conditions for the installation. Studying these factors helps not only to improve the process, but also to significantly reduce operating costs, while increasing production and environmental performance.

The kinetics of desulphurisation determines how quickly and efficiently the adsorption of sulphur compounds occurs on the surface of the adsorbent (Al-Khodor & Albayati, 2023). This aspect is key to optimising the operating cycle of the installation. Important parameters to consider are the duration of contact of the gas mixture with the adsorbent and the rate of gas flow through the reactor. The longer the contact of the gas with the adsorbent, the higher the probability that sulphur compounds will be effectively removed from the gas stream. However, it is important to balance this parameter with the energy costs and throughput of the installation.

In parallel with the duration of contact, the gas flow rate through the installation is also important. A high flow rate can speed up the process, but the degree of adsorption will decrease, since the gas will not be in contact with the adsorbent for a long time. On the contrary, too low a flow rate can lead to insufficient equipment efficiency and excessive costs for maintaining the necessary conditions.

The dynamics of the process, in contrast to kinetics, considers the behaviour of a gas mixture over time and its interaction with an adsorbent (Karimi *et al.*, 2021). An important aspect of the dynamics is to ensure an even

distribution of gas throughout the reactor volume. If the gas passes through the adsorbent unevenly, this can lead to the development of “dead zones” – areas where the gas does not come into contact with the adsorbent properly, which significantly reduces the effectiveness of desulphurisation. Thus, it is important to adjust the gas flow parameters to prevent the occurrence of such zones and ensure an even distribution of the mixture components. One solution to increase dynamic efficiency is to use flow distributors or technologies with improved gas-adsorbent contact. These technologies allow minimising the loss of working material and significantly improving the degree of gas purification from sulphur.

In order to accurately determine the optimal parameters of the kinetics and dynamics of the process, it is necessary to conduct experimental studies to collect data for building models. Such data may include information on the rate of adsorption of sulphur compounds at various temperatures, pressures, and gas mixture compositions. The use of mathematical modelling allows predicting the behaviour of the system and optimise the parameters in real production conditions.

Several approaches can be used to develop mathematical models of the desulphurisation process during propane-propylene processing. The main elements to be considered include the adsorption coefficient, the dynamics of changes in the concentration of sulphur compounds, energy costs, and operating costs (Naderi *et al.*, 2024). Basic mathematical models have been proposed that can be used to analyse and optimise this process.

The adsorption model can be based on the classical theory of adsorption, where the concentration of sulphur compounds in the gas phase decreases over time, depending on the process parameters. The basic model for this process is the adsorption rate equation, which can be written as (1):

$$\frac{dC}{dt} = K_a \cdot C, \quad (1)$$

where C – concentration of sulphur compounds in the gas mixture (mg/m^3); t – time (h); K_a – adsorption coefficient ($\text{m}^3/\text{mg}\cdot\text{h}$), which depends on the type of adsorbent and temperature.

The solution of this equation gives the dependence of the sulphur concentration on time (2):

$$C(t) = C_0 \cdot e^{-K_a t}, \quad (2)$$

where C_0 – initial concentration of sulphur compounds (mg/m^3); $C(t)$ – concentration of sulphur at time t .

The duration of the desulphurisation cycle depends on the capacity of the adsorbent and the volume of gas to be treated. The model for the cycle duration has a form (3):

$$t_c = \frac{m \cdot q_{max}}{F \cdot C}, \quad (3)$$

where t_c – duration of the desulphurisation cycle (h); m – weight of the adsorbent (g); q_{max} – maximum

capacity of the adsorbent (mg/g); F – volume flow rate of gas (m³/h); C – concentration of sulphur compounds in the gas mixture (mg/m³).

This model allows estimating the operating time of the installation before the adsorbent needs to be replaced or regenerated. The energy costs of maintaining temperature and pressure can be expressed in terms of equipment capacity and operating time (4):

$$E = P \cdot t, \tag{4}$$

where E – energy cost (kWh); P – power of the equipment (kW); t – operating time of the installation (h).

This model will help to calculate energy consumption for different operating modes of the installation, which is important for optimising processes. The total cost of operating the plant consists of several components: the cost of adsorbent, energy costs, and maintenance costs. The model for the total cost of operation is as follows (5):

$$C_{total} = C_{ads} + C_{energy} + C_{maint} \tag{5}$$

where C_{total} – total cost of operation (USD); C_{ads} – adsorbent cost (USD); C_{energy} – energy cost (USD); C_{maint} – equipment maintenance and replacement costs (USD).

