MODERN METHODS OF ANALYSIS OF SUBSTANCES AND MATERIALS

Research Article
УДК 543.27(573+579)
https://doi.org/10.20915/2077-1177-2024-20-3-65-80

Non-Isothermal Thermogravimetric Analysis of Carbonation Reaction for Enhanced CO_2 Capture

Md Tariqur R. Shaon[1] ✉, Mahamudul H. Antor[1], Md Mahabubur R. Sharon[2]

[1]Ural Federal University, Yekaterinburg, Russia
✉ potterh274@gmail.com

[2]Khulna University of Engineering and technology, Khulna, Bangladesh

Abstract: An in-depth investigation into *CaO*-based carbonation reaction kinetics for CO_2 sorption is being conducted using simultaneous thermal analysis (*STA*), with the application of advanced thermogravimetric and differential scanning calorimetry techniques. Utilizing advanced thermal analysis system for real-time monitoring of simultaneous measurements of mass changes and thermal effects are conducted, ensuring precision and versatility in data acquisition. The study explores the intricacies of the non-isothermal carbonation process across a wide range of temperatures, shedding light on the temperature-dependent trends in reaction rates. Innovative statistical methods, combining regression techniques and Arrhenius equation, are employed to determine energy and reaction kinetics. The sensitivity of carbonation process to varying pressure conditions is meticulously examined in the study, providing pivotal discernment for optimization of reaction parameters across diverse applications. The integration of *STA* with statistical modeling alongside systematic analysis of temperature-dependent trends and pressure-order relationships not only enhances the understanding of CO_2 capture efficiency but also improves the robustness and accuracy of the findings. Furthermore, meticulous cross-validation with existing studies provides a critical evaluation of the experimental approach's precision and limitations. This study enhances understanding of *CaO* carbonation kinetics, providing practical implications for carbon capture processes and contributing to sustainable industrial processes.

Keywords: carbonation kinetics, thermogravimetric analysis, non-isothermal condition, sorbent performance, carbon capture and storage

For citation: Shaon Md T. R., Antor M. H., Sharon Md M. R. Non-isothermal thermogravimetric analysis of carbonation reaction for enhanced CO_2 capture. *Measurement Standards. Reference Materials*. 2024;20(3):65–80. https://doi.org/10.20915/2077-1177-2024-20-3-65-80

The article was submitted 22.02.2024; approved after reviewing 04.06.2024; accepted for publication 25.09.2024.

СОВРЕМЕННЫЕ МЕТОДЫ АНАЛИЗА ВЕЩЕСТВ И МАТЕРИАЛОВ

Научная статья

Неизотермический термогравиметрический анализ реакции карбонизации для усиленного улавливания CO_2

Мд Т. Р. Шаон[1], М. Х. Антор[1], Мд М. Р. Шарон[2]

[1]Уральский федеральный университет имени первого Президента России Б. Н. Ельцина, Екатеринбург, Россия
potterh274@gmail. com

[2]Инженерно-технологический университет Кхулны, Кхулна, Бангладеш

Аннотация: Углубленное исследование кинетики реакции карбонизации на основе CaO для сорбции CO_2 проводится с помощью одновременного термического анализа с применением передовых методов термогравиметрии и дифференциальной сканирующей калориметрии. Использование передовой системы термического анализа для мониторинга в реальном времени одновременных измерений изменения массы и тепловых эффектов обеспечивает точность и универсальность сбора данных. В исследовании изучаются тонкости неизотермического процесса карбонизации в широком диапазоне температур, проливая свет на зависящие от температуры тенденции в скорости реакции. Для определения энергии и кинетики реакции используются инновационные статистические методы, сочетающие регрессионные методы и уравнение Аррениуса. В исследовании тщательно изучается чувствительность процесса карбонизации к различным условиям давления, что позволяет оптимизировать параметры реакции в различных областях применения. Интеграция одновременного термического анализа со статистическим моделированием, а также систематический анализ зависимых от температуры тенденций и соотношений между давлением и порядком не только углубляет понимание эффективности улавливания CO_2, но и повышает надежность и точность полученных результатов. Кроме того, тщательная перекрестная валидация с существующими исследованиями дает критическую оценку точности и ограничений экспериментального подхода. Данное исследование углубляет понимание кинетики карбонизации CaO, обеспечивая практическое значение для процессов улавливания углерода и способствуя развитию устойчивых промышленных процессов.

Ключевые слова: кинетика карбонизации, термогравиметрический анализ, неизотермические условия, эффективность сорбента, улавливание и хранение углерода

Статья поступила в редакцию 22.02.2024; одобрена после рецензирования 04.06.2024; принята к публикации 25.09.2024.

Introduction

The escalating levels of carbon dioxide (CO_2) emissions resulting from combustion of fossil fuels such as coal have spurred a global initiative to explore innovative strategies for carbon capture and storage, with the aim of reducing carbon footprint associated with energy production and industrial processes [1]. With over 40 % of the world's CO_2 emissions originating from burning of coal, oil, and natural gas in power plants to generate energy[2], [3] the imperative to mitigate climate change has prompted into carbon capture and storage *(CCS)* technologies [4]. Current *CCS* methods, while effective [5], often suffer from resourceintensive and site-specific limitations [6], hindering their widespread adoption. Recognizing the need for more efficient and versatile solutions, studies have shifted their focus towards the development of novel sorbents [7] and advanced technologies that can enhance the overall efficacy of CO_2 sorption [8]. Among various approaches being investigated, reversible calcium-based sorbents carbonation process has emerged as a promising avenue[9]. This process involves the use of calcium oxide *(CaO)* as a CO_2 absorber, making it a sustainable and economically viable option for carbon capture[10], [11]. The promising opportunities in this area, particularly under different conditions, makes the development of optimized carbon capture systems and sustainable CO_2 mitigation technologies. The variability in experimental conditions and lack of standardized methodologies further complicate the comparison of results across diverse applications of CaO [12]. A comprehensive thermogravimetric study is needed to analyze the kinetics of CaO for enhanced CO_2 capture, examining the relationships between temperature, reaction rates, and efficiency. This will not only contribute to the understanding of CaO carbonation but also provide practical insights for system design and improvement.

In this study, we investigate carbonation kinetics of calcium oxide *(CaO)* under thermogravimetric experimental conditions using simultaneous thermal analysis *(STA)* and mass spectrometry *(MS).* The objectives include analyzing the experimental conditions and setup, conducting non-isothermal experiments by employing specific configurations, investigating reaction kinetics and thermodynamics, analyzing, and interpreting experimental results, and comparing and validating calculated activation energy with existing studies. The study aims to advance our understanding of calcium oxide's carbonation kinetics, contributing to the optimization of carbon capture and mineralization processes. By delving into intricacies of the reaction under varying conditions, our work provides valuable revelation for the design and improvement of systems utilizing CaO in carbon capture strategies. The study enhances the efficiency and applicability of CaO-based carbonation in addressing carbon emissions. The primary focus of this investigation is on carbonation kinetics of *CaO,* encompassing the examination of thermodynamic and kinetic aspects under diverse experimental conditions. The study aims to shed light on temperature-dependent behavior of carbonation process, providing a detailed analysis of the reaction kinetics and associated factors. Special attention is given to the configuration of the experimental setup, choice of materials, and utilization of advanced analytical techniques for a comprehensive understanding of carbonation kinetics of *CaO.*

In essence, this study investigation delves into intricacies of CaO-based carbonation process, aiming to contribute valuable understanding into the kinetics of CO_2 capture. Outcomes of the study not only advance our understanding of sustainable carbon capture technologies but also hold promise of facilitating development of more efficient and widely applicable solutions for mitigating the impact of anthropogenic CO_2 emissions on global climate. Furthermore, the chosen non-isothermal approach, involving distinct temperature programs, adds a layer of complexity to the study, allowing to simulate real-world conditions where temperature fluctuations are common. The non-isothermal kinetic analysis includes validation and comparison with existing studies, ensuring consistency with established studies. The study contributes to the broader field of carbon capture and mineralization research by deepening our understanding of how CaO behaves under non-isothermal conditions, fostering advancements in sustainable technologies aimed at reducing carbon emissions. Findings have implications for industrial applications, environmental sustainability, and global efforts to mitigate the impact of carbon emissions on the climate.

Our study significantly advances understanding of CaO carbonation kinetics through a multifaceted approach, leveraging simultaneous thermal analysis and statistical modeling. The study is structured into six distinctive sections. Initially, literature review of existing studies in section two through reveals the research gap within this domain, establishing the theoretical framework and highlighting the novelty and contribution of the proposed study. The experimental setup and theoretical foundation for kinetic calculations form the basis for subsequent analyses in section three. In the core of the study, thermogravimetric analysis and results unveil intricate kinetics in section four. A critical comparison with existing studies and key findings takes place in discussion section five, and the study concludes in section 6 by succinctly outlining the broader implications and future direction for sustainable industrial practices.

Literature Review

In the context of mitigating escalating CO_2 emissions and the associated global warming, adoption of low-carbon technologies, such as Carbon Capture and Storage *(CCS),* is underscored as crucial for achieving reduction in global CO_2 emissions. Notably, investigation of sorbent-based carbonation reactions holds significant relevance in this domain [13], [14]. Efforts in current existing research are centered on optimizing CaO-based carbonation reaction to elevate the effectiveness of CO_2 capture [15], [16] thus representing a prominent issue in present-day discussions and analysis.

