Draft Publikasi_Internasional_09012024_Parafrase#4

by Ely S

Submission date: 22-Jan-2024 11:35PM (UTC-0800)
Submission ID: 2182917948
File name: Draft_Publikasi_Internasional_09012024_Parafrase_4.docx (136.23K)
Word count: 2323
Character count: 11995

Kinetic Study of Steam Gasification Pattukku Sub-bituminous char with CaO catalyst

Takdir Syarif* , Andi Aladin, Munira, Gusnawati
[1]Chemical Engineering Department, Faculty of Industrial Technology, Universitas Muslim Indonesia
Jl. Urip Sumoharjo Km. 05 Makassar

Abstract

To study the mechanism of gasification process, it is very important to know the kinetic parameters. Mathematical models can be used to obtain the gasification process's reaction rate. Although mathematical models cannot give exact results, they can quantitatively show the effect of feedstock and other process constants. This study aimed to obtain the reaction rate constant using random pore and volumetric models. Based on the random pore model calculation obtained, reaction rate constant is $k = 0.543\exp\left(-\frac{29.879}{RT}\right)$ (kJ/mol) (catalyst mass 15 grams), and SSE of 0.46% were obtained. Meanwhile, by using a volumetric model, $k = 0.0499\exp\left(-\frac{27.582}{RT}\right)$ (kJ/mol) (catalyst mass 15 grams) and SSE of 8.76% were obtained.

Keywords: kinetic parameters, random pore model, reaction rate, steam gasification, volumetric model.

1. Introduction

Clean energy and alternative energy is one of the main themes of several studies on sustainable energy development. As petroleum reserves are decreasing, the advancement of alternative energy is essential to prevent a fuel crisis [1–3]. Indonesia has plenty of coal reserves, but its quality is low. Therefore, its use needs to be improved. One method that can be used to improve the quality of coal as a fuel is gasification. Gasification is an effective and accurate technique for changing solid carbon materials into electricity-generating gas or synthesis gas. These gases can be used for electricity generation, thermal energy production, or synthetic precursors. [4, 6].

* Corresponding author.
E-mail address: takdir_syarif@umi.ac.id

Understanding the influence of feedstock, operational parameters, and interacting physical and chemical mechanisms during the gasification process is the basis for optimal gasifier design [5, 6, 7].

Reaction rate are very important parameters to obtain information about the mechanism of reaction in the gasification process [8]. Several researchers have investigated the influence of kinetic variables of gasification systems. Babu and Sheth [11] predicted steady state temperature and composition profiles for the reducing region in biomass gasification. They concluded that the char reactivity in the the reduction region can be directly explained by the char reactivity coefficient. Goebel *et al*. [10] develop mathematical models from mass and energy balance, chemical equilibrium, and Langmuir-Hinshelwood to explain coal kinetic response. From this study, Gobel *et al*. [10] concluded that coal reaction kinetics is based on a mathematical model based on the Langmuir-Hinshelwood equation, mass and energy balance in simple single-dimensional flow and chemical equilibrium at the gas phase. We conclude that it can be explained by. D. P. Ye and J. B. Agnew [11] studied the effect of active cations (Na, K, Ni, Ca) for the reactivity of low quality coal from South Australia. These experiments showed that acid washing of coal causes the loss of carboxyl functional groups, and removing or adding active cations will change the reactivity of the coal. Furthermore, for the same anion, catalytic activity increases in the order of Na > K > Ca > Ni.

Several scientists has developed reaction kinetic equations to analyze the reaction kinetics of gasification, for example random pore model (RPM), volume model (VM), and shrink core model (SCM). However, when evaluating the reaction rate constant of coal gasification processes, the use of random pore models gives better results than homogeneous models [12].

