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INFLUENCE OF THE OXIDIZER ON THE FORMATION AND PURIFICATION EFFICIENCY OF ACID GASES PRODUCED DURING ASPHALTENE GASIFICATION

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The relevance *of the study is determined by the need to understand the influence of the oxidizer on the formation of acid gases (CO_2, H_2S, COS and CS_2) during thermal decomposition of high-viscosity hydrocarbons. This is important for predicting the purification efficiency of the produced gasification products and estimating the economic costs.*

The aim: *using the simulation to study the effect of an oxidizer in the form of steam on the composition and properties of asphaltene gasification products obtained from natural bitumen, as well as to determine the cleaning efficiency depending on the amount of steam and the absorbent based on NaOH water-alkaline solution.*

Object: *asphaltene of natural bitumen of Ashalchinskoe field of the Tatarstan Republic (Russia), oxidizer in the form of steam, the value of which varied from 0,1 to 1 depending on the amount of asphaltene.*

Methods: *simulation of asphaltene gasification and acid gas absorption taking into account influence of an oxidizer in a form of steam with regard for basic chemical kinetics, ultimate analysis and TGA.*

Simulation results of gasification and absorption showed that steam used as an oxidizer during asphaltene gasification has a significant influence on the composition and properties of gasification products, as well as on the purification of syngas. With the increase of steam, a parabolic dependence of the concentrations of syngas components is observed, which values decrease with time, except for CO_2. The calorific value of syngas decreases from 11,3 to 7,2 MJ/m^3 and the cold gas efficiency increases from 53,4 to 62,5 % due to growth of syngas yield. As the amount of steam increases, the amount of absorbent decreases and the purification efficiency of acid gases rises. Thus, the amount of absorbed CO_2 increases by 20,7 % while the absorbent decreases by 6,7 %. At the same time the amount of absorbed H_2S increased by 0,39 % with decrease of NaOH by 40,9 %.

Key words:
Asphaltene, gasification, syngas, acid gas purification, NaOH.

Introduction

According to the International Energy Agency, in 2021 global CO_2 emissions increased by nearly 4,8 percent to 33 Gigatons, thereby approaching the 2018–2019 peak [1]. This increase, as noted by the International Energy Agency, is due to a recovery in demand for classic energy sources such as coal, oil and gas in the second year of the Covid-19 pandemic. In this regard, the use of conventional energy technologies will lead to an increase in acid gases, which will not only worsen the environmental situation, but also have a negative impact on energy equipment. One way to solve this problem is to use clean technologies, which reduce the negative impact on the environment by significantly improving energy efficiency, sustainable use of resources or environmental protection activities. Clean technologies include a wide range of technologies related to recycling, renewable energy, etc.

In this regard, the use of fuel gasification is a more environmentally attractive technology compared to direct combustion. According to the Global Syngas Technologies Council, there are several hundred gasification plants work in the USA, Europe, Asia, South Africa and other countries which process various raw materials for the production of liquid and gaseous fuels [2]. Oil sands and bitumen are the important sources of raw materials and are being studied in Canada, USA, Venezuela and other countries. According to [3], bitumen reserves are estimated at 5,9 billion tons in the United States, 24,1 billion tons in Canada, and 36,4 billion tons in Venezuela. A significant amount of bitumen in Russia is concentrated in the Tatarstan Republic (about 7 billion tons). Gasification of bitumen will produce syngas and related products for various industries.

Natural gas, associated petroleum gas, syngas may contain acid gaseous components – carbon dioxide (CO_2) and hydrogen sulfide (H_2S), as well as sulfur compounds – carbonyl sulfide (COS), carbon disulfide (CS_2), and other impurities that negatively affect the environment and equipment. For example, the presence of CO_2 and H_2S creates conditions for metal corrosion and also reduces the efficiency of catalytic processes. In addition, H_2S and COS are highly toxic substances. Removal of these acid gases is driven by operational, economic, and environmental factors [4].

Various absorbents and methods, including alkanolamines [5], organic solvents [6], membrane separation [7], adsorption, and biological methods [8], are used to purify acid gases. One way to purify acid gases in industry is to use aqueous-alkaline solutions, particularly based on sodium hydroxide (NaOH) [9]. One of the advantages of the latter is that it does not contain harmful impurities. Waste NaOH can be used for simple neutralization or in pulp and paper mills after quality control analysis [10].