In addressing rising carbon dioxide emissions and global warming, authors [17] highlight low-carbon technology, including *CCS. CCS,* especially with $Ca(Ac)_2$, is essential to lowering global CO_2 emissions by 50 % by 2050. $Ca(Ac)_2$ to CaO is studied using *TGA, XRD,* and *TEM.* Testing shows that heating rate considerably impacts CaO formation temperature and sintering. Slower breakdown yields bigger, porous CaO particles that may trap CO_2. The review suggests modifying calcination temperature, heating rate, and particle spacers to limit CaO sintering and increase CO_2 uptake in future experiments. The calcium additions CaO and $CaCO3$ impact maize cob pyrolysis to obtaining kinetic parameters is studied [18]. CaO enhances activation energy while $CaCO_3$ lowers it. Kinetic Coats-Redfern integral investigation exposes thermal degradation. Challenges to linear regression models emphasize the need for optimization. Results indicate that maize cob can be a sustainable energy source and highlight the function of pyrolysis catalysts. A new solid sorbent technology for atmospheric CO_2 removal is studied [19]. This initiative develops low temperature CO_2 sorbents based on potassium, specifically *3K/CaO.* Thermogravimetric, FTIR, and X-ray diffraction study the sorbent's properties and processes. The study prioritizes sorbent stability and avoids potassium carbonate loading, which damages pores. The high surface area and potassium carbonate concentration of 3*K/CaO* make CO_2 extraction possible and fast. The Greenhouse Calcium Looping *(GCL)* process may solve greenhouse heating issues [20]. Photosynthesis and nighttime heat require CO_2 in greenhouses. The *GCL* method produces CO_2 and heat using limestone sorbent cyclic carbonation/calcination, according to the study. Aspen Plus simulations and thermogravimetric research generate *GCL* carbonation/calcination reaction kinetic parameters. After identifying suitable kinetic models, the study illuminate's reaction mechanisms and *GCL* process operational needs. We also found temperature-dependent carbonation and calcination kinetics. Compared to burner systems, *GCL* emits little CO_2. CaO-based biomass materials for CO_2 sorption and separation are covered in [21]. The study highlights such material's CO_2 capture capabilities, cost- effectiveness, and benefits. An exothermic carbonation reaction is used to regenerate the endothermic CaO-based sorbent during calcination-carbonation. For example, calcination residence time, biomass with SiO_2 and Al_2O_3, and alkaline ions affect sorbent performance. Biomass like cockle shell, empty fruit bunches, rice husk, and coal bottom ash being studied for sorbent synthesis. The study found that biomass components improve sorbent cyclic stability and CO_2 capture. In chemical looping reforming, a CO_2 reduction method, naturally generated dolomite is examined [22]. Dolomite, mostly CaO and MgO, undergoes calcination and carbonation cycles. Study examines how sample weight, set-up scale, and steam affect CO_2 capture performance. Incomplete dolomite calcination due to non-uniform temperature gradients and sintering is seen at macroscale. Over cycles, steam stabilizes sorbent, reducing sintering. Experimental results suggest that sorbent regeneration without steam may improve in situ CO_2 collection for chemical looping reforming. This study underlines the need of maximizing dolomite's use in chemical looping systems for stability, efficiency, and repeated cycles.

Existing studies predominantly concentrate on specific facets, such as the breakdown of calcium acetate *(CaAc)* to calcium oxide *(CaO),* the influence of temperature and heating rate on CaO formation, and utilization of CaO in diverse contexts, including maize cob pyrolysis and CO_2 sorbent technology. Nevertheless, there exists an opportunity for integration of empirical observations and theoretical models across these discrete investigations. The augmentation of a comprehensive comprehension regarding the intrinsic kinetics, activation energy, and reaction rates within these varied applications is imperative. A methodical approach is requisite to amalgamate variables across distinct experimental configurations, given that the divergence in experimental conditions and absence of a standardized methodology pose challenges in comparison and generalization of findings across studies. Additionally, an investigation into potential synergies arising from distinct applications of CaO in mitigating carbon emissions emerges as a fertile area for study. Addressing these aspects would significantly contribute to a more holistic understanding of carbonation kinetics of CaO to CO_2 sorption and its manifold applications.

In this study, we investigate the kinetics of CO_2 capture through CaO-based carbonation processes using *STA* and *MS.* This innovative approach allows real-time monitoring of evolution and simultaneous measurement of thermal effects and mass changes during carbonation reaction, providing a comprehensive understanding of reaction kinetics and evolution dynamics. The experimental setup is characterized using cutting-edge instrumentation such as thermogravimetric analysis device and *QMS* 403*C AËOLOS* mass spectrometer. This study delves into the intricate kinetics of carbonation reaction, unraveling activation energy, reaction rate constants, and half-lives across diverse temperature ranges. The utilization of Arrhenius plots has unveiled the intriguing temperature dependence of reaction rates, shedding light on the energy barriers within the carbonation process. Furthermore, the study has ventured into exploring the pressure-order relationship, elucidating the profound impact of pressure variations on enhancing CO_2 capture efficiency. The study demonstrates temperature-dependent CO_2 capture capacity, identifying temperature thresholds and efficiency variations at different temperature ranges. This provides critical insights into optimal temperature conditions for enhancing CO_2 capture efficiency and informs the design and optimization of CO_2 capture technologies. Comparisons with existing studies validate the accuracy and reliability of the findings, enhancing the credibility of the study and highlighting the proposed methodology's significance in advancing CO_2 capture and utilization. The contribution of the study are as follows:

a) The study utilizes advanced instrumentations such as thermogravimetric analysis *(NETZSCH STA* 449 *F3 Jupiter)* device and mass spectrometer *(QMS* 403C *AËOLOS)* for precise and real-time data acquisition, enhancing experimental results reliability and accuracy.

b) Analysis of carbonation process across various temperatures reveals temperature- dependent trends in reaction rates, crucial for optimizing reaction conditions in industrial applications for process efficiency.

c) The study investigates the pressure-order relationship in carbonation, revealing how pressure changes affect CO_2 capture efficiency that offers valuable insights for designing and optimizing CO_2 capture systems in industrial settings.

d) The study explores temperature-dependent CO_2 capture capacity, identifying thresholds and efficiency variations across different temperature ranges which improves understanding of optimal CO_2 capture conditions and informs CO_2 capture technology design, advancing sustainable emission reduction strategies.

e) The dual-method approach, combining linear regression and least-squares methods, enhances the robustness of statistical models in analyzing activation energy and reaction rates.

Methodology

This section details the experimental setup and kinetics modeling used to study the carbonation process of calcium oxide and carbon dioxide for CO_2 capture applications. The setup includes simultaneous thermal analysis and mass spectrometry, integrating components like the *STA* 449 *F*3 thermogravimetric analysis device and *QMS* 403C *AËOLOS* mass spectrometer.

Configuration of experimental setup

Thermal analysis is a comprehensive analytical approach that involves the concurrent application of thermogravimetric (*TGA*) and differential scanning calorimetry (*DSC*) techniques to a singular sample within a unified instrument [23]. Figure 1 represents the workflow diagram of the study. *TGA – DSC* allow simultaneous measurement of heat flow and mass changes, providing a more comprehensive understanding of reaction kinetics [24]. Mass Spectrometry (*MS*) has been used in the experiment to analyze the gas composition and evolution as the carbonation reaction progressed. *MS* in *STA* enables real-time monitoring of gas evolution, identifying reaction intermediates, and quantifying gas concentrations [25].

STA is a method that allows non-isothermal experiments, providing insights into temperature-dependent behavior [26]. It uses data from *TGA* and *DSC,* along with *MS* analysis, to calculate critical kinetic parameters, such as activation energy, for predicting reaction rates under different conditions [27]. *STA* and *MS* help optimize systems for CO_2 capture, improving reaction efficiency and overall design. *TGA* monitors changes in a sample's mass over time as temperature varies, providing insights into physical phenomena like phase transitions, absorption, desorption, and chemical processes like thermal decomposition and solid-gas reactions [28], [29]. The integration of synchronous thermal analysis with *MS* involves components such as *NETZSCH STA* 449 *F3* thermogravimetric analysis device, *QMS*403C *AËOLOS* mass spectrometer, high-precision pulsed gas supply, steam generator unit, and auxiliary apparatus. *Netzsch STA F3* Jupiter enables simultaneous measurements of mass change and thermal effects using the same sample, accommodating a wide range of thermogravimetric applications [30]. The introduction of argon into the furnace safeguards the balance block from gases, with controlled gas flow for thorough mixing and heating, followed by gas analysis in a mass spectrometer [31]. In our study, Table 1 delineates the experimental conditions utilized for our comprehensive analysis, while Figure 2 presents the block diagram depicting the intricacies of mass spectrometry.

