

## Kinetic Modeling of Lignite Devolatilization: Comparative Perspectives of DAEM and Iso-conversional Methods

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**Abstract.** DAEM and iso-conversional methods are reviewed for kinetically modeling lignite devolatilization, a critical initial stage in coal utilization that profoundly impacts energy efficiency and emissions. Lignite presents unique challenges due to its high volatile content (60 – 70 wt%) and complex multi-stage decomposition reactions. DAEM addresses this by assuming devolatilization as a series of parallel, first-order reactions with a continuous distribution of activation energies, mostly Gaussian or Weibull; multi-Gaussian DAEM extensions further enhance accuracy for intricate decomposition profiles. Conversely, iso-conversional methods like Friedman, FWO, and KAS estimate effective activation energies ( $E_a$ ) at various conversions, offering a robust way to analyze kinetic data from multiple heating rates. Comparative analyses indicate that multi-Gaussian DAEM more effectively captures the staged devolatilization of lignite, with reported  $E_a$  for low-rank coal ranging from 142 to 248 kJ/mol and significantly improved sum of squared error (SSE) ratios (e.g., 1.73x – 244x). While iso-conversional methods are computationally efficient and provide consistent profiles ( $R^2 > 0.98$ ), DAEM yields more complete kinetic parameters. Both require quality TGA data and primarily describe chemical kinetics, often neglecting physical transport limitations pertinent to reactor design. Future research focuses on refining these models and integrating them with broader system simulations.

**Keywords:** *activation energy, DAEM, Gaussian, kinetic modeling, lignite, TGA.*

### 1 Introduction

Coal remains critical in Indonesia's energy sector, with over 775 million tonnes (Mt) produced in 2023, primarily low-rank varieties such as sub-bituminous and lignite, as reported by the IEA in [1] and [2]. The process of coal utilization commences with devolatilization, during which the high volatile matter content (60–70 wt%) of lignite is released in the form of gases and tars, resulting in a char residue. The rate and extent of this initial step significantly influence subsequent energy efficiency, burnout, and pollutant formation [3], [4]. Consequently, reliable kinetic models are essential for accurately predicting volatile release, informing reactor design, and optimizing emissions [5]. Early kinetic models employing

single-step Arrhenius equations, as reported by Kobayashi *et al.* (1977) in [6], encounter difficulties in addressing the complex, multi-stage chemistry of lignite. This challenge has led to the adoption of more adaptable frameworks, such as the Distributed Activation Energy Model (DAEM) and iso-conversional (model-free) analyses, which customize activation-energy distributions to enable precise simulations of gasifiers, pyrolyzers, and boilers [6].

This review focuses on empirical and distributed approaches, specifically DAEM and iso-conversional techniques, while acknowledging but not addressing mechanism-intensive models such as CPD, FLASHCHAIN, and FG-DVC. The detailed structural requirements and computational demands of these models restrict their routine application in thermogravimetric analysis (TGA).

## 2 Coal Devolatilization Fundamentals

Coal devolatilization is the initial and critical step in thermal conversion processes such as combustion, gasification, and pyrolysis. When exposed to elevated temperatures in an oxygen-deficient environment, coal undergoes thermal decomposition, releasing volatile matter (VM), a mixture of condensable tars and non-condensable gases, and leaving behind char. This transformation is governed by the breakdown of weaker chemical bonds, particularly aliphatic bridges and oxygenated functional groups, which form a transient liquid-like phase known as metaplast. The formation and mobility of metaplast significantly influence volatile release, especially in low-rank coals with high oxygen content [7], [8], [9].

The complexity of devolatilization is amplified by secondary reactions such as tar cracking and repolymerization, which occur under high temperature and pressure, altering gas composition and contributing to soot or secondary char formation [10], [11]. Additionally, physical transport limitations—particularly at high heating rates or in large particles—can restrict volatile release, making diffusion a rate-limiting factor [12].

