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ANALYTICAL JUSTIFICATION OF THE THERMOCHEMICAL INTERACTION BETWEEN BLAST REAGENTS AND CARBON-CONTAINING PRODUCTS UNDER THE INFLUENCE OF MAGNETIC FIELDS

Purpose. To justify and develop a model that describes the effect of magnetic treatment of blast reagents and carbon-containing products on the gasification process for predicting the intensification of gas formation.

Methodology. The study involves theoretical modeling based on experimental data to investigate the influence of magnetic fields on the underground coal gasification process and co-gasification of coal and carbon-containing products. The Arrhenius equation was used to estimate the rate constants of gasification reactions in the temperature range of 800–1,000 °C. The effect of the magnetic field was incorporated by adjusting the activation energy (E_a). The results of analytical and experimental studies were processed using methods of computer and mathematical modeling.

Findings. The results show that the application of magnetic fields significantly intensifies the gasification process of carbon containing products. Increasing the reactivity of the blast reagents, particularly water and oxygen, leads to a higher overall yield of combustible gases. The use of magnetic fields in the gasification process substantially increases the reaction rate (k) due to the reduction in activation energy (E_a), improving the overall efficiency of gasification.

Originality. For the first time, an analytical model has been developed to describe the effect of magnetic treatment of blast reagents and carbon-containing products on the gasification process in the temperature range of 800–1,000 °C. The obtained reaction rates follow an exponential trend. The established and correlation-validated pattern shows the relationship between changes in the approximation coefficient (F) and the change in the carbon fraction (C, %) during the magnetic treatment of blast components within the specified temperature range.

Practical value. The results of this study can be applied to enhance the efficiency of industrial gasification processes, particularly underground coal gasification and co-gasification of coal and carbon-containing productss.

Keywords: *magnetic field, gasification, underground coal gasification, co-gasification thermochemical interaction, syngas, intensification*

Introduction. The global energy crisis, exacerbated by the depletion of readily accessible fossil fuel reserves and rising environmental concerns, has driven the demand for more efficient and sustainable energy production methods [1, 2]. Traditional energy sources such as coal, oil, and natural gas are becoming increasingly expensive to extract, and their environmental impact is drawing heightened scrutiny [3, 4]. Topical issues include the exploration of prospective methods for coal mine methane utilization, which offers the potential to generate an additional valuable energy resource for the regional development of coal-mining areas [5]. As a result, alternative methods for energy production are being actively pursued, with underground coal gasification (UCG) emerging as one of the most promising technologies. UCG enables the conversion of coal into syngas directly at the site of its occurrence, offering a method to exploit coal seams that are otherwise too deep, thin, or hazardous to mine through conventional means [6]. This process not only provides access to previously untapped coal resources but also minimizes surface disruption, reducing the overall environmental footprint of coal extraction.

While UCG presents a compelling solution, the efficiency of the gasification process is often limited by factors such as coal seam characteristics and the quality of the blast (air, oxygen, and steam) used to facilitate the reaction [7]. In particular, the thermochemical interaction between blast reagents and carbon-based materials plays a crucial role in determining the overall yield and quality of syngas [8]. Therefore, intensifying the gasification process to enhance syngas production is a key area of focus for researchers.

One promising avenue for process intensification is the application of magnetic fields to the gasification process [9]. Magnetic fields can influence the behavior of both blast reagents and carbon-based products by altering the spin states of molecules, particularly oxygen and water [10]. This modification of molecular properties can result in more efficient chemical reactions, increasing the carbon participation rate and improving the overall gasification process. Studies have shown that the use of magnetic fields can lead to a higher yield of combustible gases, making the gasification process more effective and economically viable.

Analysis of recent research and publications. The growing need for efficient and sustainable energy production has led to extensive research into underground coal gasification (UCG) as a method to exploit coal seams that are otherwise inaccessible through conventional mining techniques. UCG allows for the in-situ conversion of coal into syngas, a mixture of carbon monoxide, hydrogen, and methane, which can be used for energy production or as feedstock for chemical processes. The application of magnetic fields to intensify gasification processes is a relatively new approach that promises to enhance energy efficiency and reduce the environmental impact of traditional coal utilization.

Underground coal gasification is a technique for converting coal into synthesis gas in situ, offering potential for integration with carbon capture and storage [11]. Several studies have explored the fundamentals of gasification processes, focusing on the interaction between carbonaceous materials and gasification agents such as oxygen, water, and steam. The reaction mechanisms underlying these processes have been extensively documented, highlighting the role of exothermic reactions like carbon combustion and endothermic reactions such as the water-gas shift reaction [12]. Thermochemical models, such as the Arrhenius-based reaction rate equations, have been instrumental in predicting the behavior of these reactions under various temperature and pressure conditions [13]. However, these models typically do not account for the influence of external factors such as magnetic fields on the reaction kinetics, an area this study seeks to address.

