Metallurgical Coke Gasification by Carbon Dioxide under Nonisothermal Conditions: A Kinetic Study

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ABSTRACT: Metallurgical coke gasification by carbon dioxide was kinetically investigated through the use of thermogravimetric analysis under nonisothermal conditions. The results showed that the activation energy, gained by the Cai–Chen iterative model-free method, was estimated to be 183.15 kJ·mol⁻¹. Notwithstanding, the mechanism function \( f(\alpha) \) cannot be directly determined due to the fact that \( f(\alpha) \) and the pre-exponential factor \( A_p \) were lumped together as \( [A_p f(\alpha)] \); this situation may be tackled by means of the master-plot methods. The most probable mechanism function, determined by the Mélek master-plot method (based on \( Z(\alpha) \) master plots), was discovered to be the Johnson–Mehl–Avrami equation. The usefulness of the compound kinetic calculation technique founded upon complemental application of the Mélek master-plot and Cai–Chen model-free methods in estimating reaction kinetics of metallurgical coke gasification was verified. The comparison between original and reconstructed kinetic curves judged the accuracy of the gained kinetic parameters. By means of gained nonisothermal kinetic results, the forecasting of kinetic curves in isothermal as well as nonisothermal conditions was performed. In this work, new kinetic equations were presented and applied to reproducing and forecasting kinetic curves.

INTRODUCTION

The characterization of the investigated reactive behavior is commonly exhibited in the form of a so-called kinetic triplet (namely, the pre-exponential Arrhenius factor, the conversion factor, and the activation energy), which is the classic result of an ordinary kinetic study. The kinetic triplet is widely studied, probably because it can be used for describing the reaction process, forecasting the reactive behavior beyond the scope of the experimental temperature, enabling the rational planning of experimental programs, and designing gas–solid contacting systems. Ordinarily, it is not easy for one to derive the most precise kinetic triplet from the kinetic data. Under dynamic regimes, the rate of conversion is always affected by the conversion factor as well as the reaction constant; consequently, when evaluating a kinetic triplet, one will confront a situation: an imprecise evaluation of any constituent of the triplet would lead other constituents of the triplet to be incorrectly evaluated. Accordingly, during a kinetic computation, one should try one’s best to accurately evaluate all constituents of the triplet, especially the constituent that is first evaluated and afterward is used in the evaluation of other constituents. The first evaluated kinetic parameter, in the present work, is the activation energy, of which the calculation procedures were widely developed and could be generally categorized into two types: model-free and model-fitting methods. The model-free methods are universally accepted to be more dependable than model-fitting ones. An iterative linear integral isoconversional method, a model-free method published by Cai et al. and designated as the Cai–Chen method, was adopted.

This present study is aimed specifically at showing the usefulness of a compound kinetic approach, founded upon complemental application of the master-plot method as well as the model-free method, in deriving the kinetic triplet from the experimental thermoanalytical (TA) data of carbon dioxide gasification of metallurgical coke under nonisothermal conditions. It is expected that the present research can be helpful for comprehending the process of metallurgical coke gasification and designing as well as operating the gasifier.

EXPERIMENTAL SECTION

The metallurgical coke, which Ansteel (China) generously supplied, of which the properties are described in Table 1, was used as the material for the present research. In the present study, all experimental tests were performed in a SETSYS Evolution thermogravimetric analyzer (TGA) bought from Setaram Co., France. Prior to running each gasification test, the
heating rates of 2, 5, 10, and 15 K respectively. The four selected heating rates, at which the samples were heated from the ambient temperature to 1500 K under high-purity carbon dioxide (which is the gasification agent and of which the gas flow rate is 40 mL·min⁻¹), are 2, 5, 10, and 15 K·min⁻¹. So that the results of all tests can be reproduced, in the present work each test was redone at least twice.

The carbon conversion can be defined as the next equation, whereby one can change the experimental thermogravimetry curves into curves of α vs T.

\[
\alpha = \frac{m_0 - m}{m_0 - m_\infty}
\]  
(1)

where \(m_0\), \(m\), and \(m_\infty\), are the initial, immediate, and final masses, respectively.

Figure 1 displays the α vs T curves of the nonisothermal gasification of metallurgical coke at constant heating rates; from this figure, it can be seen that the more the heating rate increases, the higher temperature the curve of α vs T transfers to.

