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# A New Diagnostic when Determining the Activation Energy by the Advanced Isoconversional Method

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## Highlights

- An Optimization Indicator is introduced which identifies and diagnoses possible error in TGA data.
- The results suggest that limestone activation energies  $<200 \text{ kJ}\cdot\text{mol}^{-1}$  for calcination in nitrogen are questionable.
- Strong activation energy vs. conversion trends for limestone calcination are likely due to errors.

## Abstract

The Advanced Isoconversional (AIC) method involves minimization of a function which uses conversion data at a minimum of three heating rates to determine an activation energy ( $E_a$ ) at different values of conversion ( $\alpha$ ). Reactions that can be described by a single model give an  $E_a$  which is independent of  $\alpha$ , while reactions which are described by more than one model give an  $E_a$  which varies with  $\alpha$ . Shifts in the conversion curves due to error can lead to  $E_a$  vs.  $\alpha$  trends which falsely indicate, or mask, true multi-model kinetics. It was found that the minimum value obtained during optimization of what we call the 'Optimization Indicator' ( $\Omega$ ) can indicate whether trends in  $E_a$  vs.  $\alpha$  are likely to be error-derived in the case of single-model reactions or artifacts in the case of multi-model reactions.  $E_a$  and  $\Omega$  for the calcination of  $\text{CaCO}_3$  are used to demonstrate the experimental application of this new diagnostic.

## Keywords

Nonisothermal kinetics

Advanced Isoconversional method

Optimization Indicator

## 1. Introduction

The kinetic equation for a single-mechanism, solid-state reaction at a particular heating rate ( $\beta$ ) describes the rate of reaction ( $d\alpha/dT$ ) as a function of two variables: temperature ( $T$ ) and conversion ( $\alpha$ ):

$$\frac{d\alpha}{dT} = \frac{A}{\beta} \exp\left(\frac{-E_a}{RT}\right) f(\alpha) \quad (1)$$

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