The application of magnetic fields to enhance chemical reactivity has garnered attention in recent years. Magnetic fields can significantly influence chemical reactions, particularly under specific conditions. Research shows that magnetic fields can influence electron spin states, particularly in paramagnetic species like oxygen, thereby altering their reactivity. Weak magnetic fields may induce changes in rate constants of radical reactions, leading to bifurcation of steady states and abrupt changes in temperature and concentration in non-equilibrium systems [14]. High magnetic fields can influence chemical reactions, affecting reaction pathways, nanomaterial growth, product phases, and the spins of catalyst surfaces [15]. Magnetic fields can alter the energy levels of active species in catalytic reactions by interacting with their spin states [16]. While most studies have focused on small-scale reactions, their findings provide a foundation for applying magnetic fields in larger industrial processes like UCG.

The interaction of magnetic fields with gasification processes has only recently begun to be explored. Early studies indicate that magnetic fields can significantly affect the thermochemical behavior of both carbonaceous materials and gasification agents, leading to an increase in syngas yield. Recent studies have explored the use of magnetic fields to enhance gasification processes [10] found that magnetic field-activated injected blast can intensify underground coal gasification, increasing the yield of combustible components. Similarly, [17] investigated the effects of gradient magnetic fields on co-firing, focusing on field-enhanced heat and mass transfer. Researchers have noted that the presence of a magnetic field can lower the activation energy for key reactions, such as the partial oxidation of carbon and the reaction of steam with coal, thereby accelerating the gasification process. This aligns with the current study's findings, where magnetic treatment of blast reagents enhanced the overall efficiency of gasification by increasing carbon participation rates. [18] further explored the impact of gradient magnetic fields on swirling flame dynamics during biomass gasification, observing enhanced burnout of volatiles and cleaner heat energy production. These studies collectively suggest that magnetic fields can be effectively applied to various gasification processes to improve efficiency, control combustion characteristics, and potentially reduce emissions. Also, studies suggest that magnetic field enhancement can significantly improve various gasification processes, offering potential for more efficient energy production from carbon-containing raw materials.

Identification of unresolved part of the general problem. Despite extensive research into underground coal gasification and the influence of magnetic fields on chemical reactions, a critical unresolved aspect remains the precise mechanisms by which magnetic fields affect the thermochemical interactions between blast reagents and carbon-containing products in large-scale gasification processes. While previous studies have demonstrated the potential for magnetic fields to lower activation energy and enhance reaction rates, especially in small-scale settings, there is still a lack of comprehensive models that accurately predict these effects in industrial-scale UCG. Specifically, the correlation between magnetic field strength, carbon participation in varying temperature ranges has yet to be fully understood and quantified. Addressing these gaps is essential for optimizing the efficiency and sustainability of UCG as a clean energy solution.

The purpose of this research is to develop a model that describes the effect of magnetic fields on the co-gasification process of carbon-based materials. By exploring how magnetic fields influence the thermochemical interactions between blast reagents and coal, this study aims to provide a deeper understanding of how UCG can be optimized for better energy production. This model will help identify the key parameters required to maximize the efficiency of the gasification process, paving the way for future innovations in clean energy technology.

Theoretical background. ***Thermochemical interaction in gasification.*** Gasification, particularly in underground coal gasification, is a complex thermochemical process where carbonaceous materials like coal react with blast reagents – typically a combination of air, oxygen, and steam – to produce syngas [19]. The efficiency of this process largely depends on the interactions between the carbon in coal and the blast reagents, primarily through a series of chemical reactions that release energy and form a mixture of gases including carbon monoxide (CO), hydrogen (H_2), carbon dioxide (CO_2), and methane (CH_4). These gases are then used for various energy applications [20].

In the UCG process, carbon (C) primarily reacts with water (H_2O) and oxygen (O_2) from the blast to produce syngas. The primary reactions involved are [12]

