Application Brief

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Introduction to Highway TA

- Heating Rate Conversion Simulation Software -

1. Introduction

TG/DTA and DSC are widely used in thermal analysis to measure evaporation, breakdown, melting and reaction heat. However, the heating rate in TG/DTA and DSC measurements is generally 10°C/min so measurement time can be considerable, depending on the temperature range used.

Furthermore, analysis problems can occur in standard measurements if two reactions occur near the same temperature because the reactions overlap. To separate the two reactions, the measurement must be repeated using a slower heating rate.

Highway simulation thermal analysis (Highway TA) was developed to solve these problems[1]. Highway TA is a unique thermal analysis method that converts the time scale of measurements. This brief introduces the principles of Highway TA and measurement examples.

2. Principle of Highway TA

Highway TA is a thermal analysis technique with a simulation function. It converts data measured at one heating rate (for example, 50°C/min) to measurement data at another heating rate (for example, 10°C/min). To use Highway TA, software to convert the measurement data must be installed.

The conversion principles of Highway TA are shown in Figure 1. For phenomenon that can be kinetically analyzed following Arrhenius law, heating rate differences can be converted into temperature differences using activation energy ΔE (slope).

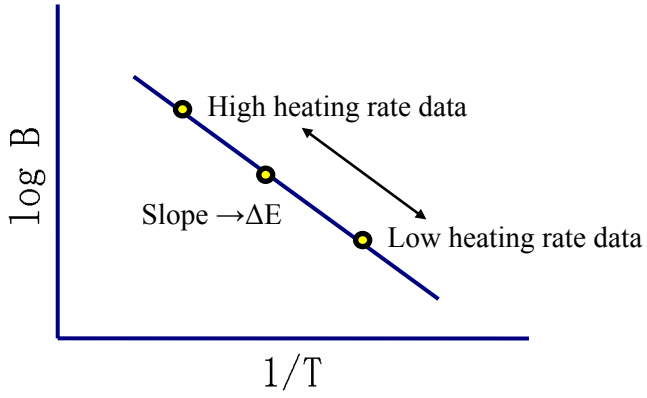

Figure 1 Highway TA conversion principles
B: Heating rate
T: Temperature

Furthermore, Highway TA organically combines with conventional methods to achieve new thermal analysis simulations. Actual measurement data can be converted to data at another heating rate by combining the following four methods (patent pending).

1. Thermal analysis data (TG data or DSC data)
2. Peak separation (when multiple DTG or DSC peaks overlap)
3. Calculation of activation energy (Δ E) for each peak
4. Temperature-time conversion following Arrhenius law

Highway TA has the following features.

- Simulations cut measurement time by 50% to 90%.
- Can be added as an optional function to current systems.
- Can complete simulations using data measured at high heating rates.
- Can be used with TG/DTA and DSC.

3. Measurements

3-1 TG Measurement of Calcium Oxalate

Figure 2 shows the results of converting data for calcium oxalate measured at 100°C/min to data measured at 10°C/min. Data from actual measurements at 10°C/min is also shown. The simulation data corresponded well with this actual data and essentially overlapped it. A measurement of only about 9 minutes produced results similar to a measurement that typically requires 90 minutes.

3-2 TG Measurement of Nylon

Figure 3 shows the results of converting TG data for nylon decomposition measured at 20°C/min to data measured at 2°C/min. The result matches well with actual data from measurements at 2°C/min. In this case, measurement data that typically requires 5 hours was acquired in a mere 30 minutes.