In this study, volumetric and random pore models were applied to evaluate the reaction rate constants of steam gasification. Gasification is carried out in an updraft reactor with different temperatures and atmospheric pressure, namely 600, 700, and 800 °C. The mass of charcoal used was 10 grams and the mass of CaO catalyst was varied as 0, 5, 10, and 15 grams. The random pore model results were compared with the volumetric model

2. Kinetic Models

2.1. Volumetric Model (VM)

This model assumes that all active sites are homogeneously located on the coal surface and the particle size is kept as constant as possible during gasification [13],[11]. Based on this assumption, the rate of reaction can be represented as:

$$\frac{dX_A}{dt} = k_{VM}\left(1 - X_A\right) \tag{1}$$

Equation (1) could be integrated to give equation (2)

$$\int_0^X \frac{dX_A}{\left(1 - X_A\right)} = \int_0^t k_{VM}\, dt$$

$$X_A = 1 - \exp\left(-k_{VM} t\right) \tag{2}$$

where k_{VM} is expressed in The Arrhenius equation as below:

$$k_{VM} = k_o \exp\left(-\frac{Ea}{RT}\right) \tag{3}$$

Furthermore, equation (3) could be expressed in linear expression as follow:

$$\ln k_{VM} = \ln k_o - \left(\frac{Ea}{R}\right)\frac{1}{T} \tag{4}$$

The activated energy (E_a) and collision factor (k_o) can be obtained by plotting $\ln k_{VM}$ versus $\frac{1}{T}$.

2.2. Random Pore Model (RPM)

This model supposes that reaction starts in the pore surface and then a gaseous product layer forms near the coal surface. The reactants diffuse to the reaction surface where the reaction occurs through the gas-producing layer. This model takes into account the changes in physical structure during gasification [16]. The reaction rate was expressed in the following format:

$$\frac{dX_A}{dt} = k_{RPM}\left(1 - X_A\right)\sqrt{1 - \psi\left(1 - X_A\right)} \tag{5}$$

where k_{RPM} is expressed as follow:

$$k_{RPM} = k_o \exp\left(-\frac{Ea}{RT}\right) \tag{6}$$

3. Result and discussion

3.1. Evaluation of the kinetic parameters

3.1.1. Volumetric model

Figure 5a-c shows correlations of char conversion and time of reaction for gasification using charcoal and steam at temperatures of 600, 700, and 800°C for 60 minutes and mass of CaO 0, 5, 10, and 15 grams. Dashed lines represent calculated results, and dotted symbols represent experimental results.

The volumetric model is only fit for reaction time less than 45 minutes or char conversion smaller than 50%, as shown in Fig. 5a-c. It is indicated that the volumetric model cannot fully express this process. This experiment corresponds to the work of previous research [16], [17].

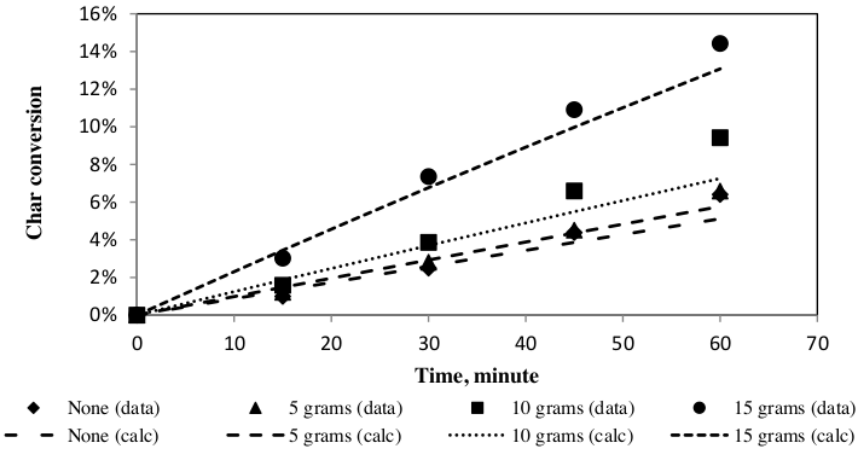

Fig. 5a. Comparison of conversion chart of observation results with calculation results using volumetric model for catalyst mass variation of 0, 5, 10, and 15 grams and temperature of 600 C.