These physicochemical processes critically affect reactor performance. The timing and extent of volatile release influence ignition behavior, flame stability, and burnout efficiency. In gasification, volatile composition directly determines syngas quality. Furthermore, devolatilization dictates the structural and reactive properties of the resulting char. Morphological changes such as softening, swelling, and pore development during this stage impact char reactivity in subsequent combustion or gasification steps [13], [14], [15]

Key influencing factors include coal rank, maceral composition, mineral content, heating rate, pressure, and particle size. Rapid heating promotes higher volatile yields by favoring bond scission over cross-linking. Conversely, high pressures and larger particle sizes enhance secondary reactions and reduce tar yield. Accurate

modeling of these effects is essential for designing efficient and clean energy conversion systems.

### 3 Kinetic Modeling Approaches of Coal Devolatilization

Kinetic models predict the rate and extent of volatile release. Simple models use single first-order reactions but lack accuracy. Multi-step models (e.g., two competing reactions) improve fits but require assumptions about sub-reactions [16], [17].

DAEM (Distributed Activation Energy Model) addresses this by modeling a continuous distribution of activation energies, reflecting coal's diverse bond strengths [3].

Isoconversional methods (e.g., FWO, KAS, Friedmann) are model-free approaches that estimate activation energy at different conversion levels using data from multiple heating rates. These are valuable for evaluating kinetics without assuming a specific reaction mechanism [18], [19], [20], [21].

## 4 Distributed Activation Energy Model (DAEM)

### 4.1 Theoretical Background

The Distributed Activation Energy Model (DAEM) interprets coal devolatilization as a superposition of a theoretically infinite number of independent, parallel, first-order reactions. Each reaction proceeds with a unique activation energy  $E_a$  and these are assumed to follow a continuous statistical distribution described by a probability density function  $f(E)$ . This framework was originally proposed by [22] and later adapted to coal pyrolysis by [3].

A common simplification in DAEM is the assumption of a constant pre-exponential factor  $k_0$  for all reactions. This is primarily for mathematical tractability, as simultaneously determining both  $f(E)$  and a distribution of  $k_0$  values are challenging due to strong correlations between  $k_0$  and the mean activation energy  $E_0$ . For instance, [23] reported a high correlation coefficient (0.971) between these parameters in their experimental work. As a result, the derived  $f(E)$  becomes an effective distribution that may implicitly incorporate variations in both activation energy and  $k_0$ .

### 4.2 Mathematical Formulation

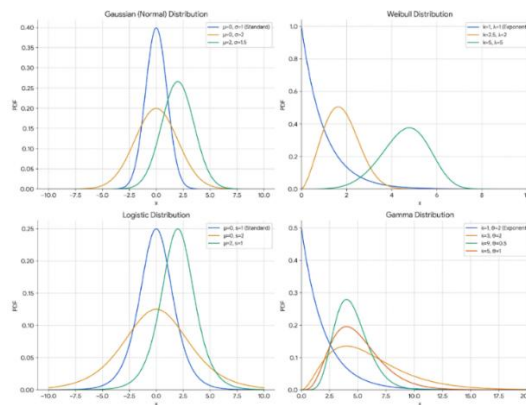
The rate of conversion for a single first-order reaction with activation energy  $E$  and pre-exponential factor  $k_0$  is given by the Arrhenius law. In DAEM, the overall rate of volatile release or the remaining fraction of potential volatiles is obtained by

integrating the contributions of all these parallel reactions over the distribution of activation energies.

Let  $V(t)$  be the amount of volatile evolved up to time  $t$ , and  $V^*$  be the total potential volatile yield. The fraction of unreacted volatile precursors corresponding to reactions with activation energy  $E$  at time  $t$  is given by  $\exp\left(-\frac{E}{RT(t)}\right)$ . The overall fraction of remaining potential volatiles,  $1 - \frac{V(t)}{V^*}$ , can be calculated using equation (1).

$$1 - \frac{V(t)}{V^*} = \int_0^\infty \exp\left[-k_0 \int_0^t \exp\left(-\frac{E}{RT(t)}\right) dt\right] f(E) dE \quad (1)$$

The core objective of applying DAEM is to determine the kinetic parameters: the pre-exponential factor  $k_0$  (often assumed or fixed) and the parameters that define the shape and location of the activation energy distribution function  $f(E)$  (e.g., the mean  $E_0$  and standard deviation  $\sigma E$  for a Gaussian distribution) by fitting this equation to experimental data (typically TGA curves obtained at multiple heating rates).