Here, the adsorbent cost may depend on the amount of material used, energy consumption on the installation capacity and operating time, and maintenance costs on the frequency of equipment replacement and maintenance. Graph of changes in the concentration of sulphur compounds over time: based on the equation for adsorption (2), a graph can be constructed that shows a decrease in sulphur concentration depending on time at different values of the adsorption coefficient K_a (Fig. 1). The initial concentration values of $C_0 = 100$ mg/m³ and adsorption coefficients $K_a = 0.1, 0.2, 0.3$ mg/m³ were used in the calculations. Such data help to estimate how fast the desulphurisation process takes place at the specified parameters.

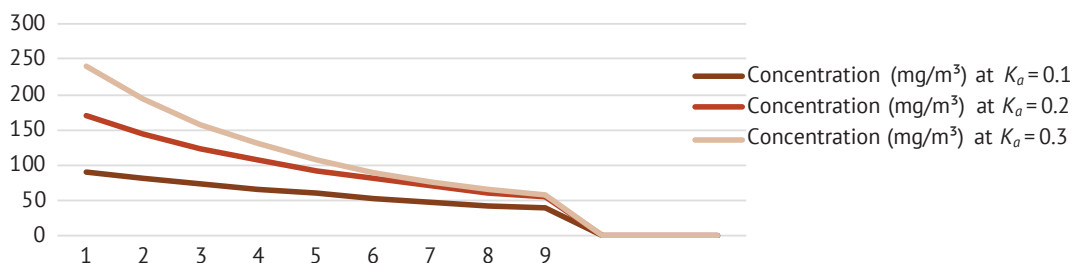


Figure 1. Graph of changes in the concentration of sulphur compounds as a function of time at different values of the adsorption coefficient

Source: compiled by the authors

Graph of the dependence of the total cost of operation on the parameters of the installation: a graph can be constructed that shows the variation of total cost of operation as a function of plant capacity, operating time, adsorbent cost, and energy consumption (Fig. 2). The total cost was calculated using the equation (5).

For calculations, the values of equipment power $P = 50, 75, 100$ kW, operating time $t = 100, 200$ h, and electricity price 0.1 USD/kWh, and the cost of adsorbent in the range from USD 1,500 to 4,000 were used. These data allow visually showing how the installation parameters affect the economics of the process.

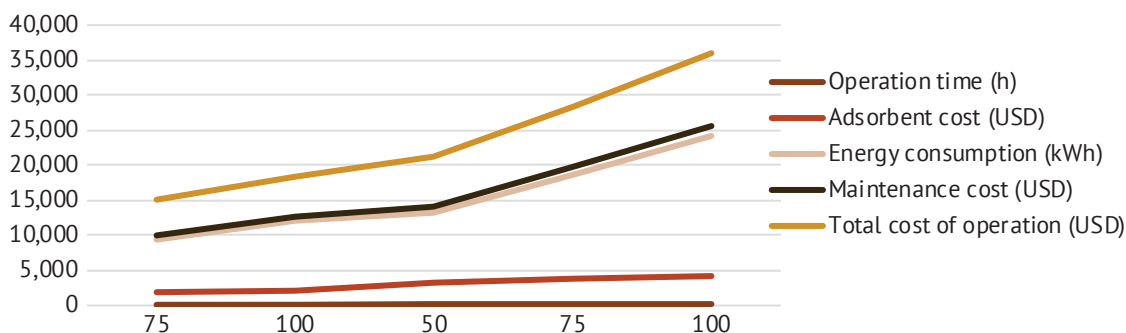


Figure 2. Graph of the dependence of the total cost of operation of the installation on the capacity of the equipment and the operating time

Source: compiled by the authors

In engineering applications, the importance of optimisation lies in ensuring the reliability and accuracy of data for system design. For example, when

designing desulphurisation plants, dynamic parameter changes such as temperature or pressure fluctuations must be considered to minimise the risks of equipment

failure. Accurate mathematical models allow predicting possible deviations and developing compensating mechanisms, which increases the overall safety of the installation (Ahn *et al.*, 2023). Energy aspects are also central to the process. Efficient energy management, for

example by choosing a low-energy adsorbent or optimising pressure, reduces the load on the company's energy systems. This is especially important in the context of modern requirements for reducing carbon dioxide emissions and energy conservation (Table 2).