Kinetics Modeling for CaO- based Carbonation

CaO served as absorber in the experimental setup, with test average sample mass of 30.664 *mg.* The experiment has been conducted three times to ensure the acquisition of precise and dependable data. *CaO* particles range in size from a few micrometers to tens of micrometers, with a uniform distribution in *TGA*. Their low to moderate porosity affects their reactivity and surface area, influencing the reaction with CO_2 to form *CaCO3.* CaO particles have a relatively low surface area, which plays a significant role in their reactivity with CO_2. They exhibit high thermal stability at elevated temperatures, with minimal weight loss until reacting with CO_2 to form CaC03.When converting *CaO* to *CaCO3,* the size and porosity of the particles change. The size decreases due to the solid-state transformation, while the porosity may decrease due to the filling of pores. *TGA* analysis typically shows changes in the weight loss curve, providing insights into the reaction's kinetics and extent. *STA* 449 *F3 Jupiter* instrument accommodates various crucible

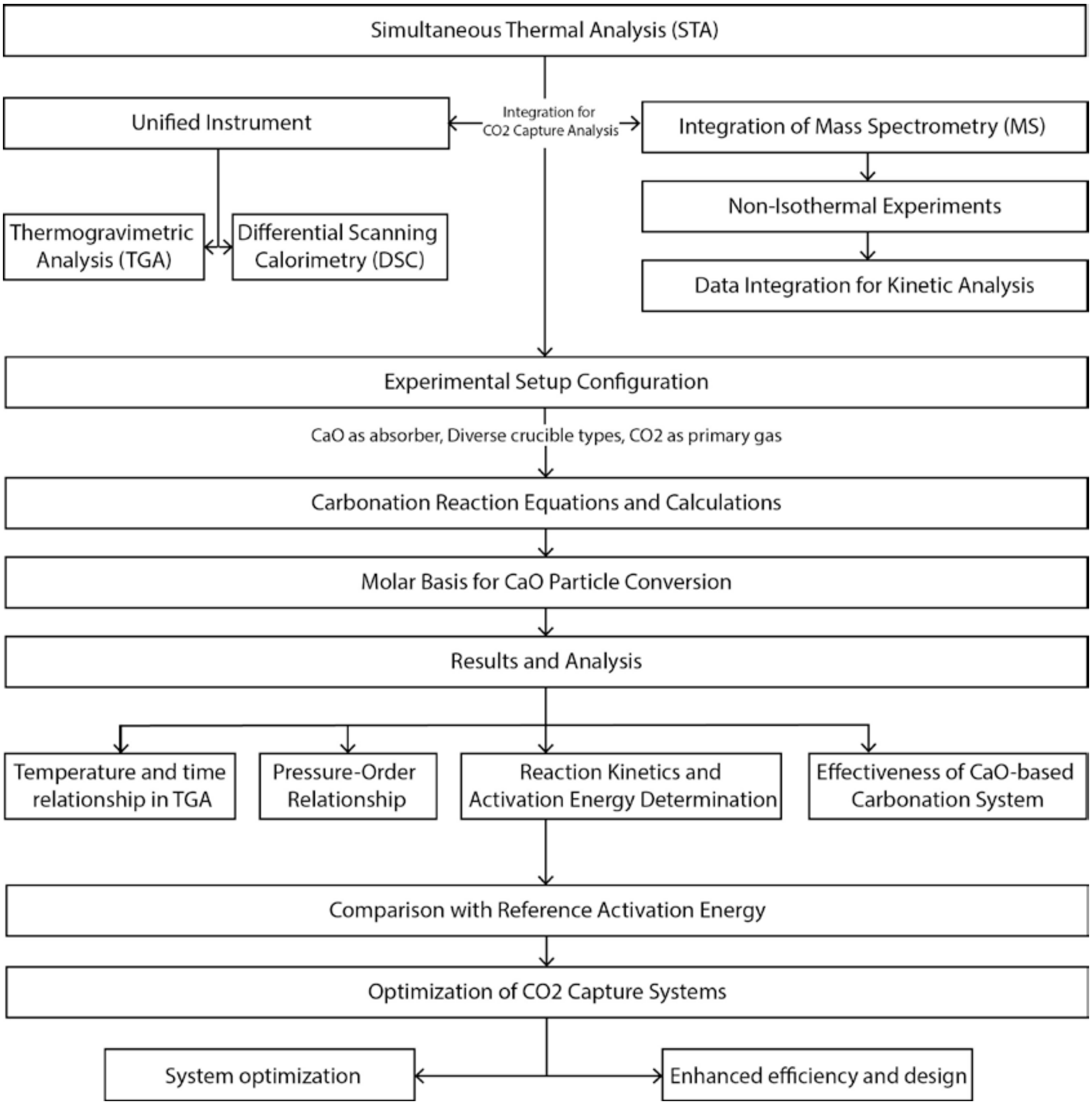


Fig. 1. A schematic framework for the analysis of CO_2 capture by CaO-based carbonation processes

types for diverse applications, and for this experiment, a *DSC/TG* pan made of $Al2O3$ was employed as the crucible. The experimental duration extended over 48 minutes. The primary gas employed was CO_2, while argon was utilized to safeguard the weighing unit. The experiment was conducted in a non-isothermal mode, wherein the sample underwent heating from room temperature to 1240 K at a rate of 20 °*K/min.* This heating rate has been chosen to accurately represent the reaction's kinetic and thermodynamic characteristics within experimental conditions. The carbon absorption reaction under investigation during the experiment is represented by Eq. (1) which involves the absorption of CO_2 by CaO, resulting in the formation of calcium carbonate *(*$CaCO3$*)*. This chemical transformation is central to various industrial applications, such as carbon capture and utilization [32].

$$CaO + CO_2 \rightarrow CaCO_3 \tag{1}$$

To ascertain theoretical mass of $CaCO_3$, a series of calculations is being conducted. Subsequently, molar mass of CaO is determined to be 56 *g/mol.* and molar mass of $CaCO3$ is established at 100.09 *g/mol.* The theoretical mass of $CaCO_3$ is then calculated 54.73 *mg*, revealing a theoretical mass that corresponds to 178.480 % of the actual mass. In the context of carbonation reactions, CaO plays a pivotal role as a reactant. To determine reaction kinetics, general equation for a gas-solid reaction is expressed as Eq. (2). which provides a framework for analyzing kinetics

Table 1 Experimental Conditions for Therma Analysis

SL	Parameters	Specification	Units	Description / Remarks
1	Absorber	*CaO*	–	Sample to analyze reactivity, performance in carbonation
2	Mass	30.664 (average)	*mg*	Mass of test sample
3	Crucible Type	Al_2O_2	–	Alumina as *DSC – TGA* pan
4	Crucible Holder	*STA* 449 *F3 Jupiter*	–	Sample holder used in STA apparatus
5	Main Gas	CO_2	–	To simulate carbonation conditions, degradation and assesses *CaO*-based materials
	Flow Rate	133.33	*mL/min*	–
6	Protective Gas	*Ar*	–	Ar as inert gas to prevent unwanted reactions, particularly when studying heat degradation and carbonization
	Flow Rate	40	*mL/min*	–
7	Experimental Mode	Nonisothermal	–	To study carbonation kinetics, *CaO*-based performance under dynamic temperatures
8	Temperature	298 to 1240	*K*	Heating profile
	Heating Rate	20	*°K/min*	–

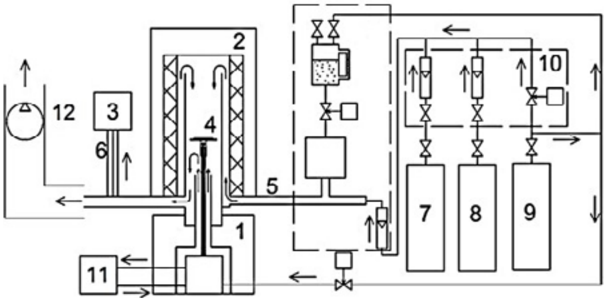


Fig. 2. Synchronous thermal analysis complex featuring mass spectrometry: 1 – weighing unit, 2 – furnace, 3 – mass spectrometer, 4 – sample holder, 5 – heated gas supply line, 6 – heated gas sampling line at the outlet of the furnace, 7, 8 – CO_2 gas cylinders, 9 – argon cylinder, 10 – PulseTA prefix, 11 – thermostat, 12 – exhaust system

of gas-solid reactions and offers insight into factors such as gas pressure ($P_{CO\,2,eq}$), temperature, and reaction mechanism influencing reaction rates.

$$\frac{dx}{dt} = k \times f(x) \times (P_{CO_2} - P_{CO_{2,eq}})^n \qquad (2)$$

Here, dt represents time, n denotes reaction order, $f(x)$ signifies a function for reaction mechanism, and κ is reaction rate constant. CaO-based carbonation reaction's mechanism can be depicted by diffusion function $f(x) = x^2$. This representation, which yields the optimal linear fit, indicates that CaO-based carbonation reaction follows a first- order kinetics. The equilibrium pressure ($P_{CO\,2,eq}$) of 0 is established through the introduction of CO_2 from external source, distinct from the sample itself. Additionally, determining partial pressure of CO_2 ($P_{CO\,2}$) involves multiplying atmospheric pressure (P_{atm}) by CO_2 volume fraction (r_{CO_2}), specifically set at 1 (100 %). The quantification of *CaO* particle conversion through carbonation is imperative for understanding reaction kinetics and optimizing process parameters. The molar basis, as expressed by Eq. (3), facilitates a comprehensive assessment of this conversion process. Investigating the conversion of *CaO* particles provide crucial insights into the efficiency and dynamics of carbonation reaction, offering valuable information for the design and improvement of systems employing *CaO* as a key component in carbon capture and mineralization strategies. It is worth mentioning that while it seems counterintuitive to conduct decarbonation reactions in a CO_2 environment due to potential thermal degradation of calcium carbonate, we chose this approach to maintain consistent experimental conditions and simulate real-world scenarios where CO_2 is present.