**Figure 1** Distribution Functions with Varying Parameters

Several distribution functions have been employed, with the selection often based on mathematical convenience or the ability to provide a good fit to the experimental data. The prevalent choices for the distribution function  $f(E)$ , visualized by Figure 1 include Gaussian (normal), Weibull, Gamma, and Logistic Distributions. The multi-Gaussian DAEM posits that  $f(E)$  is a weighted sum of multiple Gaussian distributions ( $f(E) = \sum w_i f_i(E)$ ), each corresponding to a distinct stage with its own parameters. This approach yields improved fits to complex TGA/DTG curves [23]. The DAEM formulation described here is applied in Section 6.1 to new TGA data for East Kalimantan lignite, allowing for a direct comparison with existing literature models.

## 5 Iso-conversional (Model-Free) Methods

Several widely applied iso-conversional methods—namely the Friedman (FR), Flynn-Wall-Ozawa (FWO), and Kissinger-Akahira-Sunose (KAS) methods—differ primarily in their mathematical formulations and sensitivity to data quality. As summarized in Table 1, the Friedman method adopts a differential approach based on the logarithmic form of the rate equation and does not require approximating the temperature integral. This enables high accuracy but also renders it highly susceptible to experimental noise, particularly in regions with low signal-to-noise ratios. In contrast, the FWO and KAS methods employ integral formulations that utilize approximations, Doyle's and Coats-Redfern, respectively, to simplify the temperature integral. While the FWO method is straightforward and less sensitive to noise, its reliance on Doyle's approximation may compromise accuracy for complex reactions. The KAS method offers improved precision over FWO by employing a more accurate integral approximation, albeit with certain limitations still in place. Collectively, these methods facilitate the estimation of activation energy  $E_a$  as a function of conversion without requiring a predefined reaction model, but each presents a trade-off between computational simplicity, accuracy, and robustness to noise[24].

**Table 1** Comparison of Common Iso-conversional Methods

Aspect	Friedman (FR)	Flynn-Wall-Ozawa (FWO)	Kissinger-Akahira-Sunose (KAS)
Type	Differential	Integral	Integral
Equation Basis	$\ln\left(\frac{d\alpha}{dt}\right)_{\alpha,i} = \ln(A_\alpha f(\alpha)) - \frac{E_a}{RT_{\alpha,i}}$	$\ln(\beta_i) = \text{Constant} - \frac{1.052E_a}{RT_{\alpha,i}}$	$\ln\left(\frac{\beta_i}{T_{\alpha,i}^2}\right) = \text{Constant} - \frac{E_a}{RT_{\alpha,i}}$
Temperature Integral Approximation	Not required (uses raw data)	Doyle's approximation	Coats-Redfern approximation (more accurate)
Main Advantage	High accuracy (no integral approximation)	Simple; less sensitive to noise	More accurate than FWO; moderate noise sensitivity
Main Disadvantage	Highly sensitive to experimental noise	Approximation may reduce accuracy	Assumes model stability; still uses an approximation
Data Requirement	High-resolution $d\alpha/dt$ at multiple $\beta$	Multiple heating rates at fixed $\alpha$	Multiple heating rates at fixed $\alpha$
Accuracy Trend	High if noise-free	Moderate	Higher than FWO; lower than FR if noisy

## 6 Comparative Perspectives: DAEM vs. Iso-conversional

These comparative perspectives utilize several aspects, including comparative results, strengths and weaknesses, data requirements and computations, and the accuracy in predicting devolatilization behavior.

### 6.1 Comparative Kinetic Parameters Results

As shown in Table 2 the kinetic parameters derived show that DAEM with multi-Gaussian distributions captures the staged devolatilization behavior of lignite more effectively, with activation energies in low rank coal ranging from 142 to 248 kJ/mol [9] and the ratio of SSE can be achieved by 1.73x – 244x by adding the Gaussian distribution function (2-3 DAEM), which indicates excellent fit quality. Compared to literature values, the activation energy obtained for EK Lignite is within the range observed for lignite and sub-bituminous coals. The  $R^2$  metrics demonstrate good fit quality, supporting the suitability of the DAEM approach in modeling this regional fuel. Figure 2 is the DTG-Conversion curve fitting result derived from actual TG data using three-Gaussian DAEM inspired by Wang et al., in [9].