Primary reactions, kJ/mol

$$C + O_2 \rightarrow CO_2 + 394; \quad (1)$$

$$2C + O_2 \rightarrow 2CO + 221; \quad (2)$$

$$C + H_2O \rightarrow CO + H_2 - 130; \quad (3)$$

$$C + 2H_2O \rightarrow CO_2 + 2H_2 - 80.3. \quad (4)$$

Reaction of carbon with oxygen (combustion) (1) is exothermic reaction releases a significant amount of heat, which helps sustain the high temperatures necessary for other endothermic gasification reactions [21]. The combustion of carbon with oxygen is fundamental in maintaining the process's thermal balance [22]. Partial oxidation of carbon (2) produces carbon monoxide, an essential fuel gas that contributes to the overall energy yield of syngas. This reaction is also exothermic and aids in maintaining the gasification temperature. Reaction of carbon with water vapor (steam) (3) is endothermic, meaning it absorbs heat. It is crucial for generating hydrogen (H_2), a valuable component of syngas, and carbon monoxide (CO), a fuel gas. This reaction forms the basis of the water-gas shift reaction used in gasification processes to balance the ratio of CO and H_2 in the syngas. Reaction of carbon with excess water vapor (4) is secondary reaction also produces hydrogen and carbon dioxide (CO_2). The higher yield of CO_2 reduces the energy content of syngas, making it less efficient for combustion. Therefore, controlling the steam-to-carbon ratio is essential to prevent excessive CO_2 formation [23].

The introduction of magnetic fields can influence the thermochemical reactions involved in UCG, particularly through the modification of the spin states of molecules like oxygen and water. Research has shown that magnetic fields can affect the alignment of electron spins, altering the reactivity of oxygen and enhancing the formation of syngas. This phenomenon is particularly relevant when considering the co-gasification of carbonaceous products in UCG. Studies, as highlighted in previous [10] have demonstrated that magnetic fields can intensify the gasification process by increasing carbon participation and boosting the yield of combustible gases.

The application of magnetic fields leads to a higher internal energy state of the reactant molecules, facilitating more efficient reaction pathways. For instance, water molecules exposed to magnetic fields tend to exhibit higher reactivity, which accelerates the steam-carbon reactions, thereby enhancing hydrogen production. Similarly, oxygen molecules in a magnetic field become more reactive, promoting partial oxidation and increasing the production of carbon monoxide.

The effectiveness of UCG is largely determined by how well the key parameters – temperature, pressure, and blast composition – are controlled [24]. Magnetic fields offer a promising method for optimizing these parameters by influencing the molecular interactions between the blast reagents and the coal. The resulting model of magnetic field-enhanced gasification processes will provide insights into how to maximize syngas production while minimizing unwanted by-products like CO_2. In this case the thermochemical interactions in UCG involve a delicate balance of reactions between carbon, water, and oxygen. Understanding and optimizing these interactions, particularly through the use of magnetic fields, will lead to more efficient and sustainable gasification processes.

Magnetic fields and molecular activation in gasification. Magnetic fields can significantly influence the behavior of gasification reactants, particularly water (H_2O) and oxygen (O_2)

molecules. These effects are rooted in quantum mechanical principles, particularly the Pauli exclusion principle and intercombination transitions, which affect the spin states of electrons and enhance the chemical reactivity of these molecules [25]. By altering the spin configuration of electrons, magnetic fields modify the way molecules participate in chemical reactions, making the gasification process more efficient. At the quantum level, each electron in an atom or molecule possesses two types of angular momentum: orbital angular momentum, which arises from the electron's motion around the nucleus, and spin angular momentum, an intrinsic property of the electron. These spins are crucial in determining how electrons interact and form chemical bonds.

The Pauli exclusion principle states that no two electrons in an atom or molecule can occupy the same quantum state simultaneously [26]. This means that electrons in the same orbital must have opposite spins (a "paired" state). In normal conditions, the electrons in water and oxygen molecules are paired, resulting in stable, low-energy molecular configurations. However, when a molecule is exposed to an external magnetic field, this stability is disrupted.

A magnetic field can cause the reorientation of electron spins, especially when the field is inhomogeneous (i.e., varies in strength across space). This reorientation can force some electrons to move from their paired, low-energy singlet state into an unpaired triplet state, where the spins are aligned in the same direction [27, 28]. This transition is known as an intercombination transition. The triplet state is higher in energy and less stable, which means the molecules in this state become more chemically reactive.

For example, oxygen is a paramagnetic molecule, meaning that it naturally has two unpaired electrons in its ground state. These electrons form a weak bond that can be disrupted more easily under the influence of a magnetic field, leading to higher reactivity. By transitioning to an excited triplet state, oxygen molecules in a magnetic field are more prone to dissociate into highly reactive oxygen atoms, which enhances the oxidation reactions essential for gasification. Similarly, water molecules, which are normally diamagnetic (non-magnetic with paired electrons), can transition into a paramagnetic state when exposed to a magnetic field. This reorientation of the electrons in water molecules increases their chemical reactivity, especially in reactions with carbon in the gasification process.

Under normal conditions, the water molecule's hydrogen atoms form bonds with oxygen via p-electrons, whose spins are aligned oppositely according to the Pauli exclusion principle, resulting in a singlet state. This singlet state is a stable configuration with paired spins, contributing to the low reactivity of water under standard conditions.