$$x = \frac{\dfrac{m_{CaO}(t) - m_{CaO}(0)}{44}}{\dfrac{m_{CaO}(0)}{56}} \qquad (3)$$

In order to determine activation energy *(E_a)*, reaction rate constant (k), and half-life ($t_{1/2}$) for the degree of conversion ($0 < x < 1$) in a first-order reaction ($n = 1$), a crucial step involves the establishment of the relationship $InR\tau = f\ (1/T)$, where $R\tau$ represents the gaseous conversion rate in sec^{-1} and $1/T$ denotes the reciprocal of temperature in $1/K$. The expression for $R\tau$ is defined in Eq. (4).

$$R\tau = \frac{d\tau \times dm}{mt} \tag{4}$$

Where *dm* is mass changes in kg, mt is mass of the sample at present in kg, and $d\tau$ is time in seconds. For the calculation of kinetic constants, temperature interval corresponding to the initiation of sample weight change is utilized. In this interval, rate of mass change is determined by the rate of the chemical reaction using Eq. (5).

$$R\tau(T) = k \times e^{\frac{R \times T}{E_a}} \tag{5}$$

Where k represents reaction rate constant in sec^{-1}, Ea is activation energy in J/mol, R is universal gas constant in $J/(mol \times K)$, and T is temperature in K. The half-life ($t_{1/2}$) for a first-order reaction is defined in Eq (6) as the reaction rate constant κ divided by natural logarithm of 2.

$$t_{1/2} = \frac{k}{ln2} \tag{6}$$

The study considers the impact of sorption and desorption processes on reactions, using thermogravimetric analysis and mass spectrometry. Kinetics modeling considers reaction mechanisms, kinetics, and activation energy. Experimental conditions simulate carbonation conditions, highlighting the potential effects of these processes. This study provides a comprehensive understanding of crucial steps in carbon capture and mineralization methods, focusing on the role of CaO in carbonation reactions. The complex interaction of factors yields vital information for reaction optimization in industrial applications. By employing linear regression *(LR)* and least-squares *(LS)* methods, the study delves into the kinetics of the carbonation reaction of CaO with CO_2, crucial for optimizing CO_2 capture systems. These methods involve fitting experimental data to mathematical models, extracting relevant parameters, and minimizing the differences between observed and predicted values [33], [34]. Additionally, they aid in estimating reaction kinetics parameters, validating models, and optimizing CO_2 capture systems by identifying suitable operating conditions and guiding system design and scale-up.

Result

The temperature and time relationship with mass retrieval and conversion of CaO in *TGA* for *CaO-base* carbonation reaction is significant. Figure 3 provides valuable insights into kinetics and thermodynamics of the reaction, offering a deeper understanding of the underlying processes. The low-temperature region of chemical reaction is characterized by initiation phase with minimal mass loss, indicating a slow reaction. As the temperature surpasses 323 *K*, a more pronounced mass loss becomes evident, signifying an acceleration of the reaction with a steady decrease in mass over time. The transition stage within this region witnesses a moderate to rapid increase in temperature, accompanied by sustained mass loss, indicative of an active reaction. This temperature range is likely associated with the primary phase of the reaction, where CaO reacts with CO_2 to form calcium carbonate. The relationship between mass loss and conversion becomes particularly intriguing in this region. The modest mass loss, coupled with a gradual rise in conversion, implies a controlled and nuanced transformation of the reactant. This suggests that the decomposition reaction unfolds not only in response to temperature variations but also in consideration of the intrinsic properties of the material. In the high-temperature region (823–1233 *K)*, a notable trend emerges as the temperature surpasses 823 *K;* although the temperature continues to rise, the rate of mass loss stabilizes, suggesting a potential completion of the reaction or the establishment of a dynamic equilibrium. The consistent time intervals indicate a sustained state in the later stages of the regime. In the range of 973 *K to* 1233 *K*, a potential steady- state behavior is observed, as the mass loss reaches a plateau, indicating a relatively stable condition. The interaction between mass loss and conversion within this temperature range underscores the nuanced nature of the CaO to $CaCO_3$ transformation. The significance of comprehending the interdependence between temperature, mass loss, and conversion becomes evident in understanding the underlying mechanisms of the carbon capture process.

Figure 3(b) reveals that mass changes in carbonization and decarbonation reactions are non-symmetric due to various factors. These include temperature dependence, thermodynamic factors, kinetic effects, intermediate formation, catalytic effects, and microstructural changes. Carbonization dominates at lower temperatures due to carbonaceous residue stability, while decarbonation prevails at higher temperatures due to increased energy availability. Kinetic effects also influence the asymmetry, with certain temperature ranges showing more substantial mass changes. Intermediate formation can also affect the overall reaction pathway.

Arrhenius plot is employed to investigate the relationship between temperature and rate at which carbonation reactions occur. Figure 4 (a)-(f) illustrate Arrhenius plot depicting carbonation process, with a specific emphasis on different temperature ranges. Activation energy is an essential indicator for comprehending the kinetics of chemical reaction. It signifies the energy barrier that must be surpassed for the reaction to take place. Activation energy can be readily determined from Arrhenius plot. Within the framework of Arrhenius plot for carbonation, linear regression *(LR)* method can be employed to ascertain the correlation between the logarithm of reaction rate $(In\ R\tau)$ and the inverse of temperature $(1/T)$. Activation energy and pre-exponential factor for the reaction can be found by applying a linear equation to the data. Conversely, least squares *(LS)* method is employed to determine the optimal curve that fits a given set of data points. The *LS* method can be used in Arrhenius plot for carbonation to minimize the sum of the squared differences between the observed and anticipated reaction rates at various temperatures. By finding the most accurate curve that shows the relationship between the reaction rate and temperature, this method makes it easier to figure out Arrhenius equation's parameters, such as activation energy and pre-exponential factor. The observed temperature dependency is a prevalent pattern in chemical reactions, consistent with the principles of reaction kinetics from CO_2 sorting point of view. The precise equations derived from the *LS* method provide mathematical comprehension of the relationship between activation energy and temperature, offering useful insights for estimating reaction rates in diverse circumstances.

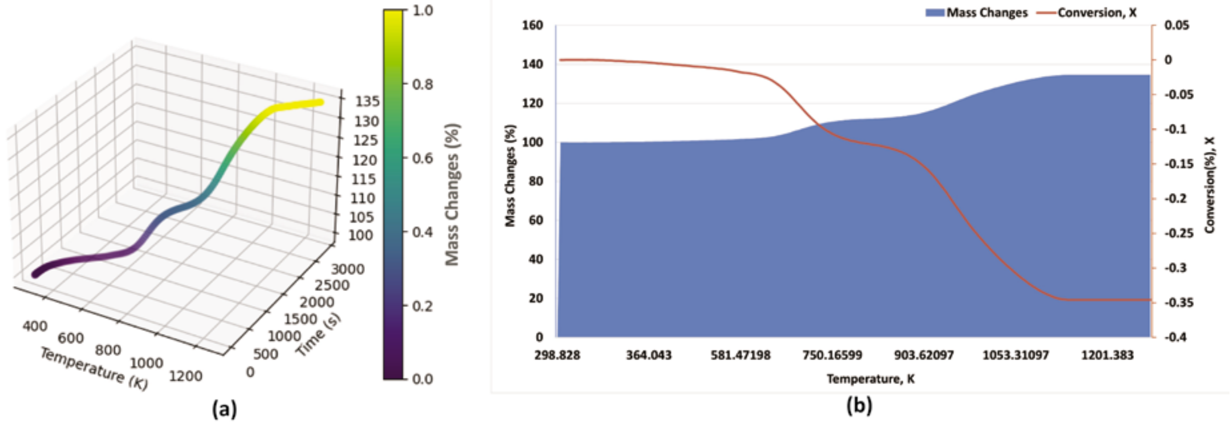


Fig. 3. Unraveling effects of temperature and time on *TGA*: (a) temperature and time on mass changes (%) (b) temperature and time on mass changes (%) and conversion (%)