**Table 2** Comparative Results of The Kinetic Parameters from Literature and The Present Study (EK-Lignite)

Type of Sample	Method (DAEM/Iso-conversional)	$E_a$ Range (kJ/mol)	Pre-exponential Factor $k_0$ ( $s^{-1}$ or $min^{-1}$ )	Fit Metrics	Ref.
Shenmu Coal (low rank)	DAEM – Miura integral method	H <sub>2</sub> atm: 175–215; CH <sub>4</sub> atm: 225–230 (concentrated ranges)	Not explicitly stated as a single value, derived with $E_a$	$R^2$ in hydrogen atmosphere > 0.95 in $\alpha$ 0.2-0.7	[25]
Sub-bituminous	DAEM – Two Gaussian	200 – 233	Fixed $k_0 = 8 \times 10^{12} s^{-1}$	SSE 1-DAEM/2-DAEM: 244	[23]
Low rank coal	DAEM – Three Gaussian	142 - 248	Fixed $k_0 = 5 \times 10^{11} s^{-1}$	SSE 2-DAEM/3-DAEM: 1.73	[9]
East Kalimantan Lignite	DAEM – Three Gaussian	1 <sup>st</sup> $E_0 = 101.4$ kJ/mol 2 <sup>nd</sup> $E_0 = 171.3$ kJ/mol 3 <sup>rd</sup> $E_0 = 238.9$ kJ/mol	Fixed $k_0 = 5 \times 10^{11} s^{-1}$	$R^2 = 0.9996$ RMSE = 0.5790	Actual TGA data
Indian Lignite	FWO, KAS, Tang	FWO= 60.34–140.94 KAS= 51.77–138.84 Tang= 52.31–139.13	Not reported	Good agreement	[26]
Lignite coal (gasification)	FWO, KAS, Friedman	FWO= 275 KAS= 271.8 Friedman= 256.8	Heat rate 5= $5.2 \times 10^{13}$ Heat rate 20 = $2.8 \times 10^{15}$	$R^2 = 0.99$ in $\alpha$ 0.4 – 0.9	[27]

Type of Sample	Method (DAEM/Iso-conversional)	$E_a$ Range (kJ/mol)	Pre-exponential Factor $k_0$ ( $s^{-1}$ or $min^{-1}$ )	Fit Metrics	Ref.
Canadian Lignite	FWO, KAS, Friedman	FWO= 282 KAS= 275 Friedman= 283	Kissinger (non iso-conversional) = $2.61 \times 10^{17} min^{-1}$	$R^2 \approx 0.99$ (iso-conversional), 0.9858 (Kissinger)	[28]
East Kalimantan Lignite	FWO, KAS	FWO = 35.4 – 350.7 KAS = 27.6 – 338.9 For conversion 0 – 0.6	FWO = $5.01 \times 10^{27}$ KAS = $2.27 \times 10^{21}$	$R^2 = 0.76$ (FWO) $R^2 = 0.749$ (KAS)	Actual TGA Data

In contrast, the iso-conversional methods, while computationally efficient, exhibited reliability only up to  $\alpha \approx 0.6$ , beyond which the derived activation energies became erratic or negative (EK-Lignite). This is consistent with known limitations of these methods at high  $\alpha$ , where devolatilization reactions overlap and the mass loss rate declines significantly. This limitation, particularly evident in the FWO method, is partially attributed to the use of Doyle's approximation, which becomes less accurate at lower  $E/RT$  ratios typically observed at high  $\alpha$  levels.