When a magnetic field is applied, the spins of some p-electrons in water molecules are reoriented. This spin reorientation leads to a triplet state, where one of the paired electrons flips its spin, creating a molecule with unpaired electrons. This makes the water molecule paramagnetic and increases its internal energy. In the triplet state, the molecule becomes much more reactive because the magnetic field weakens the hydrogen bonds that normally hold the water molecules together.

In gasification, this transition is crucial. Water molecules in their paramagnetic triplet state react more readily with carbon, participating in endothermic reactions that produce syngas (hydrogen and carbon monoxide). The increased reactivity of water due to magnetic fields makes it a more efficient reactant, enhancing the overall gasification process.

The hydrogen bonds between water molecules play a significant role in determining their chemical behavior. These bonds, which are relatively weak compared to covalent bonds, form between the hydrogen atom of one water molecule and the oxygen atom of another. In the gasification process, breaking these hydrogen bonds is essential for the efficient conversion of steam into reactive components.

A magnetic field can disrupt these hydrogen bonds through its effect on the electron spins in the water molecules. As the spins of the bonding electrons in water are reoriented into a triplet state, the stability of the hydrogen bonds decreases [29, 30]. The probability of hydrogen bond formation is reduced by half under the influence of a magnetic field. This occurs because the electrons in the excited triplet state are less likely to form the stable configurations needed for hydrogen bonds.

As a result, water molecules treated with a magnetic field become more chemically active, and their internal energy increases. In the context of gasification, this enhanced chemical activity leads to more efficient reactions with carbon, facilitating the production of hydrogen and carbon monoxide from water vapor. Since less energy is required to break the weakened hydrogen bonds, the overall efficiency of the gasification process improves.

Oxygen (O_2) is a key reactant in the gasification process, particularly in its role as an oxidizer [31]. Under normal conditions, oxygen molecules exist in a paramagnetic state due to the presence of two unpaired electrons, which form a three-electron bond that is relatively weak. In a magnetic field, these unpaired electrons undergo spin reorientation, leading to antibonding orbitals and further weakening the bond between the oxygen atoms. As the bond weakens, oxygen molecules become more likely to dissociate into highly reactive oxygen atoms. These reactive atoms can then more efficiently oxidize carbon, driving the combustion reactions that provide the necessary heat for gasification. The increase in chemical reactivity of oxygen due to the magnetic field thus directly contributes to the enhancement of gasification efficiency.

In the steam gasification process, the efficiency of steam as a reactant is significantly influenced by its molecular structure [32]. Water molecules treated with magnetic fields have fewer hydrogen bonds, making them easier to dissociate into H_2 and O_2 during gasification. This increases the efficiency of the steam-carbon reaction, particularly in the production of hydrogen, which is a critical component of syngas. By reducing the number of hydrogen bonds, the magnetic field allows steam to react more readily with carbon, producing syngas at higher rates. This reduction in bond strength also means that less energy is required to initiate and sustain the gasification reactions, making the process more energy-efficient.

Methodology. The hypothesis that magnetic fields intensify gasification processes by increasing the internal energy of water and oxygen molecules is grounded in the quantum mechanics of electron behavior in these molecules. By influencing the spin states of electrons, magnetic fields can reorient their configuration, thereby increasing the molecules' internal energy and enhancing their reactivity. This section explores the physical and chemical principles behind this effect, focusing on electron spin reorientation and its impact on gasification.

The central hypothesis is that magnetic fields enhance the gasification process by altering the electron spin states of gas molecules such as H_2O and O_2, leading to an increase in internal energy. This results in more efficient chemical reactions between blast reagents and carbon during gasification. The following chain of events outlines this hypothesis:

- magnetic fields induce changes in the spin states of electrons in water and oxygen molecules;
- this reorientation increases the internal energy of these molecules, making them more reactive;
- higher reactivity leads to faster and more efficient reactions in the gasification process;
- as a result, the gas yield (primarily hydrogen and carbon monoxide) is enhanced, improving the overall efficiency of the gasification process.

To understand how magnetic fields impact the gasification process, it is essential to delve into the physics of electron spin and magnetic field interactions. Electrons possess an intrinsic property called spin, which generates a magnetic moment.

This magnetic moment can interact with external magnetic fields, altering the behavior of the electrons within a molecule.

In a typical molecule, electrons are paired according to the Pauli exclusion principle, which dictates that no two electrons in the same orbital can have the same spin orientation. In the ground state, electrons occupy the lowest energy levels with paired, opposite spins, creating a singlet state. This configuration is stable, and the molecule's chemical reactivity is relatively low.