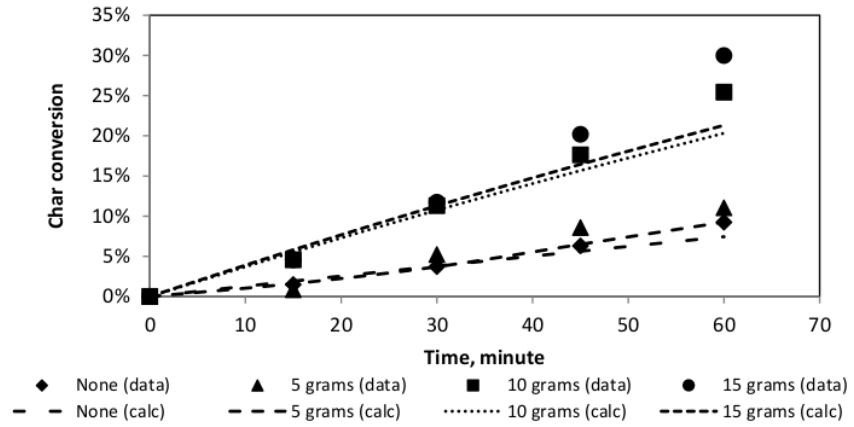

Fig. 5b. Comparison of conversion chart of observation results with calculation results using volumetric model for catalyst mass variation of 0, 5, 10, and 15 grams and temperature of 700 °C.

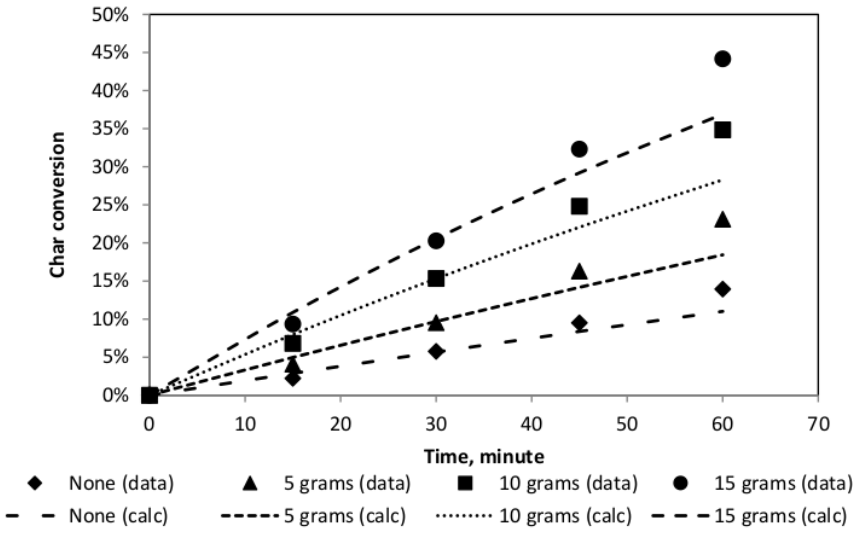

Fig. 5c. Comparison of conversion chart of observation results with calculation results using volumetric model for catalyst mass variation of 0, 5, 10, and 15 grams and temperature of 800 °C.

The collision factor (ko) and activation energy (Ea) will be determined by plotting lnk k versus 1/T, as shown in Figure 6. These plots were obtained by calculating the reaction rate constants from three different temperatures.