Table 2. Energy costs under different temperature and pressure conditions

Temperature (°C)	Pressure (atm)	Equipment power (P) (kW)	Operation time (t) (h)	Energy costs (E) (kWh)	Notes
150	5	50	10	500	Optimal mode for adsorbents with low temperature resistance
200	10	70	10	700	Requires stable temperature control, suitable for aluminium oxide
250	15	90	10	900	High sulphur removal efficiency, increased equipment cooling costs
300	20	120	10	1,200	Energy consumption increases significantly, the use of heat-resistant adsorbents is required

Source: compiled by the authors based on P.R. Chauhan *et al.* (2022)

Optimisation also significantly reduces operating costs. For example, a more durable adsorbent reduces the frequency of its replacement, which minimises maintenance costs. In addition, reducing energy consumption helps to reduce energy costs, which makes the process more economically attractive for enterprises. Engineering applications include the use of such models to select optimal materials, design equipment, and predict system performance. The integration of these models into automated control systems makes the process more stable and adaptive to changing conditions.

Optimisation of desulphurisation parameters is an integral part of engineering and energy applications. It not only increases the efficiency of the installation, but also ensures safety, reduces environmental risks and improves the economic performance of the enterprise, which makes the process more promising and sustainable in the long term. Thus, successful optimisation of these parameters using appropriate models can significantly improve the desulphurisation process, increasing its economic and energy efficiency, and reducing operating costs.

Discussion

In the course of the study, the key parameters influencing the process of propane-propylene desulphurisation were analysed: temperature, pressure, and type of adsorbent. The results showed that temperature significantly affects the rate of adsorption of sulphur compounds. The optimal temperature range established during the experiments ensured high efficiency of adsorbents, whereas a slowdown in adsorption was observed at lower temperatures, and degradation of the adsorbent structure at high temperatures.

This problem was also analysed by S.H. Shafeianpour *et al.* (2024), and their findings confirmed that the process of propane-propylene desulphurisation depends on temperature, since a change in temperature

regime affects the activity of catalytic processes. At high temperatures, the reaction accelerates, which can lead to faster desulphurisation, but also increases the risk of adsorbent degradation. Determining the optimal temperature range is critical to maximise the efficiency of the process without loss of adsorbent quality. A.K. Singh *et al.* (2024) demonstrated that it is important to establish a temperature regime that ensures a balance between high reactivity and maintaining the stability of the material to prevent adsorbent degradation. The choice of a suitable temperature range also affects the service life of the equipment and the cost-effectiveness of the process. Careful analysis of the thermodynamic characteristics of the adsorbent helps to avoid its destruction when operating at high temperatures.

It should be emphasised that optimising the temperature conditions for propane-propylene desulphurisation is of key importance not only for increasing the speed of the process, but also for extending the service life of adsorbents. Despite the obvious advantages of high temperatures in accelerating chemical reactions, it is important to consider their impact on the stability and durability of materials. Gas pressure also proved to be a significant factor. Experimental data have shown that an increase in pressure increases the density of the gas flow and, as a result, improves the contact of gas molecules with the adsorbent. However, with a further increase in pressure, the adsorption efficiency stopped increasing, which can be explained by the saturation of the active centres of the adsorbent. This indicates the need to fine-tune the operating parameters to prevent an unjustified increase in energy costs.

J. Sun *et al.* (2022) concluded that increasing the pressure during desulphurisation can significantly improve the contact of the gas mixture with the adsorbent, which contributes to a more efficient capture of sulphur compounds. Higher pressure increases the density of gas molecules, which increases the likelihood

of collisions with the active centres of the adsorbent. This can lead to faster and more complete removal of sulphur from the gas mixture. The study by Q. Dong *et al.* (2021) found that it is important to consider that increasing the pressure has its limitations, since too high pressure can lead to an overabundance of molecules, which makes it difficult for them to interact with the adsorbent. Determining the optimal pressure for desulphurisation is critical, as it must ensure maximum process efficiency without unnecessary energy costs and threats to system stability. This requires careful analysis and experiments aimed at identifying the maximum pressure for optimal operation of the adsorber.