When an external magnetic field is applied to the molecule, the energy levels of the electrons are split due to Zeeman splitting, where the magnetic field interacts with the magnetic moment of the electrons. This effect is described by the Zeeman effect, which explains how electron energy levels shift under the influence of a magnetic field. In the presence of a strong magnetic field, the paired electrons can reorient their spins, transitioning from a singlet to a triplet state, where the spins are aligned in parallel.

This reorientation is known as spin reorientation or an intercombination transition. The triplet state is higher in energy and less stable than the singlet state. Molecules in this state are more chemically reactive due to the increased internal energy. In the context of gasification, this enhanced reactivity allows water and oxygen molecules to participate more readily in thermochemical reactions, such as the formation of hydrogen and carbon monoxide.

The energy associated with an electron's magnetic moment is given by the following equation (quantum mechanical explanation)

$$E = -\mu_B \cdot B, \quad (5)$$

where E – the energy, J; μ_B – the Bohr magneton, which represents the magnitude of the electron's magnetic moment, J/T; B – the strength of the applied magnetic field, T.

As the magnetic field strength increases, the difference between the energy levels of the electrons also increases, causing a greater separation between the spin states. The probability of an electron flipping its spin – transitioning from a singlet to a triplet state-rises with the field strength. This is described by the Boltzmann distribution, where the population of electrons in higher energy states increases at higher temperatures or under stronger magnetic fields.

The transition from a singlet to a triplet state can be understood in terms of the Pauli exclusion principle. In a singlet state, the spins are paired (opposite), and the molecule is in a low-energy configuration. When the magnetic field is applied, the interaction between the field and the electron spins causes some of the paired electrons to flip their spins, violating the stable singlet configuration and entering the triplet state. In this state, the molecule becomes paramagnetic, meaning it has unpaired electrons that are more chemically active.

Water molecules, which are normally diamagnetic, have paired electrons in their ground state, making them relatively unreactive. When a magnetic field is applied, the spins of the p-electrons that form the bonds between oxygen and hydrogen atoms can reorient. The transition from a singlet state to a triplet state occurs when one of the paired electrons flips its spin, creating a higher-energy state with unpaired electrons. This transition increases the internal energy of the water molecule, enhancing its reactivity in gasification reactions. Specifically, the magnetic field weakens the hydrogen bonds between water molecules by disrupting the alignment of the electron spins. The result is a more chemically active steam that reacts more efficiently with carbon in the gasification process.

In chemical terms, the reduction in hydrogen bond strength allows the water molecule to dissociate more easily into hydrogen and oxygen, as represented in the following reaction $H_2O + C \rightarrow CO + H_2$. The reactivity of the water molecule is directly proportional to its internal energy. By elevating the internal energy through spin reorientation, magnetic fields accelerate the production of syngas.

Oxygen is naturally paramagnetic, meaning it already has unpaired electrons in its ground state. However, the application of a magnetic field further enhances the reactivity of oxygen molecules by increasing the number of electrons in higher-energy antibonding orbitals. In oxygen molecules, the bonding between oxygen atoms involves paired and unpaired electrons. Under the influence of a magnetic field, the unpaired electrons can occupy antibonding orbitals, destabilizing the O_2 molecule and making it more likely to dissociate into highly reactive oxygen atoms (O). This dissociation is critical in the combustion reactions during gasification, where oxygen atoms rapidly oxidize carbon to produce carbon monoxide and dioxide. The reaction of oxygen with carbon in the presence of a magnetic field can be represented as $O_2 + C \rightarrow CO_2$.The increase in oxygen atom reactivity due to the magnetic field intensifies the oxidation of carbon, providing the necessary heat for sustaining the gasification process.

To quantify the impact of magnetic fields on gasification, the following chemical and thermodynamic principles are employed. By raising the internal energy of the molecules, the activation energy required for gasification reactions decreases. The rate of reaction (k) is given by the Arrhenius equation (activation energy lowering)

$$k = Ae^{-\frac{Ea}{RT}}, \quad (6)$$

where k – the rate constant; A – the pre-exponential factor; E_a – the activation energy, J/mol; R – the gas constant, 8.314 J/mol · K; T – the temperature, K.

Activation energy (E_a) for coal gasification typically ranges between 100 to 200 kJ/mol, depending on the type of coal and the specific gasification process used. This value can vary significantly based on factors like the coal's rank, the presence of catalysts, and the conditions under which gasification occurs. The presence of a magnetic field effectively lowers the E_a by increasing the internal energy of reactant molecules, leading to a higher reaction rate.

The efficiency of gasification (thermodynamic efficiency) is also influenced by the Gibbs free energy (ΔG) of the reactions, J

$$\Delta G = \Delta H - T\Delta S, \quad (7)$$

where ΔH – the enthalpy change, J; ΔS – the entropy change, J/K; ΔH – the absolute temperature, K.