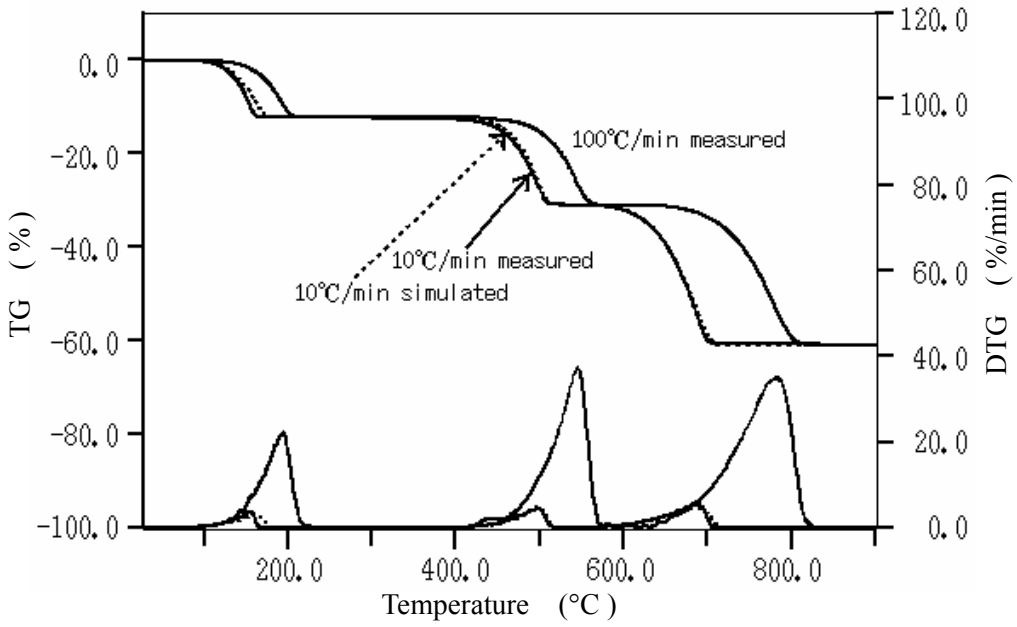

Figure 2 TG Results for Calcium Oxalate
- - - - - - - - : Simulation data
———— : Measured data