### THEORETICAL BASIS

The following rate equation widely represents the kinetics of the gas–solid reactions (e.g., carbon gasification).

\[
\frac{d\alpha}{dt} = \beta \frac{d\alpha}{dT} = k(f(\alpha)) = Af(\alpha) \exp\left(-\frac{E}{RT}\right)
\]  
(2)

where \(\alpha\) is the carbon conversion, \(t\) is the time, \(A\) is the frequency factor (i.e., the pre-exponential Arrhenius factor), \(k\) is the reaction constant, \(E\) is the activation energy, \(T\) is the temperature, \(R\) is the gas constant, \(f(\alpha)\) is the conversion factor, also referred to as the mechanism function, and \(\beta\) is the heating rate expressed as \(dT/dt\) or \((T - T_0)/t\) (the parameter \(T_0\) is the initial temperature).

Integrating eq 2 results in the integral form of \(f(\alpha)\)

\[
G(\alpha) \approx \frac{AE}{\beta R} p(u) = \frac{AE}{\beta R} \exp\left(-\frac{u}{u}\right)
\]

\[
= \frac{ART^2}{\beta E} h(u) \exp(-u)
\]  
(3)

where \(I(E, T)\) is identical to \(\int_0^{u} \exp[-E/(RT)]dT\), \(u\) is identical to \(E/(RT)\), and \(p(u)\) is a more greatly performed temperature integral than \(I(E, T)\) and is identical to \(\int_0^{u} u^{-2} \exp(-u)du\). Like both \(I(E, T)\) and \(p(u)\), these functions \((\pi(u)\) h(u)) have numeric rather than analytic solutions.

Accordingly, within a small range of conversion, from eq 3 it follows

\[
G(\alpha, \alpha - \Delta\alpha) = \frac{A e^{RT_{\alpha}}}{\beta E_{\alpha}} \left[ h(u_{\alpha}) - \frac{1}{u_{\alpha - \Delta\alpha}} h(u_{\alpha - \Delta\alpha}) \right] \exp(-u_{\alpha - \Delta\alpha})
\]  
(4)

where the subscript \(\alpha\) (or \(\alpha - \Delta\alpha\)) signifies the values when the conversion is identical to \(\alpha\) (or \(\alpha - \Delta\alpha\)).

On the basis of the above equation and on the presumption that the value of \(E\) stays invariable within the conversion interval of \(\alpha - \Delta\alpha\), a fixed conversion and a run of linear nonisothermal tests carried out with various heating rates \(\beta_i\) (i = 1, 2, ..., n), the expression of the Cai–Chen method is deduced

\[
\frac{T_{\alpha}}{\alpha - \Delta\alpha} \ln \frac{h(u_{\alpha}) - \frac{1}{u_{\alpha - \Delta\alpha}} h(u_{\alpha - \Delta\alpha})}{h(u_{\alpha - \Delta\alpha})} = \frac{E_{\alpha}}{RT_{\alpha}} + \ln \frac{R}{E_{\alpha} \int_{\alpha - \Delta\alpha}^{\alpha} \frac{d\alpha}{h(\alpha)} + \frac{E_{\alpha}}{RT_{\alpha}}}
\]  
(5)

An iterative procedure, described in detail in the literature, is applied because in eq 5 the left-hand side term, which against reciprocal temperature is supposed to result in a direct line whose slope lets activation energy be calculated (see eq 6), depends on and varies with \(E_{\alpha}\).

\[
E_{\alpha} = -R S_{\alpha}
\]  
(6)

where \(S_{\alpha}\) is the slope of the plot of the left-hand side term in eq 5 vs reciprocal temperature.

In case of the awareness of the activation energy, a method, put forward by Mälek and thus referred to as the Mälek method, is helpful in finding out the mechanism function in nonisothermal conditions; the auxiliary function \(Z(\alpha)\) employed in this method can be denoted by the next two equations.

\[
Z(\alpha) = \frac{d\alpha}{dt} \frac{\pi(u)T}{\beta}
\]  
(7)

\[
Z(\alpha) = f(\alpha)G(\alpha)
\]  
(8)
A sequence of TA curves recorded under various heating rates is applied to acquiring experimental \(Z(\alpha)\) values that are produced by plotting the right-hand side term in eq 7 vs \(\alpha\). After the substitution of the often-quoted mechanism functions into eq 8, plotting the right-hand side of eq 8 vs \(\alpha\) produces theoretical \(Z(\alpha)\) curves. Having compared the experimental and theoretical \(Z(\alpha)\) curves, one is able to acquire the most probable mechanism function whose corresponding theoretical \(Z(\alpha)\) curve corresponds closely to the experimental \(Z(\alpha)\) curve of the investigated reaction process.