Magnetic fields increase entropy (ΔS) by introducing more possible spin configurations, making the reactions thermodynamically favorable.

Results and discussion. In order to compare the experimental data from research [10] (carbon participation share with and without magnetic treatment of blast mixtures) with analytical calculations, we can consider thermodynamic principles and reaction kinetics under the influence of a magnetic field. The main reactions of carbon gasification with oxygen and steam can be described analytically using the Arrhenius equation and Gibbs free energy considerations. The Arrhenius equation for the rate constant k as a function of temperature T (6). For the gasification reactions, an increase in the temperature (as shown in the experiments where carbon participation was higher at 1,000 compared to 800 °C) will exponentially increase the reaction rate due to the decrease in E_a. From previously obtained results, with a 500 E magnetic field applied, the carbon participation increased from approximately 47.2 % at 800 °C to 59.4 % at 1,000 °C (Table 1).

The experimental data shows that the carbon participation share (%) increases with both temperature and magnetic field treatment. The magnetic field enhances molecular activation, effectively lowering the activation energy (E_a) for reactions involving both oxygen and steam. The Gibbs free energy ΔG of these reactions is temperature dependence (7). In the presence of a magnetic field, the entropy (ΔS) increases due to the higher number of accessible molecular states (from spin reorientation), which further reduces the Gibbs free energy, making reactions more spontaneous.

Table 1

Values of carbon participation share (C), in solid fuel gasification at a temperature change and magnetic treatment of the injected blast mixtures (at magnetic field strength of 500 E)

The injected blast mixtures	Temperature in gasification zone (T), °C				
	800	850	900	950	1,000
Untreated with a magnetic field, %	29.7	31.8	34.4	35.8	39.2
Treated with a magnetic field, %	47.2	49.4	53.3	55.2	59.4
Difference in data, units	17.5	17.6	18.9	19.4	20.2
Difference in data, %	58.9	55.3	54.9	54.2	51.5

For an analytical comparison, can be calculated the carbon gasification rates at different temperatures using the Arrhenius equation with and without the magnetic field impact. By incorporating the experimentally derived values, the analytical model can be refined to predict gasification efficiency across various temperatures. The enhancement from the magnetic field can be quantified by adjusting the activation energy in the Arrhenius model for treated vs untreated conditions.

To calculate the analytical data and compare it with the experimental results from [10], we will use the Arrhenius equation to estimate the rate constants for carbon gasification at different temperatures, both with and without the magnetic field influence.

Let consider several assumptions. For carbon gasification, we assume a typical value of $A = 10^6$ mol^{-1}s^{-1}. Activation energy (E_a) are as follows. Without magnetic field: E_a = 200 kJ/mol. With magnetic field: The activation energy decreases by around 10 % due to molecular activation, so we assume E_a = 180 kJ/mol under the magnetic field. The final value of E_a was calculated as the difference between the initial value and the carbon participation share difference indicated in previous research [10]. The Arrhenius equation given by (5) require gas constant that is equal to 8.314 J/mol · K.

The analytical model uses the Arrhenius equation to estimate the rate constants of gasification reactions at different temperatures, both with and without magnetic field influence. These rate constants are linked to the efficiency of carbon participation in the gasification process. Obtained results are presented on Table 2 and Fig. 1.

In Fig. 1 $-\frac{Ea}{RT}$ is exponential factor of activation energy in the Arrhenius equation. This term governs how temperature and activation energy influence the reaction rate. When exponential factor is large (due to high activation energy or low temperature), the exponential function $e^{-\frac{Ea}{RT}}$ becomes small, meaning the reaction rate decreases. Conversely, lower values of exponential factor led to a larger exponential term, increasing the reaction rate.

The Fig. 2 demonstrates the general principle of thermally activated reactions: higher temperatures lead to increased molecular activity, reducing the effective activation energy required for gasification reactions.

This results in higher rate constants, which enhance the overall efficiency of the gasification process. The presence of a magnetic field accelerates the reaction rate further, as seen by the higher rate constants compared to those without magnetic influence. This is likely due to the effect of the magnetic field on the spin states of oxygen and water molecules, increasing their reactivity by lowering the activation energy for gasification. The impact is more pronounced at higher temperatures, suggesting that the magnetic field's ability to reduce activation energy becomes more effective when combined with thermal effects. The relationships (Fig. 2) between temperature and the rate constants of gasification reactions, comparing conditions with and without the influence of a magnetic field shows that, as temperature increases (from 800 to 1,000 °C), the rate constants also increase significantly, following the Arrhenius equation, which predicts an exponential rise in reaction rates with temperature. Under both conditions (with and without a magnetic field), the rate constants increase exponentially with temperature, consistent with the Arrhenius equation. However, the magnetic field-enhanced rates are consistently higher, indicating that the magnetic treatment provides a significant advantage in boosting reaction kinetics.