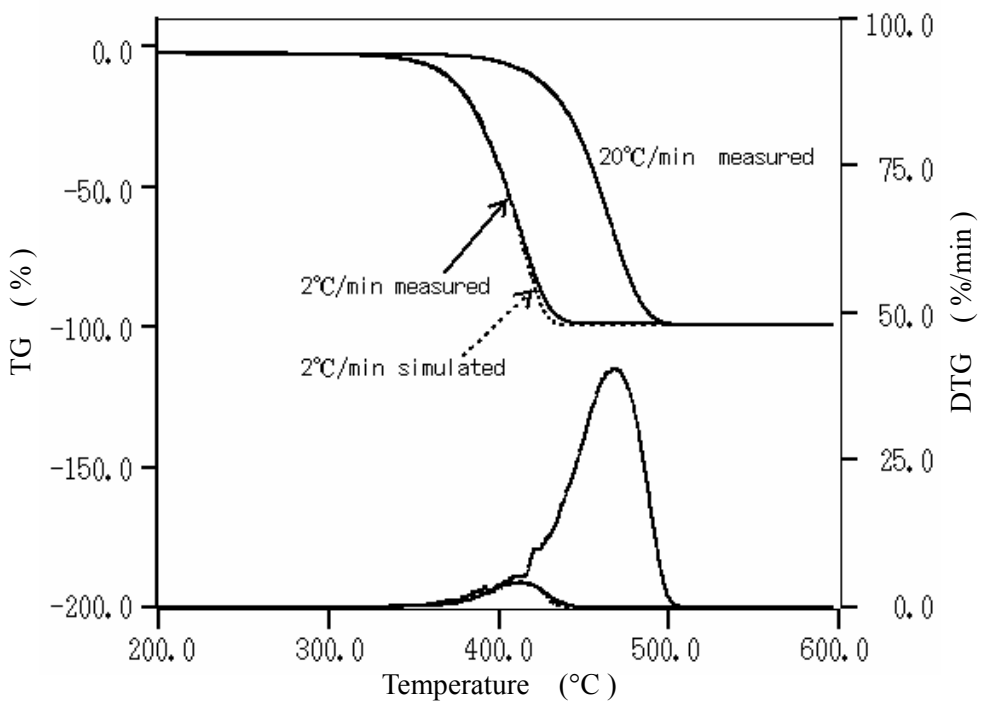

Figure 3 TG Results for Nylon

--------- : Simulation data

———— : Measured data

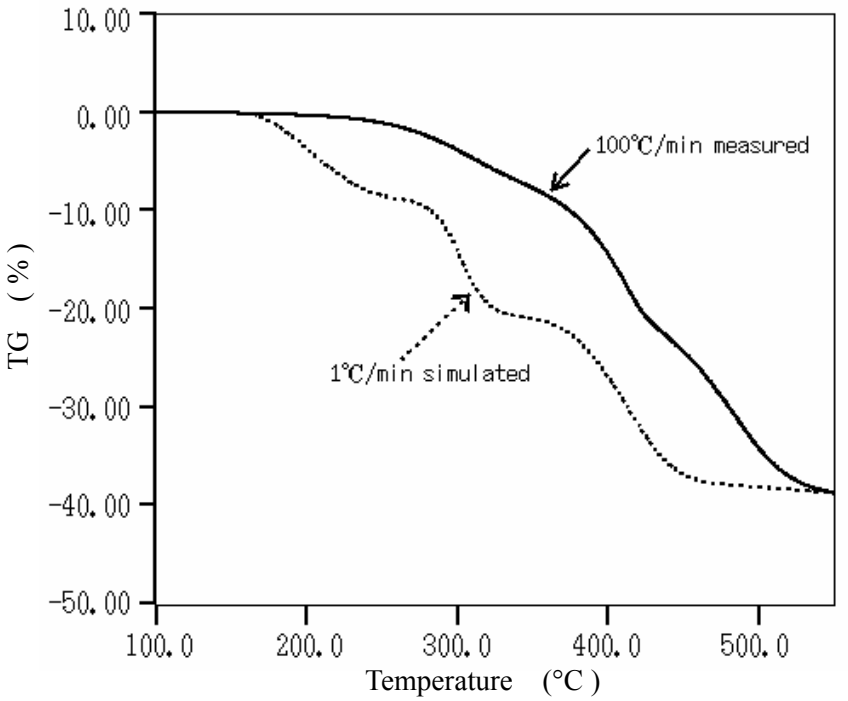

Figure 4 TG Results for Chloroprene Rubber

--------- : Simulation data

———— : Measured data

3-3 TG Measurement of Chloroprene Rubber

Figure 4 shows the results of converting data for chloroprene rubber measured at 100°C/min to data measured at 1°C/min. This simulation of measurement data at a lower heating rate confirmed a clearly defined three-stage weight decrease.

3-4 DSC Measurement of Epoxy Adhesives

Figure 5 shows the measurements results for the curing reaction of epoxy adhesive at 50°C/min. Furthermore, Figure 6 shows the results of converting this data to data measured at 10°C/min. The conversion data matches well with actual data from measurements at 10°C/ min.