The use of NaOH today is quite widespread and still relevant. A study [11] described the simultaneous removal of gaseous NO_x and SO_2 from the flue gases of coal-

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fired power plants, where NaOH was used as an absorbent in the wet scrubber cleaning process, are described.

In [12] the authors conduct a comparative analysis of the use of different membrane contactor for effective and selective removal of SO_2 from the exhaust gases of ships using NaOH.

The authors of [13] used NaOH to reduce H_2S concentrations in wastewater collection system wells, which reduced the average H_2S content by a factor of about 10.

A work [14] proposes using NaOH in a scrubber to remove H_2S from the geothermal fluid in the pilot plant of the Castelnuovo geothermal power plant. Due to the adopted countercurrent scrubber nozzle design, H_2S removal efficiency was achieved and allowed high CO_2 concentrations to be treated.

One of the recent works related to NaOH concerns its application as a catalyst together with Ni to effectively increase hydrogen production and decompose phenol in the treatment of complex phenolic wastewater [15].

NaOH is mainly used in the form of a solution in liquid form. However, the authors of the work [16] proposed a technology for purification of flue gases of power plants from CO_2 and obtaining from it a solid carbonate, which uses NaOH in solid form.

In addition to technical solutions for the use of NaOH, scientific research related to this alkali is being conducted.

Paper [17] presents a method for measuring CO_2 in synthetic biogas by passing it through a dilute NaOH solution.

The authors of the paper [18] developed a polarizable sodium hydroxide force field for modeling the structure and thermodynamics of concentrated NaOH solutions. This force field allows us to describe the structural and thermodynamic properties of NaOH salt in aqueous solutions, which is confirmed with experiments for a wide range of concentrations.

In [19] four mass transfer rate models and two enhancement factors were estimated using CFD modeling for CO_2 uptake in aqueous NaOH solution by comparing simulation results with previously published experimental data.

The purpose of this work is to evaluate the influence of the oxidizer on the formation of syngas components and the efficiency of its purification from acid gases using NaOH-based aqueous-alkaline solution.

Model development

Model description

Bitumen contains heteroatomic compounds, including sulfur, oxygen, nitrogen, metals, and high-molecular oil hydrocarbons [20]. Asphaltene of natural bitumen of the Ashalchinskoe oilfield (Russia) was chosen as the object of numerical simulation as a substance containing a significant amount of carbon and hydrogen.

The ultimate analysis and properties of asphaltene under study are presented in Table 1. According to work [21] the structural formula of asphaltene was chosen. CHNS contents were determined using elemental analyzer (EuroEA3000, Eurovector SpA, Italy). The calorific value of the sample was determined in an IKA C200 calorimeter (Germany).

Table 1. *Ultimate analysis and properties of the asphaltene under study*

Таблица 1. *Элементный анализ и свойства исследуемого асфальтена*

Formula/Формула	$C_{164}H_{150}N_4O_4S_3$
Carbon/Углерод	84,28 %
Hydrogen/Водород	6,47 %
Oxygen/Кислород	2,73 %
Nitrogen/Азот	2, 4 %
Sulfur/Сера	4,12 %
Molar mass/Молярная масса	2,337 kg/mol/кг/моль
Calorific value/Теплота сгорания	35,4 MJ/kg/МДж/кг

Fig. 1 shows a flow chart of asphaltene gasification and syngas purification. Asphaltene is sprayed in the internal space of the gasifier and interacts with the steam. As a result, syngas and a solid residue in the form of unreacted hydrocarbon are formed. The produced syngas containing sulfur products is directed to the absorber for purification, where it is purified from acid gases by a NaOH-based aqueous-alkaline solution.