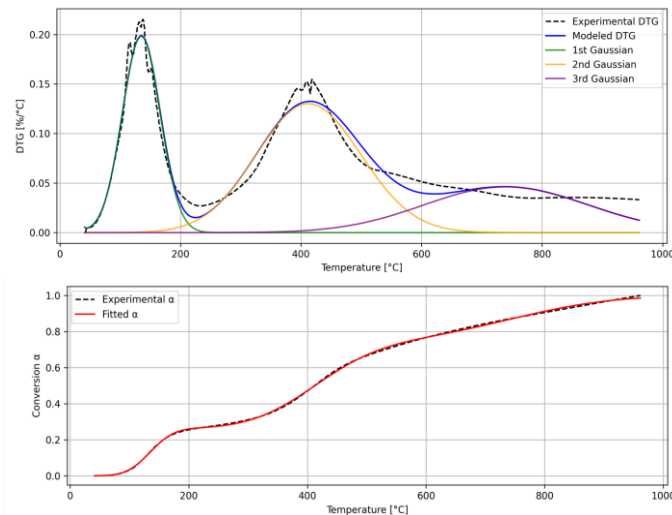


Figure 2 DTG and Conversion Curve Fitting Result by Three-Gaussian DAEM

## 6.2 Strengths and Weaknesses

Table 3 provides a structured comparison of the primary strengths and weaknesses of the Distributed Activation Energy Model (DAEM) and iso-conversional methods, highlighting key methodological distinctions along with their supporting references.

**Table 3** Strengths and Weaknesses of DAEM vs Iso-conversional Methods

Aspect	Distributed Activation Energy Model (DAEM)	Iso-conversional Methods	References
Strengths	<ul style="list-style-type: none"> <li>• Provides a complete kinetic model with <math>k_0</math> and <math>f(E)</math>; suitable for simulations</li> <li>• Reflects the heterogeneous nature of coal via distributed reactivity               <ul style="list-style-type: none"> <li>• Multi-Gaussian extensions improve accuracy in multi-stage profiles</li> </ul> </li> </ul>	<ul style="list-style-type: none"> <li>• Model-free: avoids assuming <math>f(\alpha)</math></li> <li>• Recommended by ICTAC for reliable <math>E_a</math> estimation</li> <li>• <math>E_a(\alpha)</math> profile reveals process complexity (single vs multi-step)</li> </ul>	[9], [11], [24], [29]
Weaknesses	<ul style="list-style-type: none"> <li>• Depends on the parallel first-order reaction assumption</li> <li>• Strong compensation effect complicates parameter estimation</li> <li>• High computational cost, especially for multi-stage fits</li> </ul>	<ul style="list-style-type: none"> <li>• Yields <math>E_a(\alpha)</math> only-needs extra steps to estimate <math>A_a f(\alpha)</math></li> <li>• Assumes rate separability and Arrhenius dependence</li> <li>• Sensitive to noise (Friedman) or approximation error (FWO, KAS)</li> <li>• Accuracy deteriorates beyond <math>\alpha &gt; 0.65</math> due to overlapping processes and limitations in the temperature integral approximation (e.g., Doyle's)</li> </ul>	[9], [24], [29]

### 6.3 Data Requirements and Computational Complexity

Both DAEM and iso-conversional methods require high-quality, non-isothermal thermogravimetric analysis (TGA) data collected at multiple (typically  $\geq 3$ ) linear heating rates. Single-rate data are insufficient for reliable parameter estimation in either approach.

DAEM parameter fitting involves solving a complex integral equation across all heating rates simultaneously. This typically demands non-linear optimization and, for multi-Gaussian or variable- $k_0$  models, can become computationally intensive. Additionally, numerical integration of the DAEM expression itself may present stability challenges [30].

In contrast, iso-conversional methods determine activation energy  $E_a$  as a function of conversion ( $\alpha$ ) using linear regression (e.g., Friedman, FWO, KAS) or moderate non-linear optimization (e.g., Vyazovkin). These are less demanding computationally, with most effort focused on preprocessing the TGA data-e.g., smoothing, interpolation, and differentiation [24].

Overall, iso-conversional techniques are computationally more efficient than DAEM, though they yield less detailed kinetic models.

#### 6.4 Accuracy in Predicting Devolatilization Behavior

When supported by robust multi-heating rate data and appropriate parameterization, the Distributed Activation Energy Model (DAEM) provides accurate predictions of devolatilization behavior across diverse conditions. Its accuracy depends on selecting suitable activation energy distributions, especially for multi-stage reactions. Studies confirm a strong match between DAEM predictions and experimental pyrolysis data for coal and biomass [9].