With the purpose of reproducing nonisothermal TA curves within the experimental heating rate range, in addition to \(E_a\) values, which have been known, the term \(\Delta [A_\alpha f(\alpha)]\) could be calculated via the following expression.\(^{17}\)

\[
\Delta [A_\alpha f(\alpha)] = A_\alpha f(\alpha) - A_{\alpha - \Delta \alpha} f(\alpha - \Delta \alpha)
\]

\[
= \beta \Delta \alpha \sum_{j=0}^{\alpha - \Delta \alpha} \int_{T_{j,i}}^{T_{j+\Delta \alpha,i}} \exp\left(-\frac{E_a}{RT}\right) dT^{-1}
\]

(9)

According to the above equation, if we use lowercase \(j\) to represent a left endpoint of a small interval of conversions, we get

\[
A_\alpha f(\alpha) = \beta \Delta \alpha \sum_{j=0}^{\alpha - \Delta \alpha} \int_{T_{j,i}}^{T_{j+\Delta \alpha,i}} \exp\left(-\frac{E_a}{RT}\right) dT^{-1}
\]

(10)

Substitution of both \(E_a\) and \(\Delta [A_\alpha f(\alpha)]\) into eq 2, after rearranging, yields the following equation, which can be used for reproducing the original nonisothermal experimental data and forecasting nonisothermal TA curves outside the experimental heating rate range.

\[
\frac{dT}{d\alpha} = \frac{\beta}{\Delta [A_\alpha f(\alpha)]} \exp\left(-\frac{E_a}{RT}\right), \quad j \leq \alpha \leq j + \Delta \alpha
\]

(11)

This equation is subject to the initial value condition

\[
T|_{\alpha=j} = T_j
\]

For the purpose of forecasting isothermal TA curves by means of predetermined nonisothermal kinetic results, in addition to knowing \(E_a\) values, the term \(\int_{\alpha - \Delta \alpha}^{\alpha} \{d\alpha / [A_\alpha f(\alpha)]\}\) could be calculated via the following expression.\(^{12}\)

\[
\int_{\alpha - \Delta \alpha}^{\alpha} \frac{d\alpha}{A_\alpha f(\alpha)} = -S^{-1}_\alpha \exp\left(-I_{\alpha 0}\right)
\]

(12)

where \(I_{\alpha 0}\) is the intercept of the plot of the left-hand side term in eq 5 vs reciprocal temperature.

With \(f(\alpha)\) (or \(G(\alpha)\)) presumed to stay invariable, the substitution of both \(E_a\) and \(\int_{\alpha - \Delta \alpha}^{\alpha} \{d\alpha / [A_\alpha f(\alpha)]\}\) into eq 2, after some mathematical derivations, yields the following equation, which can be used for forecasting isothermal TA curves.

\[
t_\alpha = \sum_{j=0}^{\alpha - \Delta \alpha} \int_{\alpha - \Delta \alpha}^{\alpha} \frac{d\alpha}{A_{\alpha + \Delta \alpha} f(\alpha + \Delta \alpha)} \exp\left(-\frac{E_a}{RT_{\alpha + \Delta \alpha}}\right)
\]

(13)

where \(T_{\alpha 0}\) is the isothermal temperature.

It is worth mentioning that the equations for calculating \(A_\alpha f(\alpha)\), reproducing nonisothermal kinetic curves, and forecasting isothermal kinetic curves, i.e., eqs 10, 11, and 13, are originally put forward in the present study.

**RESULTS AND DISCUSSION**

**Calculating the Activation Energy.** At various conversions, the \(E_a\) values evaluated by means of the Cai–Chen method appear in Figure 2. The errors within the beginning and end of the conversion range, as everyone knows, stand to be fairly high on account of the extremely small deflection of the TA curve away from the baseline. Accordingly, the conversion range in the present work is chosen as 0.1 \(\leq \alpha \leq 0.9\), in which the activation energy is found to be almost not connected with the conversion and then the mean activation energy \(\bar{E}\) is calculated to be 183.15 kJ mol\(^{-1}\). Fuertes et al.\(^{18}\) investigated the kinetics of CO\(_2\) gasification of metallurgical coke by means of a thermal analyzer, and the reported \(E\) value was 183 kJ mol\(^{-1}\). This value is close to the value obtained in this work.