As can be seen from Fig. 3 at 800 °C, the experimental carbon participation share is 29.7 % without a magnetic field and 47.3 % with magnetic treatment. The analytical rate constants show an increase in reaction rates by a factor of approximately 7.11 under magnetic treatment. This is calculated by comparing the analytical rate constants with and without magnetic treatment (s^{-1}), $F = \frac{13.04 \cdot 10^{-4}\ \text{s}^{-1}}{1.83 \cdot 10^{-4}\ \text{s}^{-1}}$. This correlates with the experimental increase in carbon participation from 29.7 to 47.3 %, reflecting a roughly 58.9 % increase in carbon gasification efficiency.

At 900 °C, the experimental data reports carbon participation of 34.4 % without a magnetic field and 53.3 % with magnetic treatment. The analytical rate constant increases from $12.40 \cdot 10^{-4}$ to $86.13 \cdot 10^{-4}$ s^{-1} (F = 6.94), increasing the reaction rate, which aligns with the experimental 54.9 % improvement in carbon participation.

At 1,000 °C, the experimental carbon participation is 39.2 % without the magnetic field and 59.4 % with it. The rate constant increases under magnetic treatment, going from $62.11 \cdot 10^{-4}$ to $418.84 \cdot 10^{-4}$ s^{-1} (F = 6.74), closely matching the 51.5 % increase observed in the experimental carbon participation.

Magnetic field-enhanced gasification offers practical benefits for industries that rely on coal gasification for energy production. By improving the reaction rates and reducing the en-

Table 2

Parameters of analytical model of gasification reactions at different temperatures, both with and without magnetic field influence

Temperature (T), °C/K	Untreated with a magnetic field		Treated with a magnetic field			Factor of approximately (F)
	Exponential factor, $-\frac{Ea}{RT}$	Rate constant k at E_a = 200 kJ/mol	E_a, kJ/mol	Exponential factor, $-\frac{Ea}{RT}$	Rate constant k	
800/1,073	22.42	$1.83 \cdot 10^{-10}$	182.5	20.46	$13.04 \cdot 10^{-10}$	7.11
850/1,123	21.42	$4.98 \cdot 10^{-10}$	183.4	19.54	$32.78 \cdot 10^{-10}$	6.59
900/1,173	20.51	$12.40 \cdot 10^{-10}$	181.1	18.57	$86.13 \cdot 10^{-10}$	6.94
950/1,223	19.67	$28.68 \cdot 10^{-10}$	180.6	17.76	$193.31 \cdot 10^{-10}$	6.74
1,000/1,273	18.90	$62.11 \cdot 10^{-10}$	179.8	16.99	$418.84 \cdot 10^{-10}$	6.74

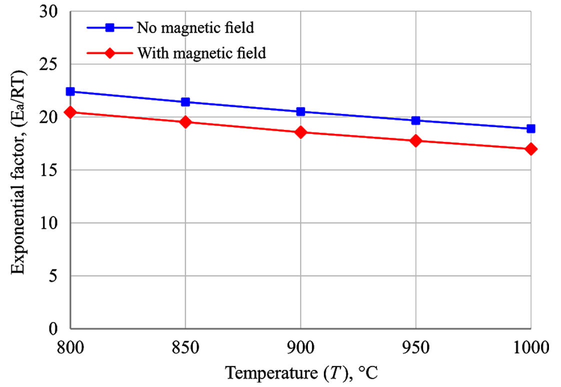

Fig. 1. Exponential factor of activation energy in the Arrhenius equation for gasification reactions at different temperatures