While iso-conversional methods such as Friedman, Flynn-Wall-Ozawa (FWO), and Kissinger-Akahira-Sunose (KAS) do not directly forecast reaction rates, the reconstruction of kinetic curves utilizing the  $E_a(\alpha)$  profile, via the compensation effect or an assumed  $f(\alpha)$ , can closely approximate experimental data. Reconstructions based on the Friedman method are frequently regarded as the most accurate, although some consider iso-conversional methods to be more qualitative in nature [29]. The limitations of the OFW method at high conversion levels ( $\alpha > 0.6$ ) are partly attributable to its reliance on Doyle's approximation for the temperature integral. This approximation assumes high  $E/RT$  values and tends to lose accuracy in the later stages of devolatilization where the temperature increases and  $E/RT$  declines. As a result, the estimated activation energies may become non-physical or highly unstable. This numerical artifact is compounded by experimental noise and overlapping secondary reactions, further degrading the reliability of iso-conversional methods at high  $\alpha$ .

When rigorously applied, both DAEM and iso-conversional approaches offer comparable predictive accuracy [29]. DAEM provides model-based interpretation, while iso-conversional methods are model-free. They can be complementary, such as using  $E_a(\alpha)$  to guide DAEM fitting. However, both approaches neglect physical transport phenomena, such as heat and mass transfer, making them most valid under kinetically controlled conditions. For realistic reactor simulations, these kinetic models must be coupled with transport models, particularly in CFD applications [31].

#### 6.5 Comparative Summary

Table 4 summarizes the key comparative aspects of DAEM and Iso-conversional methods for coal devolatilization kinetics.

**Table 4** Comparative Summary of DAEM and Iso-Conversional

Feature	Distributed Activation Energy Model (DAEM)	Iso-conversional Methods
Theoretical Basis	Assumes infinite parallel 1st-order reactions with distributed reactivity	Based on the iso-conversional principle: rate at constant $\alpha$ depends only on T

Key Assumptions	Parallel reactions, $f(E)$ distribution, often constant $k_0$	Rate = $k(T)f(\alpha)$ , Arrhenius $k(T)$ , mechanism constant at constant $\alpha$
Primary Output	Kinetic model parameters ( $k_0$ , $f(E)$ parameters like $E_0$ , $\sigma E$ )	Effective activation energy vs. conversion profile, $E_a(\alpha)$
Strengths	Provides a complete predictive model; conceptually fits heterogeneity; multi-Gaussian handles stages	Avoids assuming $f(\alpha)$ ; reveals complexity via $E_a(\alpha)$ ; robust $E_a$ determination with good multi- $\beta$ data
Weaknesses	Relies on model/ $k_0$ assumptions; complex/costly parameter estimation; compensation effect issues	Does not yield a complete model directly; potential errors from approximations (integral methods) or noise (differential methods); may misinterpret competing reactions
Data Needs	Multi-heating rate TGA data ( $\geq 3$ rates recommended)	Multi-heating rate TGA data ( $\geq 3$ rates required)
Computational Cost (Est.)	Higher (non-linear optimization for integral fit)	Lower for $E_a$ (linear regression or simpler optimization)
Predictive Accuracy	Good, if assumptions hold and fitted well to multi- $\beta$ data	Good, via reconstruction methods if $E_a(\alpha)$ is accurate
CFD Suitability	Indirect: Provides a basis for deriving/calibrating simpler CFD sub-models	Indirect: $E_a(\alpha)$ informs/calibrates simpler CFD sub-models

## 7 Emerging Trends and Future Directions

The domain of kinetic modeling for coal devolatilization is undergoing continuous advancement, propelled by the necessity for more precise predictions and enhanced integration with system-level simulations aimed at optimizing clean energy technologies. Table 5 summarizes the key emerging directions in devolatilization kinetics research.