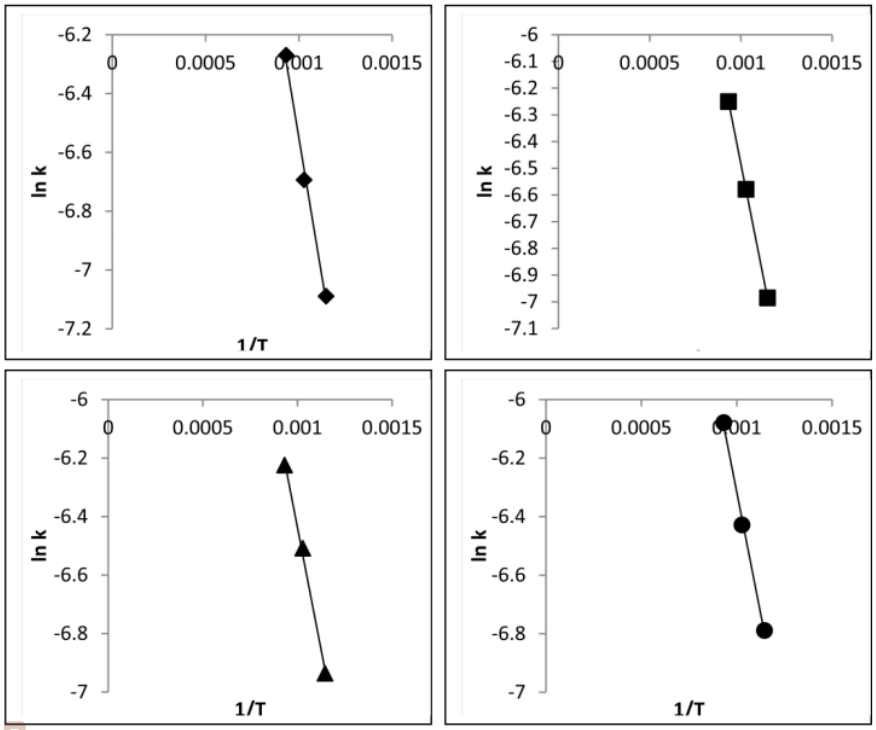

Fig. 6. Plot of ln k vs 1/T for steam gasification at 0, 5, 10, 15 grams of CaO catalyst using volumetric model.

Table 2 shows the rate parameters of steam gasification obtained from Figure 6. Table 2 shows that the activation energies for coal gasification of 0, 5, 10, and 15 grams CaO catalyst are 31.757 kJ/mol, 28.607 kJ/mol, 27.797 kJ/mol, and 27.7 kJ/mol, namely. It shows that it was 582 kJ/mol. When 5, 10, and 15 grams of CaO catalyst were added to 10 g of charcoal, the activated energy decreased for 3.15 kJ/mol, 3.96 kJ/mol, and 4.175 kJ/mol, respectively. Therefore, presence of CaO catalyst can increase the rate of steam gasification reaction. Additionally, Table 2 also considers the activation energy at 10 grams of Ca catalyst, which is close to 15 grams of CaO catalyst.

Table 2. Kinetic parameters in steam gasification process at 600 °C to 800 °C for 60 minutes using volumetric model (VM).

Mass of Ca catalyst (grams)	Activated energy ($kJ.mol^{-1}$)	Collision factor (min^{-1})	Equation of reaction kinetics constant
0	31.757	0.0652	$k = 0.0652 \exp\left(-\frac{31.757}{RT}\right)$
5	28.607	0.0453	$k = 0.0453 \exp\left(-\frac{28.607}{RT}\right)$
10	27.797	0.0477	$k = 0.0477 \exp\left(-\frac{27.797}{RT}\right)$
15	27.582	0.0499	$k = 0.0499 \exp\left(-\frac{27.582}{RT}\right)$

3.1.2. Random pore model

Figure 7a-c shows the steam gasification at temperatures of 600°C to 800°C at 60 minutes with CaO catalyst masses of 0, 5, 10, and 15 grams using the random pore model. shows the correlation between reaction time and carbon conversion rate..