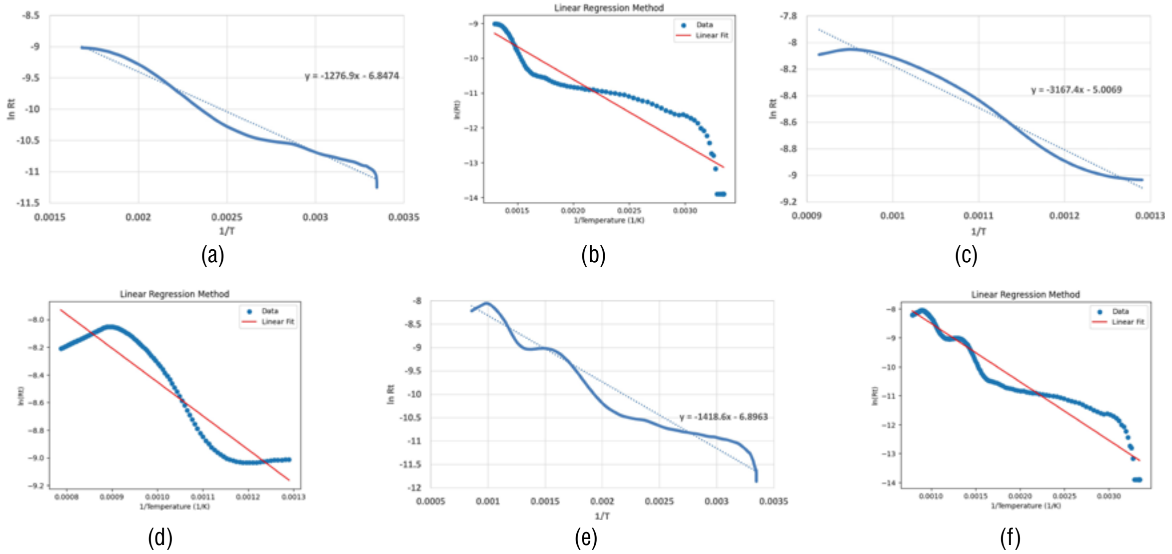


Fig.4. Arrhenius plot for carbonation reaction for different region: (a) *LS Method* – Low temperature (b) *LR Method* – Low temperature (c) *LS Method* – High temperature (d) *LR Method* – High temperature (e) *LS Method* – Overall (f) *LR Method* – Overall

Table 2. Comparative Analysis of Activation Energy and Reaction Rate Constants Using Linear Regression and Least-Squares Methods

Method	Range	Activation Energy, E_a (KJ/mol)	Pre exponential Factor, $In\ A$	From Arrhenius Plot	
				Reaction rate constant, k ($sec^{-1} \cdot Pa^{-1}$)	Half-lives (sec)
Linear regression method	Low temperature	15.59	6.86	1.036×10^{-8}	6.69×10^{7}
	High temperature	20.36	6.48	2.449×10^{-8}	2.83×10^{7}
	Overall	21.745	6	1.515×10^{-8}	4.57×10^{7}
Least-squares method	Low temperature	15.3	6.85	1.049×10^{-8}	6.60×10^{7}
	High temperature	20.44	6.89	6.609×10^{-8}	1.05×10^{7}
	Overall	26.33	5.01	9.992×10^{-8}	6.94×10^{7}

Table 2 investigates the carbonation process, focusing to determining activation energy (Ea), reaction rate constant (k), and half-lives at both low and high temperatures. The linear regression and least-squares approaches are essential in revealing the kinetics and thermodynamics of carbonation reaction. Activation energy quantifies the amount of energy needed for the reactants to undergo a transformation into products. On the other hand, $In\ A$ reflects pre-exponential factor of Arrhenius equation. The findings derived from using *LR* for low, high, and overall temperatures (15.59, 20.36, and 21.745 kJ/mol, respectively) indicate that the energy barrier for the carbonation process is greater at high temperatures. This is supported by the corresponding $In\ A$, which demonstrate a comparable pattern. Our investigation revealed a positive correlation between temperature and the rate of the carbonation reaction. The reaction rate constants (k) at low, high, and overall temperatures are 1.036×10^{-8}, 2.449×10^{-8}, and are 1.515×10^{-8} $sec^{-1} \cdot Pa^{-1}$, respectively. This is consistent with the principle that elevated temperatures typically result in accelerated reaction rates. From *LS* method, we can observe that the low, high, and overall temperatures yield κ values of 1.049×10^{-8}, 6.609×10^{-8} and 9.992×10^{-8} $sec^{-1} \cdot Pa^{-1}$ respectively. The half-lives, which represent the time required for half of the reactants to be consumed, can be obtained through subtracting the reciprocal of the reaction rate constant ($1/k$). *LR* and *LS* methods provide valuable insights into the kinetics of the carbonation process by determining half-lives at various temperatures, including low, high, and overall values. Significantly, the half-lives diminish as the temperature rises, indicating an accelerated progression of the reaction at higher temperatures.

Figure 5 depicts an in-depth assessment of the reaction kinetics over a broad range of temperatures and the corresponding rates of reaction. Figure 5(a) demonstrates a gradual decline in reaction rates as the reaction advances, with the most rapid rates happening at the beginning of the low temperature range. Reaction rates eventually become quantitative and show variations over the temperature

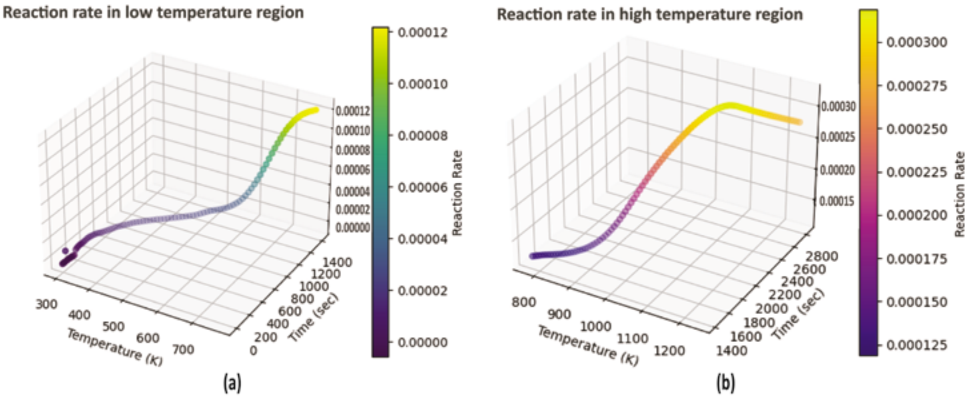
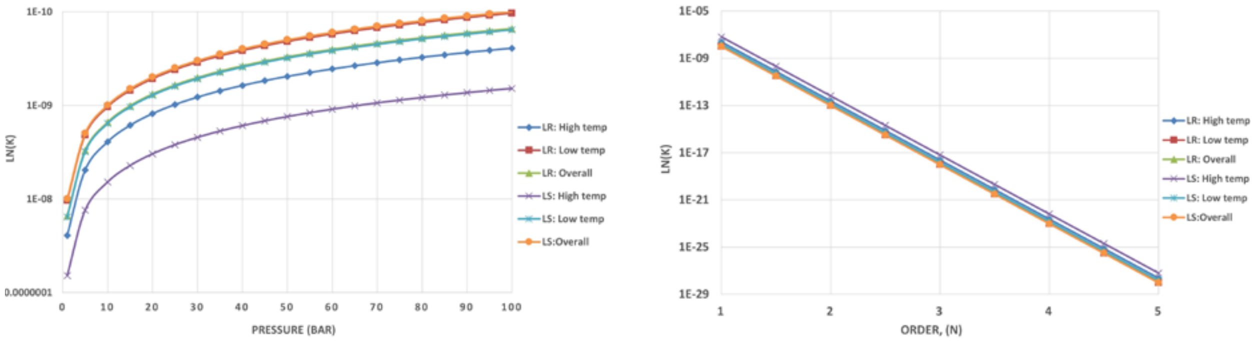


Fig. 5. Effects of temperature and time on reaction rates: (a) low temperature region (b) high temperature region

range (300–600 *K*). Lower temperatures exhibit a steady rise in reaction rates, which indicates the slower kinetics associated with these temperatures. At temperatures over 304.204 *K*, the reaction rates of carbonation process decrease significantly, indicating a substantial slowing and reaching a condition of equilibrium. Within the carbonation process, significant observations and implications can be identified at the higher temperature zone. Figure 5(b) on the relationship between time, temperature, and reaction rate demonstrates that higher temperatures have a significant impact on the rate at which reactions occur. Upon analysis in the higher temperature range, it becomes evident that reaction rates generally increase as the temperature rises. Higher temperatures lead to a greater frequency and energy of molecular collisions. Increased energy levels promote the surmounting of activation energy barriers, allowing a greater number of molecules to acquire the requisite energy for engagement in the reaction. As a result, the rates at which reactions occur are greater when temperatures are increased. When specific time intervals are analyzed within the higher temperature range, the reaction rates consistently show an increased tendency. At a temperature of 1118 *K*, reaction rate is estimated to be 3.187×10^{-4}. Subsequent observations indicate a consistent rise in reaction rates with increasing temperatures. Understanding the kinetics of the carbonation process is essential, especially in situations where controlling the reaction rate is key. This understanding relies on recognizing the temperature-dependent nature of the activity. In addition, Figure 5 (b) demonstrates that at 1 000 *K*, the reaction rates exhibit a pattern of increasing to higher values, suggesting a faster and more effective carbonation process at higher temperatures. This is important for companies and applications that need to adjust response rates to improve process efficiency and productivity. However, when analyzing individual temperature points, it is obvious that the reaction rate rises as the temperature increases, indicating the temperature's influence on the carbonation process. This is consistent with well-established concepts in chemical kinetics, where higher temperatures frequently lead to higher reaction rates because of intensified molecule collisions.