Apart from the model-free method (i.e., the Cai–Chen method in the present work), a model-fitting method (i.e., the universal integral approach\(^{19}\) denoted by eq 14) is used to calculate activation energy.

\[
\ln\frac{G(\alpha)}{T - T_0} = \ln \frac{A}{\beta} - \frac{E}{RT}
\]

(14)

For a particular mechanism function, after plotting the left-hand side term in eq 14 vs reciprocal temperature, in agreement with eq 14 a direct line is supposed to be gained. Values \(E\) and \(A\) may be estimated from the slope and intercept, respectively.

For different mechanism functions listed in Table 2,\(^{20}\) results of the application of the universal integral approach to the experimental TA data measured under 2, 5, 10, and 15 K min\(^{-1}\) are expressed as Arrhenius parameters (\(E\) and \(A\)) and the linear correlation coefficient \(R^2\) and tabulated in Table 3. As seen in Table 3, values of \(E\) and \(\ln A\) are found to be strongly influenced by the mechanism function and to be weakly influenced by the heating rate. Many mechanism functions listed in Table 2 lead to better linear correlation coefficients, which are above 0.97; the most probable mechanism function cannot be unambiguously determined according to the linear correlation coefficient. It is agreed that different mechanism functions may ostensibly fit every TA curve well on account of there being a kinetic compensation effect (KCE) between Arrhenius parameters.

![Figure 2. Relationship of \(E_a\) (calculated by the Cai–Chen method) to \(\alpha\) for the gasification of coke.](https://doi.org/10.1021/acsomega.0c06001)
The experimental and theoretical values of mechanism function words, they are considered as a group rather than separately. The master-plot method could be applied. On the condition that the Table 3. Results from Using the Universal Integral Approach for Different Mechanism Functions

| model | $E^*$ | $\ln A^*$ | $R^2$ | $E$ | $\ln A$ | $R^2$ | $E$ | $\ln A$ | $R^2$ | $E$ | $\ln A$ | $R^2$
|-------|-------|-----------|-------|-----|-------|-------|-----|-------|-------|-----|-------|-------|
| P2/3  | 358.33| 24.37     | 0.937 | 354.15| 23.34 | 0.946 | 353.58| 22.92 | 0.948 |
| P2    | 65.01 | 2.09      | 0.878 | 69.66| 1.37  | 0.900 | 71.57| -1.02 | 0.907 |
| P3    | 16.12 | -6.50     | 0.605 | 22.25| -5.49 | 0.743 | 24.57| -5.01 | 0.777 |
| P4    | -8.32 | -8.71     | 0.539 | -1.46| -7.55 | 0.031 | 1.07 | -7.01 | 0.016 |
| D1    | 505.00| 37.60     | 0.940 | 496.39| 35.70 | 0.948 | 494.59| 34.90 | 0.951 |
| D2    | 556.78| 41.99     | 0.965 | 546.12| 39.73 | 0.970 | 543.71| 38.78 | 0.972 |
| D3    | 626.63| 47.31     | 0.988 | 613.10| 44.56 | 0.991 | 609.85| 43.41 | 0.992 |
| R2    | 255.27| 14.72     | 0.978 | 253.74| 14.26 | 0.982 | 253.90| 14.10 | 0.983 |
| R3    | 272.49| 15.99     | 0.988 | 270.26| 15.42 | 0.991 | 270.21| 15.21 | 0.992 |
| A1.5  | 180.48| 8.82      | 1.000 | 180.93| 8.79  | 1.000 | 181.63| 8.82  | 1.000 |
| A2    | 114.94| 2.79      | 1.000 | 117.55| 3.16  | 0.999 | 118.86| 3.37  | 0.999 |
| A3    | 49.41 | -3.25     | 0.991 | 54.18 | -2.47 | 0.993 | 56.09 | -2.08 | 0.993 |
| F1    | 311.54| 20.90     | 0.999 | 307.69| 20.05 | 1.000 | 307.16| 19.73 | 1.000 |