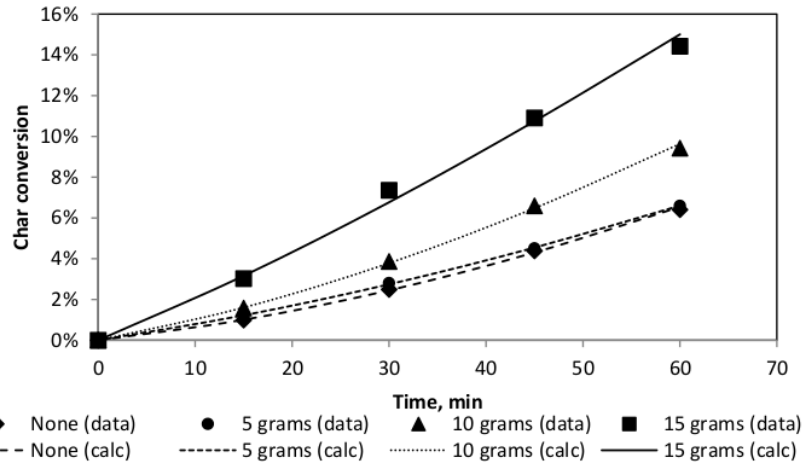

Fig. 7a. Comparison of conversion chart of observation results with calculation results using random pore model for catalyst mass variation of 0, 5, 10, and 15 grams and temperature of 600 °C.

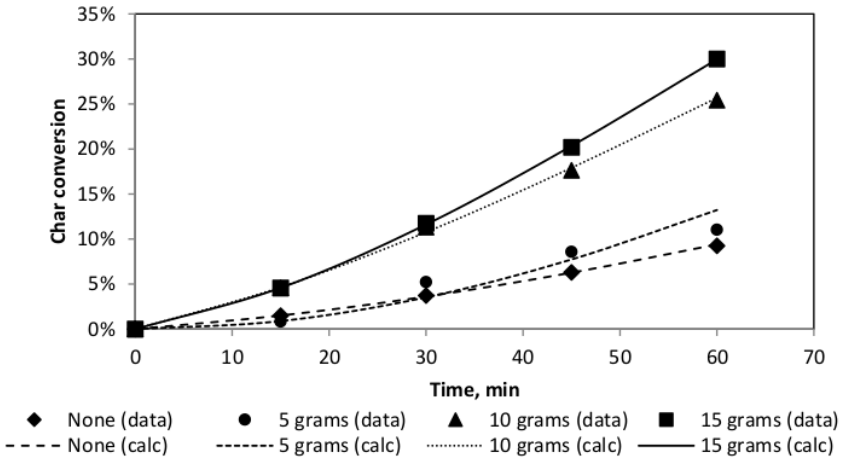

Fig. 7b. Comparison of conversion chart of observation results with calculation results using random pore model for catalyst mass variation of 0, 5, 10, and 15 grams and temperature of 700 °C.

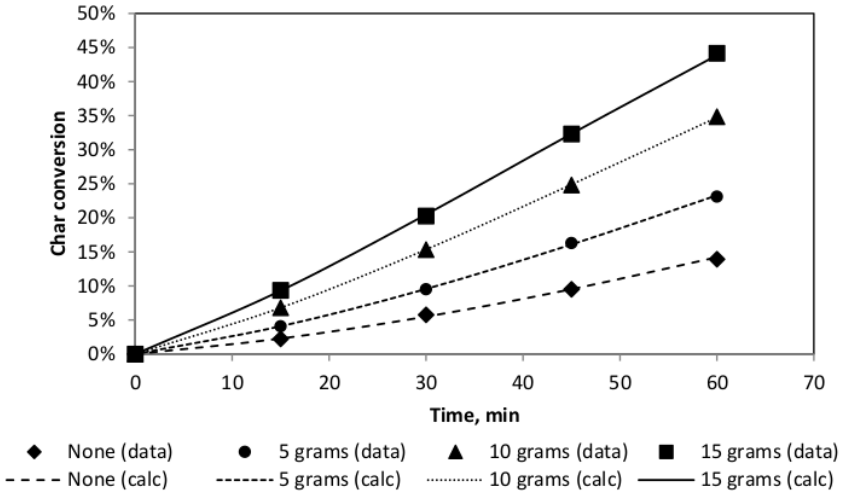

Fig. 7c. Comparison of conversion chart of observation results with calculation results using random pore model for catalyst mass variation of 0, 5, 10, and 15 grams and temperature of 800 °C.