The pressure-order relationship in CaO-to-$CaCO_3$ carbonation is illustrated in Figure 6. Carbonation converts calcium oxide to calcium carbonate by reacting with CO_2 at pressure, order, and temperature. Reaction order is the rate equation power to which a reactant concentration is elevated. As the pressure increases, the rate of carbonation tends to decrease, as indicated by Figure 6(a) of the carbonation rates for both *LR* and *LS* methods. For *LR* and *LS* at high temperature, low temperature, and overall regions provide insights into the kinetics of the carbonation process under different conditions. Both *LR* and *LS* methods offer statistical approaches to modeling the relationship between pressure and the rate of carbonation. The differences in Figure 6(a) obtained from these methods at different temperatures can indicate the sensitivity of the carbonation process to temperature variations. The comparison of *LR* and *LS* values at high and low temperatures suggests that the carbonation process is influenced by temperature, with higher temperatures generally resulting in higher carbonation rates. The overall *LR* and *LS* values provide a comprehensive view of the carbonation kinetics across the temperature range studied. Examining *LR* and *LS* values for different reaction orders reveals distinct trends in the carbonation process as shown in Figure 6(b). As the reaction order increases, *LR* and *LS* values exhibit a systematic decrease, signifying a diminishing reaction rate. This inverse relationship between reaction order and reaction rate is crucial for understanding the intricacies of the carbonation kinetics. The differentiation between *LR* values at high and low temperatures offers valuable information about the temperature dependency of the carbonation reaction. Higher *LR* values at elevated temperatures suggest a temperature-dependent enhancement of the reaction rate,



(a) (b)

Fig. 6. Exploring Reaction Rate Dependencies: (a) Pressure -Dependance of Reaction rate (b) Order-Dependance of Reaction rate

emphasizing the significance of temperature in influencing the carbonation kinetics. Comparing *LR* and *LS* values provide a comprehensive assessment of the robustness of the regression models. *LS* values, being more resilient to outliers, offer an additional layer of understanding, ensuring a more accurate representation of the relationship between reaction order and the carbonation process.

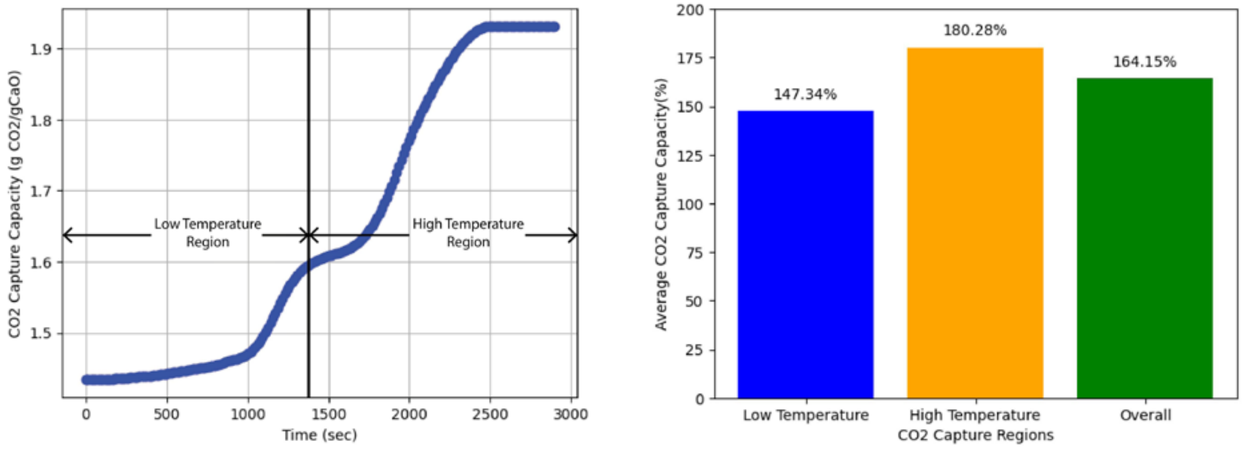
The relationship between time dependent temperature, and CO_2 capture capacity is represented in Figure 7, allowing for analytical comparison. The escalating levels of CO_2 emissions resulting from the combustion of fossil fuels, such as different coal grade in power generation [35] or other industrial processes [36], have prompted the exploration of innovative alternatives to mitigate these emissions and reduce the associated carbon footprint. The dynamic nature of the CO_2 capture process at lower temperatures is highlighted by the observed fluctuations in its capacity. The efficiency of CO_2 capture is significantly influenced by factors such as reaction kinetics and thermodynamics. Within the low temperature region, observed CO_2 capture capacity (%) stands at relatively low (Figure 6b). During low- temperature phase, *CaO* is anticipated to demonstrate distinctive CO_2 capture efficiency, marking the onset of the reaction as it begins to adsorb CO_2. In contrast CO_2 capture capacity at high temperatures reveals a consistent and discernible increase in efficiency as temperatures rise. Within high-temperature range, capacity for capturing CO_2 per gram of *CaO* exhibits a notable upward trajectory, indicating the complex interplay between thermodynamic and kinetic factors governing the underlying chemical reactions. Notably, optimal CO_2 capture capacity peaks are observed at the highest temperature regions, approximately around 1 200 *K*, suggesting the existence of temperature thresholds beyond which further improvements in capture efficiency may yield diminishing returns (Figure 7a).

In high-temperature region, *CaO* experiences the most substantial mass losses because of CO_2 absorption, signifying the peak and, consequently, the maximum capture efficiency (see Figure 7b). This observed trend aligns with fundamental thermodynamic principles, where reactions tend to be more favorable at elevated temperatures due to increased kinetic energy and enhanced reactant mobility. Understanding the temperature-dependent trend is crucial for developing CO_2 capture systems tailored for high-temperature environments. It provides valuable insights into the temperature ranges where capture process is most effective, guiding the optimization of conditions for industrial applications.

Discussion

In this study, we introduce 6ТЛ-based methodology for exploring carbonation kinetics of *CaO.* The instrument uses differential scanning calorimetry to capture thermal effects, and *LR* and *LS* methods for modeling activation energy and reaction rates. The study examines low and high-temperature regions, assessing pressure influence, to provide a holistic understanding of carbonation process across different conditions. The dual-method approach evaluates activation energy and reaction rates, ensuring the reliability of statistical models. Carbonation process's sensitivity to reaction orders, reveals dependencies on pressure and temperature. This is crucial for optimizing reaction conditions in various industrial settings. The study's precision, versatility, and the application of dual-method statistical modeling highlight its potential for enhancing the understanding of carbonation processes. In light of the foregoing analysis, the study's observations lead to the following conclusions.

a) *TGA* of the carbonation reaction reveals temperature and time dependencies, providing insights into carbon



(a) (b)

Fig.7. Effectiveness of *CaO*-based carbonation system in capturing CO_2: (a) On $gCO_2/gCaO$ basis (b) In terms of % capacity

capture capacity. In low-temperature ranges, a gradual initiation with mass loss and conversion suggests a controlled transformation of *CaO*. In high-temperature ranges, a stable condition and potential completion suggest a nuanced transformation for optimizing carbon capture processes in industrial applications.

b) Arrhenius plot and derived activation energy values offer a quantitative understanding of the temperature dependency of the carbonation process for the assessment and optimization of *CCS*. The observed temperature dependency suggests higher energy thresholds at elevated temperatures, impacting carbon capture efficiency.

c) Figures 3 and 4 reveal the carbonation process's dynamics, revealing a deceleration in reaction rates in low-temperature ranges and a surge in rates at elevated temperatures. The trajectory beyond 1 000 *K* suggests a more streamlined process, requiring optimized reaction rates for industries to improve carbon capture efficiency and productivity.

d) The study reveals that pressure-order relationships in CaO-to-$CaCO_3$ carbonation negatively impact carbon capture capacity, with higher pressures affecting efficiency. The inverse relationship between reaction order and reaction rate is crucial for understanding carbonation kinetics. Temperature control is essential for optimizing carbon capture processes, and robust *LS* values enhance accuracy in assessing reaction order.

In evaluating calculated activation energy values for carbonation process obtained through both *LR* and *LS* methods, a comparison with reference reveals insights into the accuracy and reliability of the calculated results as dissipated in Figure 8. Activation energy (E_a) obtained through *LR* method at low temperature, high temperature, and overall are in line with theoretical expectations. In comparison of calculated values, with existing studies provides additional insights. Grasa *et al.* [37] reported E_a of 21.3 *KJ/mol* at high temperatures with varying partial pressures of CO_2 (P_{CO_2}) between 0.01 and 0.1 *MPa*. Sedghkerdar *et al.* [38] obtained a value of 28.3 *KJ/mol* at high temperatures using a Thermogravimetric Analyzer operating at atmospheric pressure. Ramezani *et al.* [20] conducted experiments at low temperatures with P_{CO_2} ranging from 0.05 to 0.1 %, resulting in E_a of 19.7 *KJ/mol*. Furthermore, Fedunik-Hofman *et al.* [39] reported an overall E_a of 17.45 *KJ/mol* under isothermal conditions, where Pechini-synthesized *CaO* was initially heated isothermally under 100 % N_2 and then subjected to carbonation under a mixed atmosphere. Sun *et al.* [40] observed an overall E_a of 24 *KJ/mol* at high pressures ($P_{CO_2} > 101$ *kPa*), while another study by Grasa *et al.* [37] indicated E_a of 19.2 *KJ/mol* for cyclic carbonation and calcination reactions with varying P_{CO_2} between 0.01 and 0.1 *MPa*. Upon review of E_a, it appears that there is a discrepancy between the calculated E_a and those obtained from existing studies:

a) The calculated activation energy using both linear regression and least-squares methods generally fall within the range of the existing studies, but there are slight differences in specific temperature ranges.

b) For the high-temperature range, the calculated values from both methods tend to be lower than some of the existing studies.

c) The low-temperature calculated values, particularly with the least-squares method, are notably lower than Ramezani et al. [20].

d) Fedunik-Hofman et al. [39] overall activation energy is in closer alignment with the least-squares overall than with the linear regression overall.

e) Sun *et al.* [40] overall activation energy is within the range of the calculated values. Diverse experimental conditions, methodological choices, and complexities in reaction kinetics contribute to disparities in calculated activation energy compared to existing studies. Variances in equipment, temperature ranges, CO_2 partial pressures, reaction mechanisms, synthesis methods, and data analysis techniques introduce additional variables. Additionally, measurement uncertainties and the use of varied analytical tools impact results. It is important to mention that calculated values are approximations and are subject to limitations based on the assumptions and models employed in the linear regression and least- squares methods. The discrepancies in the total activation energy calculated by the linear regression method and the least squares method, despite similar values for the low and high temperature ranges, stems from factors such as the distribution and weighting of data points, assumptions in models, the temperature dependence of rate constants, and potential statistical fluctuations in the data.