**Table 3.** Set of Mechanism Functions Widely Applied to Kinetic Analyses

| mechanism function | code | $G(\alpha)$ | $f(\alpha)$ |
|--------------------|------|-------------|-------------|
| 1 power law        | P2/3 | $a^{1/2}$   | $(2/3) a^{1/2}$ |
| 2 power law        | P2   | $a^{1/2}$   | $2a^{1/2}$ |
| 3 power law        | P3   | $a^{1/3}$   | $3a^{1/3}$ |
| 4 power law        | P4   | $a^{1/4}$   | $4a^{1/4}$ |
| 5 parabolic law     | D1   | $a^2$       | $(1/2) a^2$ |
| 6 Valensi equation  | D2   | $(1-a)\ln(1-a) + a$ | $-\ln(1-a)^{1/3}$ |
| 7 Jander equation   | D3   | $(1-(1-a)^{1/3})^2$ | $(1/2) (1-a)^{2/3} [1-(1-a)^{1/3}]^{-1}$ |
| 8 contracting cylinder | R2  | $[1-(1-a)^{1/2}]^2$ | $2(1-a)^{1/2}$ |
| 9 contracting sphere | R3  | $[1-(1-a)^{1/3}]^2$ | $3(1-a)^{2/3}$ |
| 10 Johnson–Mehl–Avrami | A1.5 | $[-\ln(1-a)]^{2/3}$ | $(3/2) (1-a)^{1/2} [-\ln(1-a)]^{1/3}$ |
| 11 Johnson–Mehl–Avrami | A2  | $[-\ln(1-a)]^{1/2}$ | $2(1-a) [-\ln(1-a)]^{1/3}$ |
| 12 Johnson–Mehl–Avrami | A3  | $[-\ln(1-a)]^{1/2}$ | $3(1-a) [-\ln(1-a)]^{1/3}$ |
| 13 unimolecular decay law | F1  | $-\ln(1-a)$ | $(1-a)$ |

Hence, it is obvious that the application of only the model-fitting method to working out kinetic parameters may introduce errors.

**Determining the Mechanism Function and Frequency Factor.** As observed in eq 10, the mechanism function $f(\alpha)$ gets lumped in with the pre-exponential Arrhenius factor $A_\beta$; in other words, they are considered as a group rather than separately. The mechanism function $f(\alpha)$, therefore, cannot be isolated from the term $A_\beta f(\alpha)$ directly; yet, the determination of $f(\alpha)$ might be accomplished using the master-plot methods. It is observed that when the $E_\alpha$ value is not only calculated from a model-free approach but it is also virtually independent of $\alpha$, the Málek master-plot method could be applied. On the condition that the Málek method is practicable, a mean activation energy $\bar{E}$ (in this work, $\bar{E} = 183.15$ kJ mol$^{-1}$) can be substituted for the nearly invariable value of $E_\alpha$ and then be introduced into eq 7.21 As mentioned earlier, the most probable mechanism function can be recognized from the situation in which the theoretical $Z(\alpha)$ values related to this mechanism function correspond closest to the experimental data transformed by eq 7. Figure 3 compares the experimental and theoretical values of $Z(\alpha)$; as observed, the influence of $\beta$ upon experimental values of $Z(\alpha)$ may seem trivial. As also observed in Figure 3, the nonisothermal gasification of metallurgical coke by carbon dioxide can be represented by the Johnson–Mehl–Avrami equation (An)$^{22,25-27}$ $f(\alpha) = n(1-\alpha)[-\ln(1-\alpha)]^{1-n}$. With the aim of evaluating the values of $n$ in this $f(\alpha)$ under the heating rates of 2, 5, 10, and 15 K min$^{-1}$, after substituting the mean activation energy $\bar{E}$ estimated formerly as well as the differential form of the An equation into eq 2, taking logarithms, and rearranging, we write

$$\ln\left(\frac{\beta d\alpha}{dT}\right) - \ln(1-\alpha) + \frac{E}{RT} = \left(1 - \frac{1}{n}\right) \ln\left[\ln(1-\alpha)\right] + \ln n + \ln A$$