These results confirm the previously presented study, as they demonstrate a significant improvement in desulphurisation efficiency when optimising temperature and pressure conditions, which corresponds to the conclusions of previous studies. It is confirmed that the correct balance between temperature, pressure, and reaction time can significantly increase the productivity of the process, while maintaining the durability of the adsorbent. Such data also confirm the importance of an integrated approach to the development and improvement of desulphurisation technologies to achieve maximum efficiency and cost-effectiveness. The type of adsorbent used showed the greatest variability in the results. The most effective material was aluminium oxide, which provided a high degree of removal of sulphur compounds. Organometallic skeletal structures have shown promising results, but their high cost and limitations in operating conditions have so far reduced their competitiveness.

It is important to note the study by F. Ahmadijokani *et al.* (2021), in which it was also found that adsorbents based on aluminium oxides and organometallic skeleton structures have various advantages in the desulphurisation process. Aluminium oxides are known for their high stability and good adsorption properties under various temperature conditions, but their effectiveness is limited compared to more specialised materials. Whereas organometallic adsorbent framework structures offer improved selectivity and greater porosity, which can significantly increase their efficiency in removing sulphur from gas mixtures. In turn, A.T. Kadhum & T.M. Albayati (2022) concluded that the prospects for using modified adsorbents in industrial desulphurisation look promising, as they can combine the advantages of both types of materials. Modification of organometallic skeleton structures and aluminium oxides can significantly improve their resistance to high temperatures and aggressive environments, and expand their range of applications. These improvements open up new possibilities for more efficient and cost-effective desulphurisation, which can lead to significant improvements in industrial gas purification processes.

The data obtained are consistent with the statements outlined in the previous section, confirming that

optimisation of parameters such as temperature and pressure plays a key role in improving desulphurisation efficiency. The results of the study demonstrate that the correct combination of these factors can significantly improve the contact of the gas mixture with the adsorbent, which contributes to a more complete removal of sulphur compounds. Thus, observations confirm the importance of an integrated approach that considers the relationship between temperature and pressure conditions, and the need to fine-tune them to achieve maximum process performance.

The study of the kinetics of the process deserves special attention. The results showed that the duration of contact of the gas mixture with the adsorbent directly affects the effectiveness of desulphurisation. The optimal contact time ensured a balance between energy consumption and the required purification levels, while the insufficient duration did not allow achieving the desired process quality. S. Li *et al.* (2021) also conducted a study, and their results confirmed that optimising the gas-adsorbent contact time is an important aspect for reducing energy consumption during desulphurisation. Too short a contact time can lead to insufficient gas purification, while excessively long contact leads to unjustified energy costs. Therefore, it is important to determine the optimal duration of contact, which will ensure effective purification with minimal energy costs. S. Abbasi *et al.* (2023) also found that the effect of the duration of contact on the degree of purification of propane-propylene shows that there is a certain time at which the purification process reaches maximum efficiency. Increasing the contact time usually improves the degree of purification, but after reaching the optimal point, efficiency begins to decrease due to overheating and increased energy consumption. This highlights the need to fine-tune the contact duration to achieve the best balance between purification efficiency and cost-effectiveness of the process.

Comparing the data obtained during the research, it can be concluded that optimising the contact time with the adsorbent has a significant impact on the effectiveness of the desulphurisation process. While increasing the duration of contact improves the degree of purification, it must be borne in mind that after a certain threshold, a further increase in time does not significantly improve results, but increases energy consumption. These results highlight the importance of precise control of contact time, which will optimise the process, taking into account both purification efficiency and energy savings. The dynamic properties of the process also revealed the need for uniform gas distribution in the reactor. It was observed that the uneven gas flow led to the development of "dead zones" where adsorption was practically absent. The use of flow distributors and preliminary calculations of gas dynamics made it possible to significantly reduce these zones and improve the overall productivity of the process.

K. Kaczmarek & M.K. Szukiewicz (2021) concluded that the time of gas contact with the adsorbent is indeed a key factor in the desulphurisation process, affecting the degree of purification. The results showed that at the initial stages, an increase in contact time leads to a significant improvement in efficiency, since the gas has time to interact with the active centres of the adsorbent. However, after a certain point, the efficiency of the process stabilises, which confirms the need to find the optimal time to minimise energy consumption. X. Zhang *et al.* (2021) found that an excessive increase in contact time leads not only to a slight improvement in the degree of purification, but also to an increase in energy consumption, which is impractical from an economic standpoint. This approach requires careful process control to reduce unnecessary energy costs while maintaining the required purification quality. It is important that this study provides a basis for further optimisation of the conditions under which it will be possible to achieve the best results in terms of both savings and efficiency.