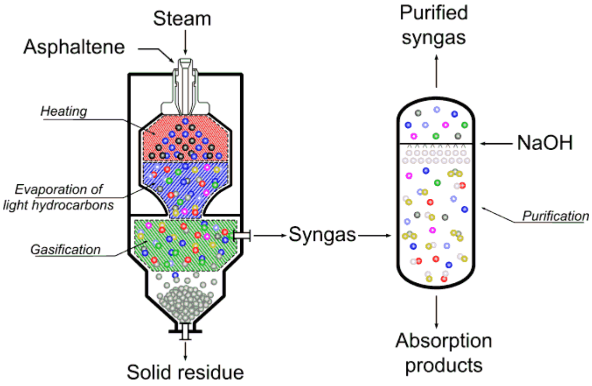

Fig. 1. *Flow chart of asphaltene gasification and syngas purification*

Рис. 1. *Схема газификации асфальтена и очистки синтез-газа*

For the numerical simulation, steam was taken as the oxidizer. The steam/asphaltene ratio (S/A) was chosen as a variable parameter, on which the amount of formed gasification products depends. A temperature value of 1400 °C corresponds to the gasification temperature of heavy oil residues according to Texaco technology. The gasification pressure was calculated based on the ideal gas law. The values given in Table 2 were used as operating parameters for asphaltene gasification simulation.

Table 2. *Operating parameters of tgasification*

Таблица 2. *Режимные параметры процесса газификации*

Gasification temperature Температура газификации	1400 °C
Asphaltene flow rate/Расход сырья	100 kg/h/кг/ч
Oxidizer/Окислитель	H_2O (steam)/(пар)
Steam/asphaltene ratio (S/A)/Пар/асфальтен	0,1–1

NaOH-based aqueous-alkaline solution was chosen as an absorbent for purification of acid gases produced during asphaltene gasification simulation. Table 3 shows the absorption specifications based on data from work [22].

Table 3. *Absorption specifications*

Таблица 3. *Характеристики процесса абсорбции*

Absorption temperature Температура абсорбции	25 °C
Absorbent/Абсорбент	NaOH
Solution concentration Концентрация раствора	10 % NaOH, 90 % H_2O
Molar mass/Молярная масса	0,019 kg/mol/кг/моль

The methodology for evaluating the oxidizer effect on the formation and purification efficiency of acid gases produced during asphaltene gasification included several steps (Fig. 2).

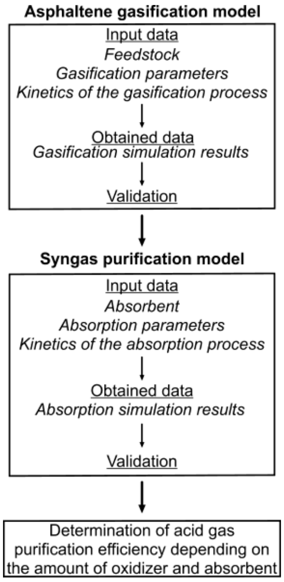

Fig. 2. *Flow chart of research*

Рис. 2. *Алгоритм исследования*

Stage 1 – development of the asphaltene gasification model, including the following tasks:

- gathering information about the gasified feedstock (elemental composition, molar mass, calorific value, formula);
- determination of operating parameters of gasification (temperature, oxidizer, oxidizer/feedstock ratio, flow rates);
- determination of the kinetics of gasification (initial concentrations of reagents, gasification reactions, reaction rate constants);
- obtaining gasification simulation results (concentrations of gasification products, calorific value of syngas, cold gas efficiency, gasification pressure);
- comparison of simulated results with the known data.

Stage 2 – development of the syngas purification model, including the following tasks:

- gathering information about the absorbent (solution composition and concentration, molar mass);
- determination of absorption specifications (temperature, acid gas and absorbent flow rates);
- determination of the absorption kinetics (initial concentrations of reagents, absorption reactions, reaction rate constants);
- obtaining absorption simulation results (concentrations of absorption products);
- comparison of simulated results with the known data.

Stage 3 – determination of acid gas purification efficiency depending on the amount of oxidizer and absorbent, including the following tasks:

- determination of maximum permissible concentrations (MPC) of acid gases in accordance with regulatory documents;
- determination of the necessary amount of absorbent to achieve safe values of the acid gas content at different S/A ratios;
- determination of the purification efficiency of acid gases at different S/A ratios.

Model assumptions

In order to simplify the simulation, some assumptions are made as follows:

- The reaction of asphaltene and steam produces syngas and a solid residue in the form of unreacted carbon (reaction R1).
- Part of the carbon interacts with CO_2, H_2 and steam.
- The produced dry syngas consists of CO, CO_2, H_2, CH_4, N_2 and H_2S.