In this study, we explore the dynamic relationship between temperature and CO_2 capture capacity, highlighting the efficiency of *CaO* at varying temperatures. The study suggests the existence of temperature thresholds, indicating diminishing returns from further enhancements. Significant mass losses at higher temperatures align with thermodynamic principles, crucial for developing CO_2 capture systems in high-temperature environments. The pivotal role of activation energy in *CaO* – based carbonation enhances reaction kinetics and aids in temperature optimization, influencing the design of energy-efficient capture systems for sustainable emission reduction.

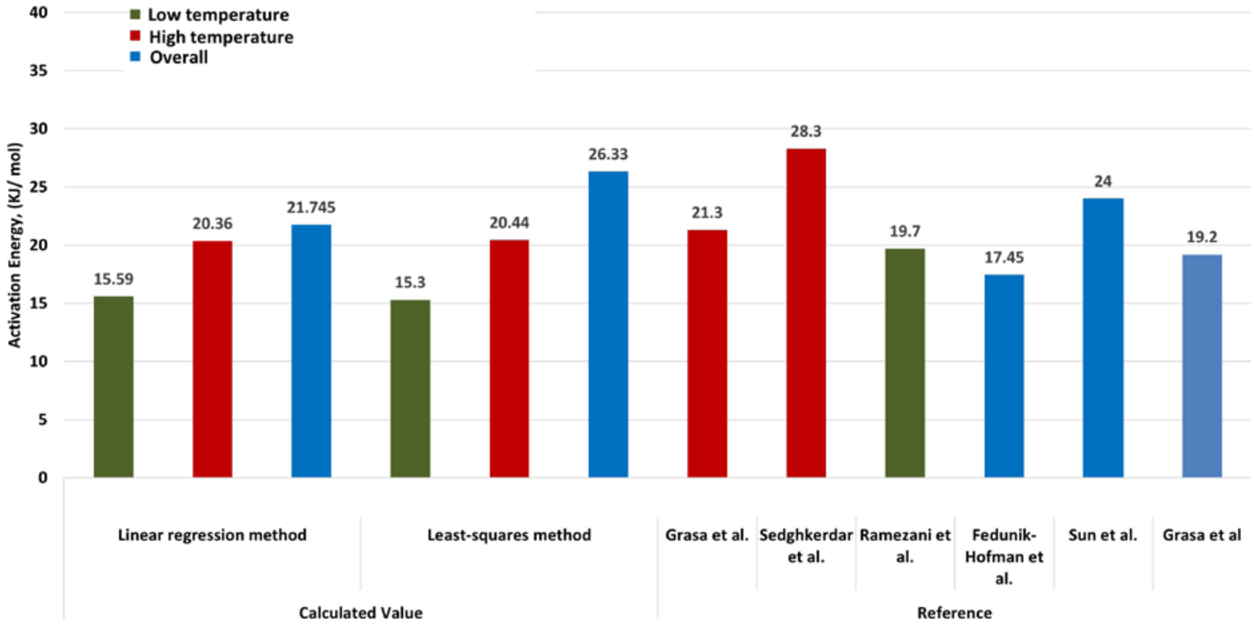


Fig. 8. Comparison of activation energy with reference

Conclusion

The thermogravimetric analysis of the carbonation reaction unveils distinct phases at low and high temperatures, shedding light on the nuanced transformations of *CaO*. Arrhenius plot and activation energy values offer a quantitative understanding of the temperature dependency, indicating higher energy thresholds at elevated temperatures, impacting carbon capture efficiency. Dual-method statistical modeling provides comprehensive analysis of the dynamic nature of the carbonation process, revealing temperature-dependent reaction rates and CO_2 capture capacity.

The findings of this study hold significant potential for the optimization of carbon capture and storage *(CCS)* technologies, with the capacity to enhance efficiency and cost- effectiveness in the management of greenhouse gas emissions. By leveraging these insights, the development of more sustainable energy solutions, particularly in the realms of power generation and industrial applications, stands to benefit. Furthermore, the study's implications extend to the advancement of scientific knowledge in fields such as chemical engineering, environmental science, and thermodynamics, thereby contributing to the progression of these disciplines. Future work could focus on exploring novel sorbent materials with enhanced long-term stability and durability, integrating computational modeling and simulation techniques. This could lead to the development of optimized sorbent materials tailored for diverse applications and sustainable synthesis routes, contributing to comprehensive sustainability and environmental impact analyses.

Contributions from co-authors: Shaon Md Tariqur Rahman made significant contributions to the introduction, methodology, analysis, interpretation of results, discussion, and conclusion. Antor Mahamudul Hashan provided valuable input in the interpretation of results and discussion. Additionally, Sharon Md Mahbubur Rahman played a key role in conducting the literature review and contributing to the methodology.

Вклад соавторов: Шаон Мд Тарикур Рахман внес значительный вклад во введение, методологию, анализ, интерпретацию результатов, обсуждение и заключение. Антор Махамудул Хашан внес ценный вклад в интерпретацию результатов и обсуждение. Кроме того, Шарон Мд Махбубур Рахман сыграл ключевую роль в проведении обзора литературы и внес вклад в разработку методологии.

Conflict of interests: The author states that they have no potential conflict of interest in relation to the study in this paper.

Конфликт интересов: Автор подтверждают, что у них нет потенциального конфликта интересов в связи с исследованием, представленным в данной статье.