**Table 5** Summary of Future Directions in Devolatilization Kinetics

Area	Key Developments	Ref.
DAEM Refinements	Multi-modal $f(E)$ ; variable $k_0$ ; discrete DAEM (DDAEM)	[9]
Iso-conversional Advances	Improved smoothing, non-linear $E_a$ methods (e.g., Vyazovkin), estimation of $A$ , $f(\alpha)$	[32], [33]

Area	Key Developments	Ref.
Hybrid Modeling	ANN + DAEM; use of $E_a(\alpha)$ profiles to guide DAEM; CPD-informed simplifications	[34]
CFD Integration	Simplified kinetic sub-models; feedback loops from CFD-derived histories	[13]
Complex Systems	Co-processing (coal + biomass/plastic), volatile speciation, mineral effects	[15]
High-Fidelity Experiments	TGA + FTIR/GC-MS; drop tube reactors for high heating rate validation	[11]

## 8 Conclusion

For modeling the complex, multi-stage devolatilization of lignite, the Distributed Activation Energy Model (DAEM), especially when employing multi-Gaussian distributions, offers a superior and more detailed kinetic representation. This approach more accurately captures the inherent heterogeneity of lignite's decomposition. Quantitatively, multi-Gaussian DAEM demonstrates significantly improved fits to experimental thermogravimetric data, as shown by substantial reductions in the sum of squared errors (SSE); a 2-Gaussian DAEM improved SSE by a factor of 244 for sub-bituminous coal, and a 3-Gaussian DAEM enhanced it by 1.73 times for low-rank coal when compared to simpler DAEM versions. Activation energies derived for low-rank coals using DAEM typically range from 142 to 248 kJ/mol. Experimental application of the three-Gaussian DAEM to East Kalimantan lignite produced activation energies of 101 – 239 kJ mol<sup>-1</sup> and achieved an  $R^2$  of 0.9996 with low RMSE, highlighting the model's robustness for regional fuel characterization. These results support broader trends observed across lignite samples and underscore the value of multi-component kinetic modeling.

Iso-conversional methods such as FWO, KAS, and Friedman provide a valuable and computationally efficient model-free pathway to determine effective activation energies ( $E_a$ ) across different conversion stages. These methods are beneficial for initial kinetic assessments and yield consistent  $E_a$  values, often with high correlation coefficients (e.g.,  $R^2 \approx 0.99$  for specific conversion ranges in lignite gasification, with  $E_a$  values around 256.8 to 275 kJ/mol). While Canadian lignite iso-conversional results report high  $R^2$  values ( $\sim 0.99$ ) over a wide  $\alpha$  range, the application of the same methods to EK-lignite was limited to  $\alpha \leq 0.6$  due to non-physical results beyond this point. The corresponding  $R^2$  values (FWO: 0.76; KAS: 0.749) confirm the breakdown of predictive accuracy, underscoring the model's sensitivity to data quality and sample heterogeneity.

Despite their strengths, both DAEM and iso-conversional methods generally fail to account for physical transport phenomena, such as heat and mass transfer, which

are critical in industrial-scale reactors. Therefore, for realistic simulations, particularly in Computational Fluid Dynamics (CFD) applications, these kinetic models must be integrated with comprehensive transport models. Future advancements, including refined DAEM variations, enhanced iso-conversional techniques, and hybrid modeling, are poised to improve predictive accuracy further. The continued development and astute application of these kinetic modeling approaches remain crucial for optimizing the design and operation of cleaner and more efficient energy conversion technologies for low-rank coals, such as lignite.

## 9 Nomenclature

$\alpha$	= Conversion (fraction of mass loss), $\alpha = \frac{m_0 - m_t}{m_0 - m_f}$
$E_0$	= Mean activation energy of the distribution function $f(E)$ (kJ/mol)
$E_a\alpha$	= Effective activation energy at conversion level $\alpha$ (kJ/mol)
$k(T)$	= Temperature-dependent rate constant ( $s^{-1}$ )
$k_0$	= Pre-exponential factor or frequency factor in Arrhenius equation ( $s^{-1}$ )
$R$	= Universal gas constant (8.314 J/mol · K)
$T$	= Temperature (K)
$\beta$	= Linear heating rate, $\beta = \frac{dT}{dt}$ (K/min)
$V(t)$	= Volatile yield at time $t$ (wt%)
$V^*$	= Total volatile yield (wt%)
$f(E)$	= Probability density function for activation energy distribution
$\sigma_E$	= Standard deviation of activation energy distribution (kJ/mol)
$w_i$	= Weight fraction of the $i$ -th pseudo-component in multi-Gaussian DAEM

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