Methods

Gasification kinetics

Gasification kinetics can be viewed as a complex of several stages (Fig. 1). Having reached the required spray temperature, fuel and oxidizer continue heating until microcracks form on the asphaltene surface due to water evaporation. As a result, light hydrocarbons are released. Then oxidation-reduction, steam-methane reforming and water-gas shift reactions take place. At this time solid residue and syngas are formed.

In developing the asphaltene gasification model, the following chemical reactions were considered.

Chemical reactions with steam and asphaltene:

$$Asphaltene+H_2O\longrightarrow H_2+CO+CO_2+CH_4+H_2O+H_2S+N_2+C \tag{R1}$$

$$CH_4+2H_2O\leftrightarrow CO_2+4H_2 \tag{R2}$$

$$H_2O\leftrightarrow H_2+0{,}5O_2 \tag{R3}$$

Steam-Reforming reaction:

$$CO+3H_2\leftrightarrow CH_4+H_2O \tag{R4}$$

$$CH_4+0{,}5O_2\longrightarrow CO+2H_2 \tag{R5}$$

Water-gas shift reaction:

$$CO_2+H_2\leftrightarrow CO+H_2O \tag{R6}$$

Methanation reaction:

$$2CO+2H_2\leftrightarrow CH_4+CO_2 \tag{R7}$$

Chemical reaction with carbon:

$$CH_4\leftrightarrow C+2H_2 \tag{R8}$$

$$C+H_2O\leftrightarrow CO+H_2 \tag{R9}$$

$$C+2H_2O\leftrightarrow CO_2+2H_2 \tag{R10}$$

$$C+CO_2\leftrightarrow 2CO \tag{R11}$$

Chemical reactions with sulfur-containing substances:

$$CH_4+2H_2S\leftrightarrow CS_2+4H_2 \tag{R12}$$

$$CO_2+H_2S\longrightarrow COS+H_2O \tag{R13}$$

$$2COS\longrightarrow CO_2+CS_2 \tag{R14}$$

$$CS_2+2H_2O \rightarrow CO_2+2H_2S \quad (R15)$$

Oxidation reaction:

$$C+0{,}5O_2 \rightarrow CO \quad (R16)$$

To determine the rate constant in the reaction R1, the experiments were carried out to determine the mass change using TGA and DSC methods and a NETZSCH STA 449 F3 thermal analyzer (Germany) [23].

Using the relation from work [24], the rate constant of the second-order reaction was calculated as:

$$k=\frac{c_0-c}{\tau\cdot c_0\cdot c},$$

τ is the time, min; c_0 is the initial sample mass, kg; c is the sample mass at time τ, kg.

The obtained average value of the rate constant for the reaction R1 was $5{,}997\cdot10^{-5}$. This value was used for asphaltene gasification model. For the other reactions R2–R16, the rate constants and equilibria were obtained from the data from the works [25–27].

Kinetics of the absorption process

The absorber is supplied with a water-alkaline solution, which is sprayed onto the incoming gas and captures the acid gases. The purified syngas is used for energy production, and the absorption products are used as feedstock in various industries.

The following reactions occurring in the interaction of hydrogen sulfide and NaOH were used for syngas absorption model [10]:

$$H_2S+NaOH \rightarrow NaHS+H_2O \quad (R17)$$

$$H_2S+2NaOH \rightarrow Na_2S+2H_2O \quad (R18)$$

The interaction of CO_2 with NaOH was based on the following kinetics [22]:

$$CO_2+NaOH \rightarrow NaHCO_3 \quad (R19)$$

$$CO_2+2NaOH \rightarrow Na_2CO_3+H_2O \quad (R20)$$

The produced additional organosulfur compounds also interact with NaOH:

$$COS+4NaOH \rightarrow Na_2S+Na_2CO_3+2H_2O \quad (R21)$$

$$CS_2+6NaOH \rightarrow 2Na_2S+Na_2CO_3+3H_2O \quad (R22)$$

According to Kopylov [22] the values of the reaction rate constants for sulfur compounds [R17, R18, R21, R22] were taken as $1{,}87\cdot10^{-4}$ and for CO_2 [R19, R20] – $1{,}23\cdot10^{-5}$.

Methods of data analysis

The cold gas efficiency (CGE) is defined as [28]:

$$CGE = (HHV_{gas}\cdot\phi) / HHV_{feedstock}.$$

Here, ϕ is the gas yield in m^3/kg; HHV_{gas} is the higher heating value of the producer gas in MJ/m^3; and $HHV_{feedstock}$ is the higher heating value of the asphaltene in MJ/kg.