An analysis of the findings shows that optimising the contact time with the adsorbent has a noticeable effect on the effectiveness of desulphurisation, allowing for better purification performance with minimal energy consumption. While increasing the contact time improves the degree of purification, it has been found that further increasing it after a certain limit does not lead to significant improvements. This highlights the importance of precise time control, which helps to save energy without compromising process quality. Thus, the analysis of the obtained results confirms that optimisation of the parameters of the desulphurisation process requires an integrated approach. The established relationships between temperature, pressure, adsorbent type, and gas flow characteristics can become the basis for further design and configuration of industrial installations. This will increase the efficiency of the process and reduce its operating costs.

Conclusions

As a result of the conducted research, the key parameters influencing the efficiency of the propane-propylene desulphurisation process were identified. It has

been established that temperature plays one of the leading roles in ensuring optimal operation of adsorbents. The use of a temperature range at which adsorbents retain their activity helps to achieve a high degree of purification of the gas mixture without loss of the working properties of the materials. The analysis of the pressure effect revealed its critical importance for process optimisation. A moderate increase in pressure contributes to a more intense contact of gas molecules with the active centres of the adsorbent, which increases the efficiency of purification. However, an excessive increase in pressure does not provide significant advantages and may lead to unnecessary energy costs. The type of adsorbent proved to be a key factor influencing the results of desulphurisation. Aluminium oxides proved to be the most effective materials. Despite the promise of organometallic skeleton structures, their cost and limitations in operating conditions limit their widespread use.

The kinetics of the process demonstrated that the duration of gas contact with the adsorbent plays a significant role. Optimal time parameters allowed achieving a high degree of purification without excessive expenditure of resources. The dynamic characteristics of the process have shown that the uniformity of gas distribution in the reactor is crucial. The use of special switchgear helped to minimise the development of "dead zones". Thus, an integrated approach to optimising the temperature, kinetic, and dynamic parameters of the process ensure high productivity and reduced operating costs. The results obtained can be applied in the design and modernisation of industrial desulphurisation plants. The main limitation of this study is that the experiments were conducted in a laboratory setting, which may not fully reflect the complexity of industrial processes. Further research is needed to investigate the long-term stability of adsorbents under actual operating conditions, including the effects of impurities and temperature fluctuations.

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Conflict of Interest

None.

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Оптимізація технологічних параметрів для покращення десульфурації в процесі переробки пропан-пропілену

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Анотація. Метою роботи була оптимізація параметрів процесу сіркоочищення пропан-пропілену для підвищення його ефективності. В роботі проаналізовано вплив температури, тиску та типу адсорбенту на ефективність процесу десульфурації пропан-пропілену. Встановлено, що підвищення температури сприяє збільшенню швидкості адсорбції сполук сірки, але цей ефект зберігається лише до певного значення температури. Після досягнення певної межі температура починає негативно впливати на адсорбент, викликаючи його деградацію. На основі отриманих даних було визначено, що оптимальна температура для максимальної ефективності процесу сіркоочищення знаходиться в діапазоні 250-300 °С. Вплив тиску на процес сіркоочищення виявився значним: підвищення тиску покращує результати, оскільки збільшує щільність газової фази, що, в свою чергу, сприяє кращому вловлюванню сполук сірки. Однак, якщо тиск є занадто високим, додаткового покращення результатів не відбувається, а енергетичні витрати на процес зростають. Крім того, оксид алюмінію виявився найефективнішим з усіх розглянутих адсорбентів. Він продемонстрував найкращі результати порівняно з активованим вугіллям і силікагелем за оптимальних температурних і тискових умов, забезпечивши найбільший ступінь видалення сірки з газової суміші. Розроблені в ході дослідження математичні моделі підтвердили, що оптимізація параметрів температури і тиску дозволяє значно підвищити ефективність процесу сіркоочищення. Це дозволяє не тільки підвищити ступінь видалення сірки, але й знизити енерговитрати та продовжити термін служби обладнання, що є важливим для його практичного застосування. Практична цінність роботи полягає в тому, що комплексний підхід, який враховує взаємозв'язок між температурою, тиском і типом адсорбенту, значно покращує процес сіркоочищення в промислових масштабах, забезпечуючи вищу ефективність та економічність.

Ключові слова: температура; тиск; адсорбент; оксид алюмінію; енергетичні витрати