REFERENCES

1. *Shaon Md T. R., Bogatova T. F.* Carbon Footprint in Industry and Opportunities to Reduce It // Теплотехника и информатика в образовании, науке и производстве: сборник докладов X Всероссийской научно-практической конференции студентов, аспирантов и молодых учёных (ТИМ'2022) с международным участием (Екатеринбург, 19–20 мая 2022 г.). Екатеринбург: УрФУ, 2022. С. 7–12.
2. *Olivier J., Peters J.* Trends in global CO_2 and total greenhouse gas emissions; 2020 report // PBL Netherlands Environmental Assessment Agency. 2020. P. 85.
3. *Freund P.* Making deep reductions in CO_2 emissions from coal-fired power plant using capture and storage of CO_2 // Proceedings of the Institution of Mechanical Engineers, Part A: Journal of Power and Energy. 2003. Vol. 217, № 1. P. 1–7. https://doi.org/10.1243/095765003321148628
4. *Garg A., Shukla P. R.* Coal and energy security for India: Role of carbon dioxide (CO_2) capture and storage (CCS) // Energy. 2009. Vol. 34, № 8. P. 1032–1041. https://doi.org/10.1016/j.energy.2009.01.005
5. Deep CCS: Moving beyond 90 % carbon dioxide capture / M. N. Dods [et al.] // Environmental Science & Technology. 2021. Vol. 55, № 13. P. 8524–8534. https://doi.org/ 10.1021/acs.est.0c07390
6. *Singh B.* Environmental evaluation of carbon capture and storage technology and large scale deployment scenarios: Doctoral thesis. Norges teknisk-naturvitenskapelige universitet, Fakultet for ingeniorvitenskap og teknologi, Program for industriell okologi, 2011.
7. *Zhang Z. et al.* A novel method for the preparation of CO_2 sorption sorbents with high performance // Applied Energy. 2014. Vol. 123. P. 179–184.
8. *Webley P. A.* Adsorption technology for CO_2 separation and capture: a perspective // Adsorption. 2014. Vol. 20, № 2–3. P. 225–231.
9. *Kuramoto K. et al.* Repetitive Carbonation-Calcination Reactions of Ca-Based Sorbents for Efficient CO_2 Sorption at Elevated Temperatures and Pressures // Ind. Eng. Chem. Res. 2003. Vol. 42, № 5. P. 975–981.
10. *Erans M., Manovic V., Anthony E. J.* Calcium looping sorbents for CO_2 capture // Applied Energy. 2016. Vol. 180. P. 722–742.
11. *Vaz S., Rodrigues De Souza A. P., Lobo Baeta B. E.* Technologies for carbon dioxide capture: A review applied to energy sectors // Cleaner Engineering and Technology. 2022. Vol. 8. P. 100456.
12. *Liu W. et al.* Performance Enhancement of Calcium Oxide Sorbents for Cyclic CO_2 Capture – A Review // Energy Fuels. 2012. Vol. 26, № 5. P. 2751–2767.
13. *Dunstan M. T. et al.* CO_2 Capture at Medium to High Temperature Using Solid OxideBased Sorbents: Fundamental Aspects, Mechanistic Insights, and Recent Advances // Chem. Rev. 2021. Vol. 121, № 20. P. 12681–12745.
14. *Halliday C., Hatton T. A.* Sorbents for the Capture of CO_2 and Other Acid Gases: A Review // Ind. Eng. Chem. Res. 2021. Vol. 60, № 26. P. 9313–9346.
15. *Naeem M. A. et al.* Optimization of the structural characteristics of CaO and its effective stabilization yield high-capacity CO_2 sorbents // Nat Commun. 2018. Vol. 9, № 1. P. 2408.
16. *Chen H. et al.* Novel Optimized Process for Utilization of CaO-Based Sorbent for Capturing CO_2 and SO_2 Sequentially // Energy Fuels. 2012. Vol. 26, № 9. P. 5596–5603.
17. *Bilton M., Brown A. P., Milne S. J.* Investigating the optimum conditions for the formation of calcium oxide, used for CO_2 sequestration, by thermal decomposition of calcium acetate // J. Phys.: Conf. Ser. 2012. Vol. 371. P. 012075.
18. *Arenas Castiblanco E. et al.* A new approach to obtain kinetic parameters of corn cob pyrolysis catalyzed with CaO and $CaCO_3$ // Heliyon. 2022. Vol. 8, № 8. P. e10195.
19. *Pojananukij N. et al.* Synthesis of Alkali Metal/CaO Sorbent for CO_2 Capture at Low Temperature. 2010. Vol. 25, № 1. P. 77.
20. *Ramezani M. et al.* Determination of Carbonation / Calcination Reaction Kinetics of a Limestone Sorbent in low CO_2 Partial Pressures Using TGA Experiments // Energy Procedia. 2017. Vol. 114. P 259–270.
21. *Mohamed M., Yusup S., Bustam M. A.* Synthesis of CaO-based Sorbent from Biomass for CO_2 Capture in Series of Calcination-carbonation Cycle // Procedia Engineering. 2016. Vol. 148. P. 78–85.
22. *Pimenidou P., Dupont V.* Dolomite study for in situ CO_2 capture for chemical looping reforming // International Journal of Ambient Energy. 2015. Vol. 36, № 4. P. 170–182.
23. *Danielsen S. P. O. et al.* Molecular Characterization of Polymer Networks // Chem. Rev. 2021. Vol. 121, № 8. P. 5042–5092.
24. *Haines P. J., Reading M., Wilburn F. W.* Differential Thermal Analysis and Differential Scanning Calorimetry // Handbook of Thermal Analysis and Calorimetry. Elsevier, 1998. Vol. 1. P. 279–361.
25. *Materazzi S., Risoluti R.* Evolved Gas Analysis by Mass Spectrometry // Applied Spectroscopy Reviews. Taylor & Francis, 2014. Vol. 49, № 8. P. 635–665.
26. *Tankov I. et al.* Non-isothermal decomposition kinetics of pyridinium nitrate under nitrogen atmosphere // Thermochimica Acta. 2018. Vol. 665. P. 85–91.
27. *Vyazovkin S. et al.* ICTAC Kinetics Committee recommendations for analysis of multistep kinetics // Thermochimica Acta. 2020. Vol. 689. P. 178597.
28. *Saadatkhah N. et al.* Experimental methods in chemical engineering: Thermogravimetric analysis – TGA // Can J Chem Eng. 2020. Vol. 98, № 1. P. 34–43.
29. *Šesták J., Hubík P., Mareš J. J.* Thermal Physics and Thermal Analysis: From Macro to Micro, Highlighting Thermodynamics, Kinetics and Nanomaterials. Springer, 2017. 585 p.

30. *Wiedemann H.-G., Bayer G.* Trends and applications of thermogravimetry // Inorganic and Physical Chemistry. Berlin, Heidelberg: Springer, 1978. P. 67–140.
31. *Никитин А. Д.* Влияние водяного пара на физико-химические процессы в парогазовой установке с внутрицикловой газификацией твердого топлива: диссертация на соискание ученой степени кандидата технических наук: 01.04.14: Thesis. б. и., 2021.
32. *Sun Z. et al.* Density functional theory study on the thermodynamics and mechanism of carbon dioxide capture by CaO and CaO regeneration // RSC Adv. The Royal Society of Chemistry, 2016. Vol. 6, № 45. P. 39460–39468.
33. *Li Z., Sun H., Cai N.* Rate Equation Theory for the Carbonation Reaction of CaO with CO_2 // Energy Fuels. American Chemical Society, 2012. Vol. 26, № 7. P. 4607–4616.
34. *Perrin C. L.* Linear or Nonlinear Least-Squares Analysis of Kinetic Data? // J. Chem. Educ. American Chemical Society, 2017. Vol. 94, № 6. P. 669–672.
35. *Rahman S. M. T., Hashan A. M., Rahman S. M. M.* Numerical Analysis of the Equilibrium Composition and Structural Features of Coal Combustion Products: preprint. In Review, 2024.
36. *Marland G., Rotty R. M.* Carbon dioxide emissions from fossil fuels: a procedure for estimation and results for 1950–1982 // Tellus B: Chemical and Physical Meteorology. 1984. Vol. 36, № 4. P. 232.
37. *Grasa G. et al.* Application of the random pore model to the carbonation cyclic reaction // AIChE Journal. 2009. Vol. 55, № 5. P. 1246–1255.
38. *Sedghkerdar M. H., Mahinpey N., Ellis N.* The effect of sawdust on the calcination and the intrinsic rate of the carbonation reaction using a thermogravimetric analyzer (TGA) // Fuel Processing Technology. 2013. Vol. 106. P. 533–538.
39. *Fedunik-Hofman L., Bayon A., Donne S. W.* Comparative Kinetic Analysis of $CaCO_3$/CaO Reaction System for Energy Storage and Carbon Capture: 21 // Applied Sciences. Multidisciplinary Digital Publishing Institute, 2019. Vol. 9, № 21. P. 4601.
40. *Sun P. et al.* Determination of intrinsic rate constants of the CaO-CO_2 reaction // Chemical Engineering Science. 2008. Vol. 63, № 1. P. 47–56.

ИНФОРМАЦИЯ ОБ АВТОРАХ

Шаон Мд Тарикур Рахман – бакалавр ядерных наук и инженерии Военного института науки и технологии, Дакка, Бангладеш, в 2020 году. Получил степень магистра по специальности «Теплоэнергетика и теплотехника» в Уральском федеральном университете, Екатеринбург, Российская Федерация. В настоящее время защищает докторскую диссертацию в Институте новых материалов и технологий (ИНМТ) того же университета.
С ним можно связаться по электронной почте:
potterh274@gmail.com
Телефон +7 (962) 323-75-50
ORCID: 0009-0007-8912-7604

Антор Махамудул Хашан – степень магистра в области инновационных программных систем «Проектирование, разработка и применение» Национального университета науки и технологий «МИСиС», Москва, Российская Федерация, в 2020 году. В настоящее время является аспирантом (Ph. D.) и работает ассистентом в Институте фундаментального образования Уральского федерального университета, Екатеринбург, Российская Федерация.
С ним можно связаться по электронной почте:
hashan.antor@gmail.com
ORCID: 0000-0001-7926-9245.

Шаон Мд Махабубур Рахман – в настоящее время получает степень бакалавра в области текстильной инженерии в Университете инженерии и технологии Кхулны, Кхулна, Бангладеш.
С ним можно связаться по электронной почте:
cssharon7@gmail.com
Телефон +8801982603947
ORCID: 0009-0001-2904-9022

AUTHOR'S INFORMATION

Shaon Md Tariqur Rahman – B. Sc. in Nuclear Science and Engineering from Military Institute of Science and Technology, Dhaka, Bangladesh in 2020. He completed his Master's degree in Thermal Power and Heat Engineering at Ural Federal University, Yekaterinburg, Russian Federation. Currently, he is pursuing a Ph.D. in the Institute of New Materials and Technologies (INMT) at the same university.

He can be contacted at Email:
potterh274@gmail.com
Telephone +7 (962) 323-75-50
ORCID: 0009-0007-8912-7604

Antor Mahamudul Hashan – M. S. c. degree in Innovative Software Systems: Design, Development & Application from National University of Science and Technology «MISIS», Moscow, Russian Federation in 2020. Currently he is a graduate student (Ph.D.) and working as a Assistant in the Institute of Fundamental Education at Ural Federal University, Yekaterinburg, Russian Federation.

He can be contacted at Email:
hashan.antor@gmail.com
ORCID: 0000-0001-7926-9245

Sharon Md Mahabubur Rahman – Currently, he is pursuing B. Sc. in Textile Engineering from Khulna University of Engineering and technology, Khulna, Bangladesh.

He can be contacted at Email:
cssharon7@gmail.com
Telephone +8801982603947
ORCID: 00090001-2904-9022.