Model Validation

As for validation purpose the results of simulation of asphaltene gasification and syngas absorption were compared with known literature data. The accuracy of the proposed models is estimated by the root mean square error (RMSE) using follow equation:

$$RMSE=\sqrt{\frac{\sum_{i=1}^{n}\left(Exp_i-Mod_i\right)^2}{n}}.$$

Here, Exp is the experimental (literary) value; Mod is the simulated value; n is the number of values.

Results and discussion

Using Comsol Multiphysics software the following results of the asphaltene gasification and syngas absorption simulation were obtained.

Gasification simulation results

Fig. 3 shows the non-stationary dependences of the concentrations of the syngas components at S/A=0,1, 0,5 and 1. As can be seen from the figure, in the beginning of gasification there is a rapid increase in the concentration of CO and H_2, then the process slows down. At the same time, there is an increase in the concentration of CO_2. With the increase of steam, a parabolic dependence of the concentrations of syngas components is observed, which values decrease with time, except for CO_2.

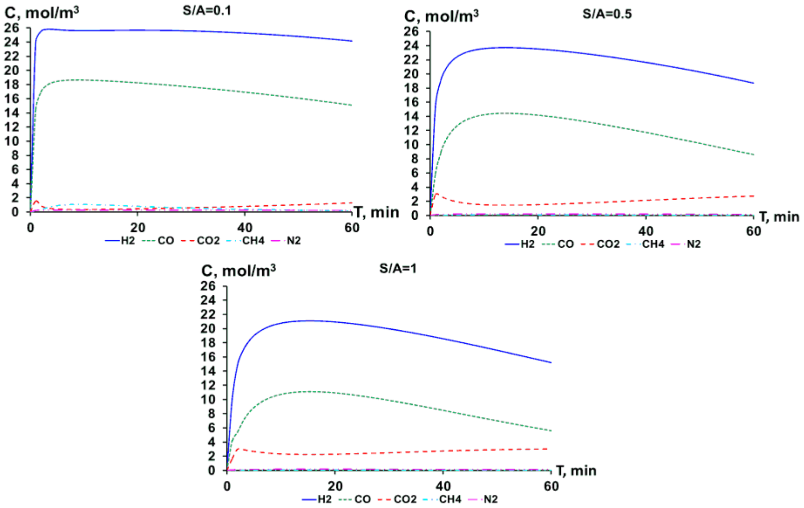

Fig. 3. *Dependences of syngas component concentrations on time at S/A=0,1, 0,5 and 1*

Рис. 3. *Зависимости нестационарных концентраций компонентов синтез-газа при S/A=0,1, 0,5 и 1*

Fig. 4 shows the dependence of the calorific value of syngas (HHV_{gas}) on the S/A ratio. It can be seen that as the amount of steam increases, the calorific value decreases from 11,3 to 7,2 MJ/m^3. Meanwhile, CGE increases from 53,4 to 62,5 % due to the increase in syngas yield.

Fig. 5 shows the dependence of the change in the average gasification pressure on S/A ratio. It can be seen that with increasing steam, the average gasification pressure declines. This is due to a decrease in the initial molar concentrations of the reagents as the S/A ratio increases.