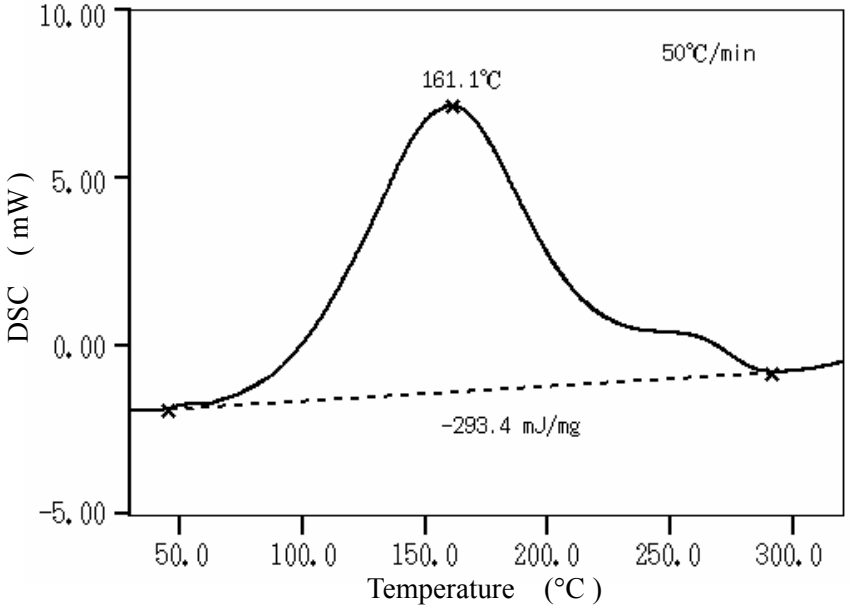

Figure 5 DSC Results for Epoxy Adhesives
Heating rate : 50°C/ min

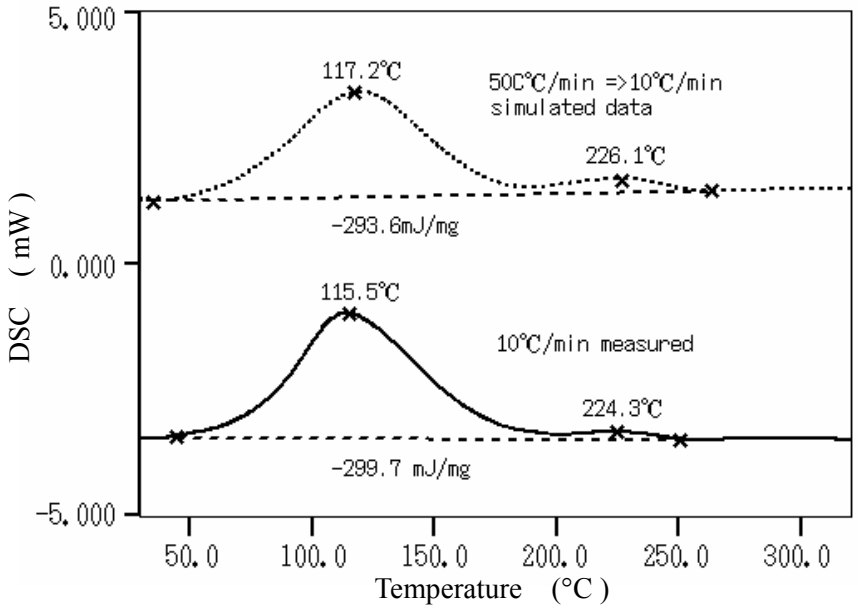

Figure 6 DSC Results for Epoxy Adhesives
Heating Rate : 10°C/ min
- - - - - - - - : Simulation data
———— : Measured data

4. Summary

Highway TA has some of the following applications.

1. Quality control

   Highway TA can save time (by speeding up the quality control process).

   Since data can be acquired at a higher heating rate, measurement time can cut by 50 to 90%.

2. Research fields

   The following evaluations can be performed using data simulations.

   Evaluation of reaction models ; For example, the validity of activation energy values can be evaluated by comparing actual and converted data..

   Separation of DTG and DSC peaks (for reactions different from activation energy).

   Estimation of measurement data for conditions with limitations in actual measurements, such as ultra-high (300°C/ min) or ultra-low (0.1°C/ min) heating rates

In the past, various cooling units, auto-samplers, and automatic analysis software have been used to save overall time and labor. Highway TA cuts measurement time by converting heating rates. Furthermore, it can provide researchers with user-friendly data simulation and it is expected to be applied to various objectives.

Reference

1) R. Kinoshita, R. Nakatani, Y. Ichimura and N. Nakamura, The 34th Japanese Conference on Calorimetry and Thermal Analysis, p42 (1998)