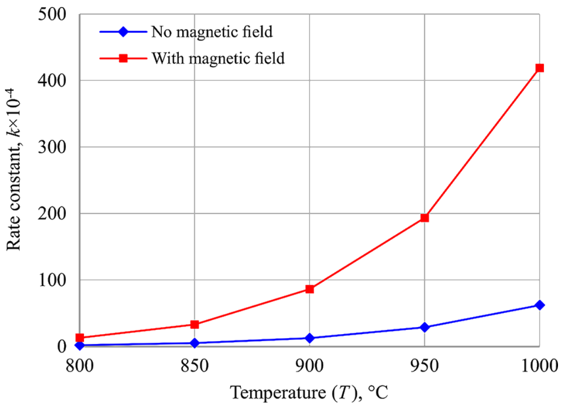

Fig. 2. Rate constants of gasification reactions at different temperatures

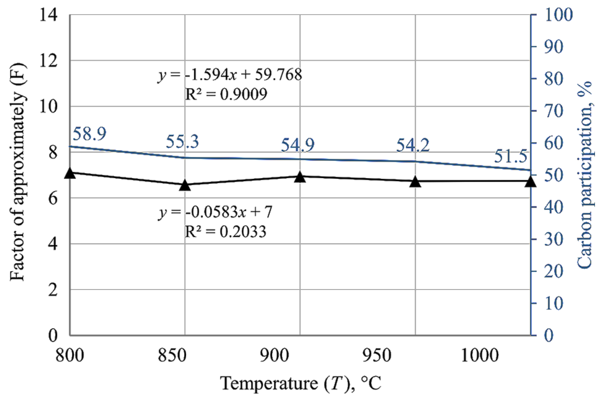

Fig. 3. The relationship between the pattern of change in the approximation factor (F) and the pattern of change in the carbon participation share (C, %) under magnetic treatment of blast air within the temperature range of 800–1,000 °C

ergy activation required for gasification, this method could make UCG and similar processes more economically viable and environmentally friendly. The technology holds potential for reducing greenhouse gas emissions by maximizing the production of hydrogen and carbon monoxide while minimizing unwanted by-products like carbon dioxide. While significant progress has been made in understanding the fundamental mechanisms of gasification, the application of magnetic fields presents an innovative approach to process intensification. Future research should focus on optimizing magnetic field parameters for large-scale applications and further refining theoretical models to predict reaction behaviors under varying magnetic field strengths.

Conclusions. The application of magnetic fields in gasification significantly enhances the reactivity of molecules like water and oxygen by increasing their internal energy through electron spin reorientation. This effect lowers the activation energy required for gasification reactions, accelerating syngas production and improving overall process efficiency. Magnetic fields also weaken hydrogen bonds in water, making the molecules more reactive and further boosting the gasification process. Analytical data based on the Arrhenius equation supports these findings, showing that magnetic fields increase reaction rates, which align closely with experimental increases in carbon participation. This demonstrates the potential of magnetic field-enhanced gasification for more efficient energy production and higher syngas yield.

The application of magnetic fields in the gasification process significantly increases the reaction rates (k), as indicated by the $-\frac{Ea}{RT}$ term in the analytical rate constants. This highlights the substantial impact of magnetic fields in enhancing the gasification process by lowering the activation energy (E_a), thereby improving reaction rates and overall carbon gasification efficiency.

Our results shows that magnetic fields can significantly enhance the efficiency of gasification by increasing the rate constants, especially at higher temperatures, making the gasification process faster and more efficient. This supports the hypothesis that magnetic fields can be used to intensify industrial gasification processes, leading to better syngas production and overall system efficiency.

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Аналітичне обґрунтування термохімічної взаємодії реагентів дуття та вуглецевмісних продуктів під дією магнітних полів

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Мета. Обґрунтування й розробка моделі, що описує вплив намагнічування реагентів дуття та вуглецевмісних продуктів на процес газифікації для прогнозування інтенсифікації газоутворення.

Методика. Дослідження включає теоретичне моделювання на основі експериментальних даних для вивчення впливу магнітних полів на процес підземної газифікації вугілля та когазифікації вугілля й вуглецевмісних продуктів. При моделюванні термохімічних взаємодій у дослідженні було використано рівняння Арреніуса для оцінки констант швидкості реакцій газифікації в діапазоні температур 800–1000 °C. Вплив магнітного поля було враховано шляхом коригування енергії активації (E_a). Обробку результатів аналітичних та експериментальних досліджень проведено з використанням методів комп'ютерного й математичного моделювання.

Результати. Отримані результати показують, що застосування магнітних полів суттєво інтенсифікує процес газифікації вуглецевмісних продуктів. Підвищення реакційної здатності реагентів дуття, зокрема води й кисню, призводить до збільшення загального виходу горючих газів. Застосування магнітних полів у процесі газифікації значно збільшує швидкість реакції (k), що є результатом зниження енергії активації (E_a), покращуючи загальну ефективність газифікації.

Наукова новизна. Уперше розроблена аналітична модель впливу намагнічування реагентів дуття й вуглецевмісних продуктів на процес газифікації в діапазоні температур 800–1000 °C. Отримані значення швидкості реакцій, що змінюються за експоненціальною закономірністю. Встановлена й кореляційно підтверджена закономірність зв'язку зміни коефіцієнту апроксимації (F) зі зміною дольової участі вуглецю (C, %) при магнітній обробці компонентів дуття в діапазоні зазначених температур.

Практична значимість. Результати дослідження можуть бути застосовані для підвищення ефективності промислових процесів газифікації, зокрема підземної газифікації та когазифікації вугілля й вуглецевмісних продуктів.

Ключові слова: *магнітне поле, газифікація, підземна газифікація вугілля, когазифікація, термохімічна взаємодія, синтез-газ, інтенсифікація*

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