As shown in Figure 7a-c, the carbonization transformation from the calculation results using the random pore model is in good agreement with the results obtained from the experimental data. These results indicate that the

changing pore structure during charcoal gasification can affect the reactivity of charcoal during the reaction. This experimental result is consistent with the study of Sangtong-Ngam and Narasingha [12].

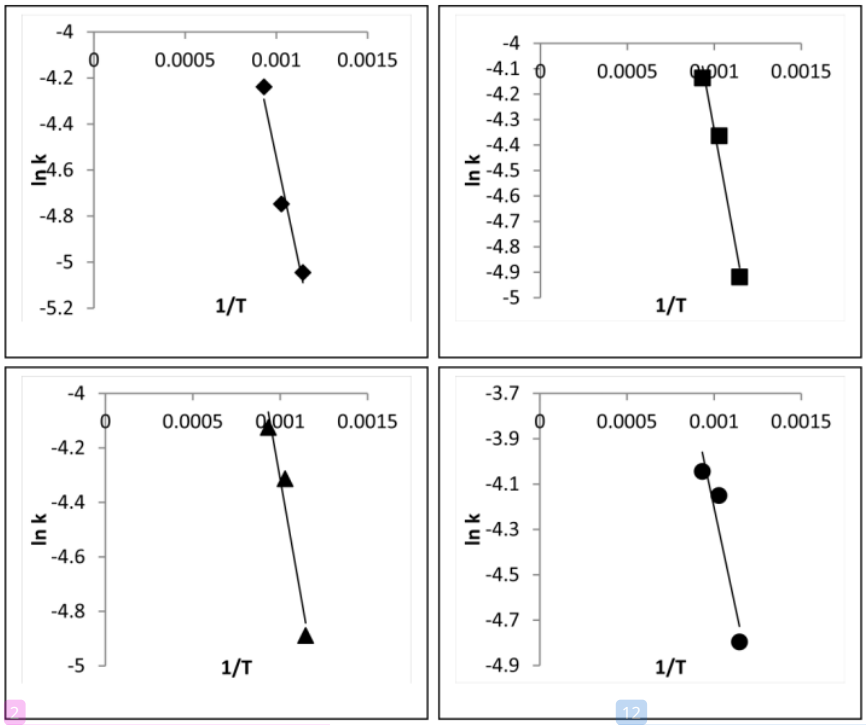

Fig. 8. Plot of ln k vs 1/T for steam gasification at (◆) 0 grams, (■) 5 grams, (▲) 10 grams, (●) 15 grams of Ca catalyst using random pore model.

Figure 8 shows the relationship between 1/T and lnk for steam gasification with four different CaO catalyst masses. A random pore model determined the reaction rate constants for three different temperatures. Table 3 presents activated energies and collision factor obtained from Figure 8.

Table 3. Kinetic parameters in steam gasification process at 600 °C to 800 °C for 60 minutes using random pore model (RPM).

Mass of Ca catalyst (grams)	Activated energy ($kJ.mol^{-1}$)	Collision factor (min^{-1})	Equation of reaction kinetics constant
0	31.002	0.0662	$k = 0.0662\exp\left(-\frac{31.002}{RT}\right)$
5	30.786	0.528	$k = 0.528\exp\left(-\frac{30.786}{RT}\right)$
10	30.140	0.532	$k = 0.532\exp\left(-\frac{30.140}{RT}\right)$
15	29.879	0.543	$k = 0.543\exp\left(-\frac{27.879}{RT}\right)$

Table 2 shows that without CaO catalyst, the activation energies of 5, 10, and 15 grams are 31.002 kJ/mol, 30.670 kJ/mol, 30.140 kJ/mol, and 29.879 kJ/mol, namely.