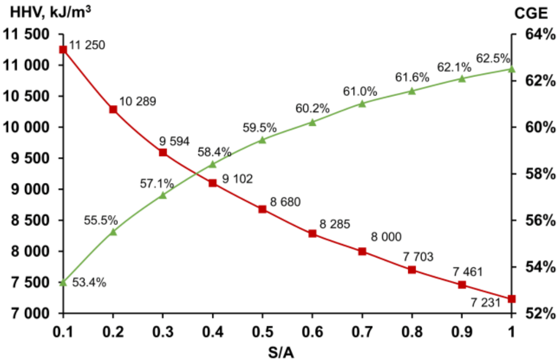

Fig. 4. *Dependence of HHV syngas and CGE value on the S/A ratio*

Рис. 4. *Зависимость теплоты сгорания синтез-газа и КПД газификации от S/A*

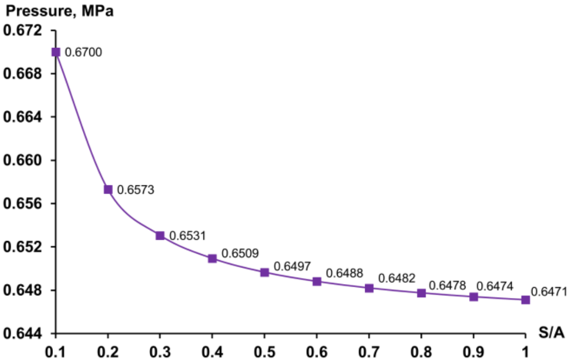

Fig. 5. *Dependence of gasification pressure on S/A*

Рис. 5. *Зависимость давления газификации от S/A*

For validation of the results of asphaltene gasification simulation, the concentrations of syngas components were compared with the data [29, 30] at S/A=0,4 and T=1400 °C (Fig. 6). Our results showed good convergence with the results of other researchers (RMSE=4,7 and RMSE=6,13 respectively). The low values of CO and CO_2 are related to the deficit of oxygen during steam gasification.

The values of acid gas concentrations obtained during asphaltene gasification simulation at different S/A ratios are presented in Table 4. For comparison, the values of maximum permissible concentrations (MPC) for acid gases according to Sanitary-hygienic standard 2.2.5.2100-06 [31] are also presented. The table shows that concentration of CO_2 exceeds the standard by 2–5 times. For H_2S this indicator is higher by 3000 times. COS and CS_2 concentrations do not exceed MPC, so we did not consider them further.

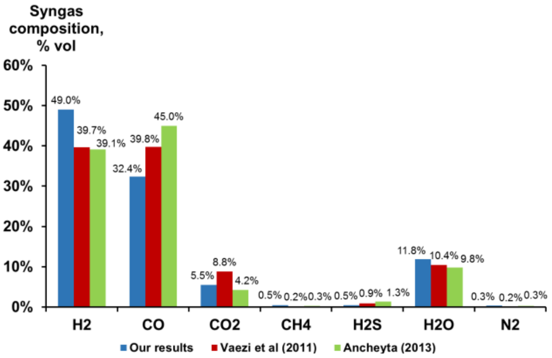

Fig. 6. *Comparison of the results of asphaltene gasification simulation with the known data*

Рис. 6. *Сравнение результатов моделирования газификации асфальтенов с известными данными*

Table 4. *Obtained values of acid gas concentrations at different S/A*

Таблица 4. *Полученные значения концентраций кислых газов при различных S/A*

S/A	CO_2	H_2S	COS	CS_2
	mg/m^3/мг/м^3			
0,1	56 109	10 307	0,251	0,936
0,2	84 894	9 042	0,198	0,362
0,3	102 309	8 164	0,165	0,188
0,4	112 446	7 556	0,143	0,115
0,5	119 579	7 046	0,126	0,073
0,6	124 929	6 577	0,111	0,046
0,7	127 965	6 243	0,101	0,032
0,8	130 394	5 901	0,091	0,022
0,9	131 815	5 626	0,084	0,016
1	132 704	5 368	0,077	0,011
МРС/ПДК	27 000	3	10	10

Absorption simulation results

As a result of syngas purification simulation, the values of purification efficiency and amount of absorbent at different S/A ratios were obtained.

Fig. 7, 8 show the dependences of the absorption degree of acid gases on the amount of absorbent at S/A=0,1, 0,5 and 1. According to results of calculation it is visible that with increase of steam, purification efficiency increases and amount of required absorbent declines. Meanwhile, the curves of CO_2 purification efficiency become parabolic with increasing S/A ratio, while for H_2S it is closer to a linear dependence.