Then, for each heating rate, values of $n$ and $\ln A$ are, respectively, found from the slope and intercept of the $\ln(\beta d\alpha/dT) - \ln(1-\alpha) + E/(RT)$ vs $\ln[-\ln(1-\alpha)]$ curve, a plot which ought to be linear. Table 4 shows $n$ values as well as $\ln A$ values. As seen in Table 4, the parameters $n$ and $\ln A$ are scarcely affected by $\beta$. As also seen in Table 4, the $n$ values at 2, 5, 10, and 15 K min$^{-1}$, respectively, were calculated to be 1.75, 1.74, 1.76, and 1.77, thereby leading to the average $n$ value of 1.75. Therefore, we reached a conclusion that the appropriate kinetic model for the CO$_2$ gasification of metallurgical coke is the Johnson–Mehl–Avrami equation (A1.5), viz., $f(\alpha) = 1.75(1-\alpha)[-\ln(1-\alpha)]^{1/1.75}$. As well as $G(\alpha) = [-\ln(1-\alpha)]^{1/1.75}$, Li et al.$^{28}$ investigated the metallurgical coke–carbon dioxide gasification reactions with/without alkali carbonates and reached the similar conclusion that in the absence of alkali carbonates, the Johnson–Mehl–Avrami equation (A2) was discovered to be the suitable mechanism function of metallurgical coke gasification.
Reproducing and Forecasting TA Curves. According to eq 11, we applied the evaluated parameters of $E_\alpha$ as well as $\Delta[A_\alpha f(\alpha)]$ to reproduce original $\alpha$ vs $T$ curves and forecast the reaction kinetics beyond the range of employed heating rates. Figure 4 presents the comparison of the original and the calculated $\alpha$ vs $T$ curves. As observed in this figure, original kinetic curves are in close accordance with the calculated ones, thereby indicating that eq 11 is appropriate to simulate the gasification process under nonisothermal conditions.

We forecast the evolution of the carbon conversion with temperature for the various linear heating rates not employed in the nonisothermal tests (see Figure 5). In low heating rate conditions, gasification starts at lower temperatures, while in high heating rate conditions, it starts at higher temperatures. For a given degree of conversion $\alpha$, the corresponding temperature $T_\alpha$ increases with the heating rate.

In addition, forecasts of conversion profiles under isothermal conditions have been given on the basis of the available nonisothermal kinetics previously determined. According to eq 13, at the chosen isothermal temperatures (1200, 1250, 1300, 1350, and 1400 K), the isothermal forecasted $\alpha$ vs $t_\alpha$ curves are procured and appear in Figure 6 from which we can notice that the entire reaction time becomes shorter with an increase in the isothermal temperature and that the evolution of $\alpha$ with $t_\alpha$ exhibits a sigmoidal shape, implying that the rate of conversion originally increases and then decreases with increasing time.

Table 4. Parameters $n$ and $\ln A$ Acquired under Different Heating Rates

| $\beta$ (K·min$^{-1}$) | $n$   | $\ln A$ (A in s$^{-1}$) |
|------------------------|-------|------------------------|
| 2                      | 1.73  | 10.171                 |
| 5                      | 1.74  | 10.182                 |
| 10                     | 1.76  | 10.208                 |
| 15                     | 1.77  | 10.221                 |
| arithmetic averages    | 1.75  | 10.196                 |

Figure 4. Comparison of original (open symbols) and calculated (dash lines) $\alpha$ vs $T$ curves for various linear heating rates.
The gasification of metallurgical coke by carbon dioxide is kinetically gone into under linear nonisothermal heating programs. The activation energy, estimated from the iterative linear integral isconversional method (the Cai–Chen method) in the absence of presuming any mechanism function in advance, is discovered to be barely affected by the conversion and therefore has a mean value of 183.15 kJ mol\(^{-1}\). The Mälek method discloses that the mechanism function \(f(\alpha) = n(1 - \alpha)^{1/n} \) \((n = 1.75)\) well represents the reaction behavior. The frequency factor is also determined: the value of \(ln A\) is estimated to be 10.196. With the aid of the joint kinetic analysis, acceptable deriving the kinetic triplet from the kinetic equations developed from the Cai–Chen method have been presented for reproducing the experimental data as well as forecasting kinetic curves, and satisfactory results have been achieved.

**CONCLUSIONS**

The gasification of metallurgical coke by carbon dioxide is kinetically gone into under linear nonisothermal heating programs. The activation energy, estimated from the iterative linear integral isconversional method (the Cai–Chen method) in the absence of presuming any mechanism function in advance, is discovered to be barely affected by the conversion and therefore has a mean value of 183.15 kJ mol\(^{-1}\). The Mälek method discloses that the mechanism function \(f(\alpha) = n(1 - \alpha)^{1/n} \) \((n = 1.75)\) well represents the reaction behavior. The frequency factor is also determined: the value of \(ln A\) is estimated to be 10.196. With the aid of the joint kinetic analysis, acceptable deriving the kinetic triplet from the kinetic equations developed from the Cai–Chen method have been presented for reproducing the experimental data as well as forecasting kinetic curves, and satisfactory results have been achieved.
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