This shows that the addition of 5, 10, and 15 grams of catalyst can reduce the activation energy by 0.216 kJ/mol, 0.862 kJ/mol, and 1.123 kJ/mol, namely. Thus, the addition of CaO can increase the reaction rate in charcoal gasification.

3.2. Comparison of the random pore and the volumetric model

Figures 5a-5c show that the volumetric model is only suitable for reaction times less than 45 min. On the other hand, Figures 7a–7c show that the random pores fit the experimental data well.

Table 4 compares the standard errors of both the volumetric pore model and random pore model. Table 4 shows that the calculated standard error with random pore model is lower than volumetric model under all conditions. Based on these results, it can be said that the random pore equation has better precision than the volumetric model.

Table 4. Comparison standard error between volumetric model and random pore model

Mass of Ca catalyst (gr)	Error (%)					
	VM			RPM		
	600 ºC	700 ºC	800 ºC	600 ºC	700 ºC	800 ºC
0	13.50	12.27	12.75	1.39	1.38	1.85
5	8.40	32.61	11.38	0.83	13.93	0.50
10	12.40	11.47	9.46	1.51	1.92	0.15
15	7.94	15.72	8.76	3.61	0.46	0.46

4. Conclusions

CaO catalyst can improve the conversion rate of coal in steam gasification. Activation energy can be reduced by using a CaO catalyst. Using random pore model, the charcoal conversion from the calculated results is consistent with the charcoal conversion from the experiment data at a temperature of 800 °C and SSE of 0.46% at 15 g of catalyst. On the other side, volumetric model is only suitable for response time is less than 45 minutes with the SSE is 8.76%.

References

[1] M. Zile, "Biomass/Geothermal Power Station Energy Management Computer Program Using Artificial Neural Networks," *Int. J. Tech. Phys. Probl. Eng.*, vol. 13, no. 4, pp. 147–151, 2021.

[2] A. M. Hashimov, Z. A. Mammadov, N. M. Tabatabaei, R. E. Kerimov, R. N. Rahmanov, and N. R. Rahmanov, "Assessment and optimal combined utilization of renewable energy sources in the remote inhabited locations," *Int. J. Tech. Phys. Probl. Eng.*, vol. 12, no. 4, pp. 82–90, 2020.

[3] M. Rafiei and M. S. Zadeh, "Optimization of a typical biomass fueled power plant using Genetic algorithm and binary particle swarm optimization," *2012 Proc. 17th Conf. Electr. Power Distrib. EPDC 2012*, no. June, pp. 15–21, 2012.

[4] Q. Xu, S. Pang, and T. Levi, “Reaction kinetics and producer gas compositions of steam gasification of coal and biomass blend chars, part 1 : Experimental investigation,” *Chem. Eng. Sci.*, vol. 66, no. 10, pp. 2141–2148, 2011.

[5] A. Molina and F. Mondrago, “Reactivity of coal gasification with steam and CO2,” *Fuel*, vol. 77, no. 15, pp. 1831–1839, 1998.

[6] M. Materazzi, P. Lettieri, L. Mazzei, R. Taylor, and C. Chapman, “Thermodynamic modelling and evaluation of a two-stage thermal process for waste gasification,” *Fuel*, vol. 108, pp. 356–369, 2013.

[7] J. Rezaiyan and N. P. Cheremisinoff, *Gasification Technologies*, 1st ed. Francis: CRC Press, 2005.

[8] C. Xu *et al*., “Kinetic models comparison for steam gasification of coal/biomass blend chars,” *Bioresour. Technol.*, vol. 171, pp. 253–259, 2014.