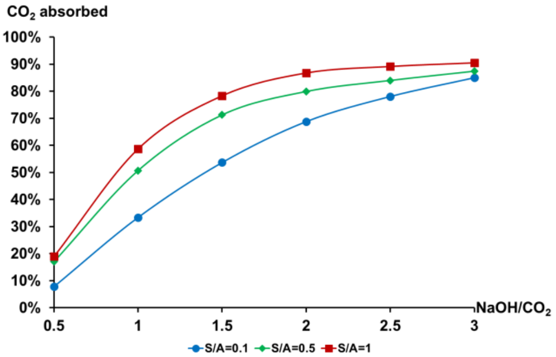

Fig. 7. *Dependence of CO_2 absorbed on the absorbent at different S/A*

Рис. 7. *Зависимость поглощенного CO_2 от абсорбента при различных S/A*

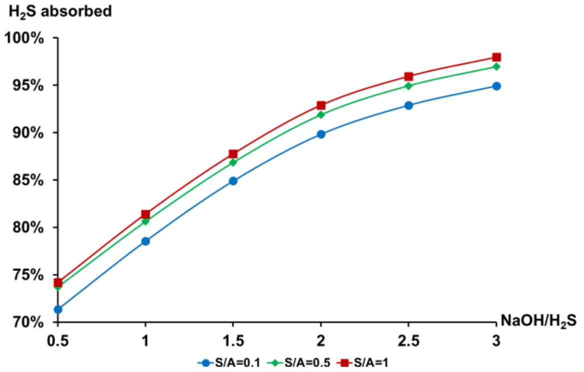

Fig. 8. *Dependence of H_2S absorbed on the absorbent at different S/A*

Рис. 8. *Зависимость поглощенного H_2S от абсорбента при различных S/A*

For validation the results of syngas purification simulation, we compared them with the known data [32, 33] under similar conditions (Figs. 9, 10) and they showed good convergence (RMSE=3,62 and 4,98 respectively).

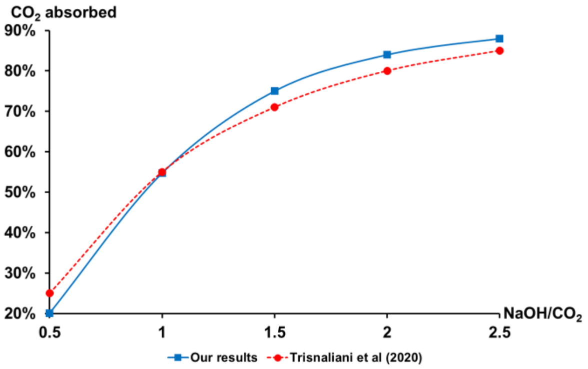

Fig. 9. *Comparison of the dependence of CO_2 absorbed with the known data*

Рис. 9. *Сравнение зависимости поглощения CO_2 с известными данными*

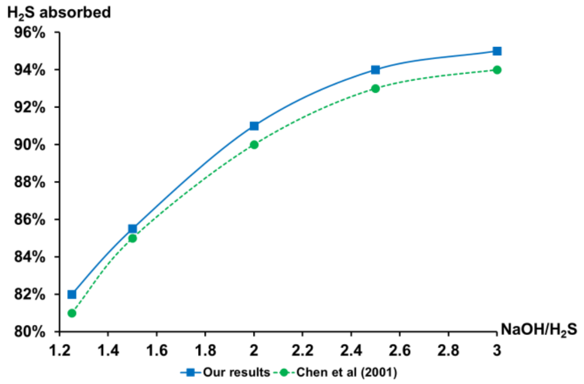

Fig. 10. *Comparison of the dependence of H_2S absorbed with the known data*

Рис. 10. *Сравнение зависимости поглощения H_2S с известными данными*

Effect of the oxidizer on acid gases

Table 5 shows the safe values of acid gases (below the MPC value) depending on the amount of absorbent, steam and purification efficiency. The table shows that as the amount of steam increases, there is a decrease in the amount of absorbent and an increase in purification efficiency. Thus, the amount of absorbed CO_2 increases by 20,7 % (from 53,68 to 74,38 %) with a decrease in the amount of NaOH for purification by 6,7 % (from 1,5 to 1,4). At the same time, the amount of absorbed H_2S increased by 0,39 % (from 96,34 to 96,73 %) with a decrease in NaOH by 40,9 % (from 4,4 to 2,6). The obtained dependence of purification efficiency on the amount of absorbent agrees with the results of Álvarez-Cruz et al. [34].