[9] B. V. Babu and P. N. Sheth, “Modeling and simulation of reduction zone of downdraft biomass gasifier: Effect of char reactivity factor,” *Energy Convers. Manag.*, vol. 47, no. 15–16, pp. 2602–2611, 2006.

[10] B. Gøbel, U. Henriksen, T. K. Jensen, B. Qvale, and N. Houbak, “The development of a computer model for a fixed bed gasifier and its use for optimization and control,” vol. 98, pp. 2043–2052, 2007.

[11] D. P. Ye, J. B. Agnew, and D. K. Zhang, “Gasification of a South Australian low-rank coal with carbon dioxide and steam : kinetics and reactivity studies,” *Fuel*, vol. 77, no. 11, pp. 1209–1219, 1998.

[12] K. Sangtong-Ngam and M. H. Narasingha, “Kinetic Study of Thai-lignite Char Gasification Using the Random Pore Model,” *Thammasat Int. J. Sc. Tech.*, vol. 13, no. 3, pp. 17–26, 2008.

[13] J. Tang, X. Wu, and J. Wang, “Kinetic study of steam gasification of two mineralogically different lignite chars : An active site / intermediate model,” *Fuel*, vol. 141, pp. 46–55, 2015.

[14] S. K. Bhatia and D. D. Perlmutter, “A Random Pore Model for Fluid-Solid Reactions : 1 . Isothermal , Kinetic Control,” *AIChE J.*, vol. 26, no. 3, pp. 379–386, 1980.

[15] I. Matsui, D. Kunii, and T. Furusawa, “Study of Char Gasification by Carbon Dioxide . 1 . Kinetic Study by Thermogravimetric Analysis,” pp. 91–95, 1987.

Draft Publikasi_Internasional_09012024_Parafrase#4

ORIGINALITY REPORT

7%	6%	5%	1%
SIMILARITY INDEX	INTERNET SOURCES	PUBLICATIONS	STUDENT PAPERS

PRIMARY SOURCES

1	repository.umi.ac.id Internet Source	1%
2	link.springer.com Internet Source	1%
3	M Rabinowitz, J Sinclair, L DeSalle, R Haselkorn, H H Swift. "Isolation of deoxyribonucleic acid from mitochondria of chick embryo heart and liver.", Proceedings of the National Academy of Sciences, 1965 Publication	1%
4	vtechworks.lib.vt.edu Internet Source	1%
5	www.researchgate.net Internet Source	1%
6	www.qucosa.de Internet Source	<1%
7	aip.scitation.org Internet Source	<1%
8	ejournal.undip.ac.id Internet Source	

		<1 %
9	Duan, Wenjun, Qingbo Yu, Tianwei Wu, Fan Yang, and Qin Qin. "The steam gasification of coal with molten blast furnace slag as heat carrier and catalyst: Kinetic study", International Journal of Hydrogen Energy, 2016. Publication	<1 %
10	delibra.bg.polsl.pl Internet Source	<1 %
11	media.neliti.com Internet Source	<1 %
12	www.ijert.org Internet Source	<1 %
13	Takdir Syarif, Hary Sulistyo, Wahyudi Budi Sediawan, Budhijanto. "Thin Reaction Zone Model for Evaluating the Mechanisms that Control the Char Gasification Process: 1. Quasi-steady State", Arabian Journal for Science and Engineering, 2017 Publication	<1 %
14	Eric A. Morris, Rex Choi, Ti Ouyang, Charles Q. Jia. "Constant Thickness Porous Layer Model for Reaction between Gas and Dense Carbonaceous Materials", Industrial & Engineering Chemistry Research, 2012	<1 %

Publication

15	Narendra Sadhwani, Sushil Adhikari, Mario R. Eden, Zhouhong Wang, Ryan Baker. "Southern pines char gasification with CO2—Kinetics and effect of alkali and alkaline earth metals", Fuel Processing Technology, 2016 Publication	<1%

Exclude quotes	Off	Exclude matches	Off
Exclude bibliography	On		