Table 5. *Safe acid gases values at different S/A*

Таблица 5. *Безопасные значения кислых газов при различных S/A*

S/A	$NaOH/CO_2$	CO_2, mg/m^3 CO_2, мг/м^3	CO_2 absorbed, % Уловленный CO_2, %	$NaOH/H_2S$	H_2S, mg/m^3 H_2S, мг/м^3	H_2S absorbed, % Уловленный H_2S, %
0,1	1,5	26552	53,68	4,4	2,93	96,34
0,2	1,5	23808	57,05	3,6	2,96	96,38
0,3	1,5	22295	60,42	3,3	2,79	96,43
0,4	1,4	24306	63,79	3,1	2,84	96,47
0,5	1,4	23096	67,16	2,9	2,98	96,52
0,6	1,4	22284	68,61	2,8	2,95	96,56
0,7	1,4	21773	70,05	2,8	2,75	96,60
0,8	1,4	21435	71,49	2,7	2,81	96,65
0,9	1,4	21148	72,94	2,6	2,93	96,69
1	1,4	21056	74,38	2,6	2,78	96,73

Conclusions

It was revealed that steam used as an oxidizer during asphaltene gasification has a significant effect on the composition and properties of gasification products, as well as on the syngas purification.

The results of asphaltene gasification simulation showed that in the beginning of gasification there is a rapid increase in the concentration of CO and H_2, then the process slows down. With the increase of steam, a parabolic dependence of the concentrations of syngas components is observed, which values decrease with time, except for CO_2. The calorific value of syngas decreases from 11,3 to 7,2 MJ/m^3 and the cold gas efficiency increases from 53,4 to 62,5 % due to an increase in syngas yield.

Comparing the obtained concentrations of acid gases with MPC, it was found that the concentration of CO_2 exceeds the standard by 2–5 times, H_2S – by 3000 times. COS and CS_2 concentrations do not exceed the MPC.

The results of syngas purification simulation showed that as the amount of steam increases, there is a decrease in the amount of absorbent and an increase in purification efficiency. Thus, the amount of absorbed CO_2 increases by 20,7 % (from 53,68 to 74,38 %) with a decrease in the amount of NaOH for purification by 6,7 % (from 1,5 to 1,4). At the same time, the amount of absorbed H_2S increased by 0,39 % (from 96,34 to 96,73 %) with a decrease in NaOH by 40,9 % (from 4,4 to 2,6).

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ВЛИЯНИЕ ОКИСЛИТЕЛЯ НА ОБРАЗОВАНИЕ И ЭФФЕКТИВНОСТЬ ОЧИСТКИ КИСЛЫХ ГАЗОВ, ПОЛУЧЕННЫХ В ПРОЦЕССЕ ГАЗИФИКАЦИИ АСФАЛЬТЕНА

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Актуальность *исследования определяется необходимостью понимания влияния окислителя на образование кислых газов (CO_2, H_2S, COS и CS_2) в процессе термического разложения высоковязких углеводородов. Это важно для прогнозирования эффективности очистки полученных продуктов газификации и оценки экономических затрат.*
Цель: *с помощью математического моделирования исследовать влияние окислителя в виде пара на состав и свойства продуктов газификации асфальтена, полученного из природных битумов, а также определить степени очистки в зависимости от количества пара и абсорбента на основе водно-щелочного раствора NaOH.*
Объект: *асфальтен природного битума Ашальчинского месторождения Республики Татарстан (Россия), окислитель в виде пара, величина которого варьировалась от 0,1 до 1 в зависимости от количества асфальтена.*
Метод: *математическое моделирование процессов газификации асфальтенов и абсорбции кислых газов при воздействии окислителя в виде пара с учетом основ химической кинетики, элементного и термогравиметрического анализов.*
Результаты моделирования процессов газификации и абсорбции показали, что пар, используемый в качестве окислителя при газификации асфальтенов, оказывает существенное влияние на состав и свойства продуктов газификации, а также на очистку синтез-газа. С увеличением пара наблюдается параболическая зависимость концентраций компонентов синтез-газа, значения которых со временем уменьшаются, за исключением CO_2. Теплотворная способность синтез-газа снижается с 11,3 до 7,2 МДж/м^3, а КПД газификации повышается с 53,4 до 62,5 % за счет увеличения выхода синтез-газа. По мере роста количества пара уменьшается количество абсорбента и увеличивается эффективность очистки синтез-газа от кислых газов. Таким образом, количество поглощенного CO_2 увеличивается на 20,7 % при снижении абсорбента на 6,7 %. При этом количество поглощенного H_2S выросло на 0,39 % при снижении NaOH на 40,9 %.

Ключевые слова:
Асфальтен, газификация, синтез-газ, очистка кислых газов, NaOH.

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