Decomposition kinetics of PET by TGA according to ASTM E1641

INTRODUCTION

Determining the kinetic parameters of a decomposition is an important step to evaluate the stability of a material. Different techniques, models and standards have been developed to be able to better understand these kinetics. Here, the decomposition of a polyethylene terephthalate sample (PET) was performed using the THEMYS ONE TGA. The method applied was the one described by the ASTM E1641-13 standard, which uses the Ozawa/Flynn/Wall isoconversional method.

Figure 1 – PET pellets

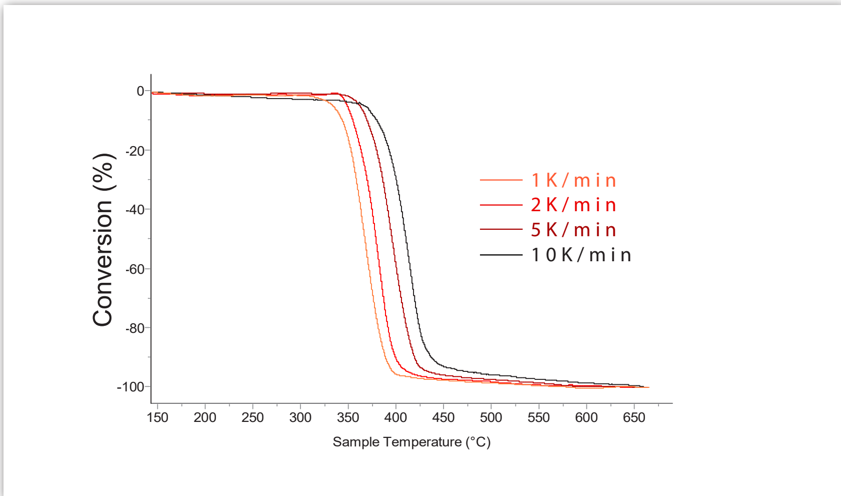


Figure 2 – Superimposition of the conversion vs. temperature signals obtained during the decomposition of PET at 1 K/min, 2 K/min, 5 K/min and 10 K/min

EXPERIMENT

THEMYS ONE TGA was used for the experiments. PET was cut in order to work with 3 ± 1mg samples for each test. A total of four experiments were run at different heating rates: 1, 2, 5 and 10K/min. The other experimental conditions were the following:

- Heating 25°C → 700°C at 1, 2, 5 or 10K/minute
- Atmosphere: nitrogen 30 ml/min
- Crucible: alumina

A blank experiment with an empty alumina crucible was run using the same experimental conditions for each heating rate. The obtained signals were used to subtract the contribution of buoyancy effects from the tests with samples.

RESULTS AND CONCLUSION

One mass loss was detected between about 300°C and 650°C for each experiment (**Figure 2**) and corresponds to a single step decomposition of the PET.

A conversion of 10% was selected as the failure criterion and the absolute temperatures corresponding to that conversion were determined. After plotting the heating rate logarithms versus the reciprocal temperatures, the slope of the curve was estimated by linear regression (**Figure 3**).

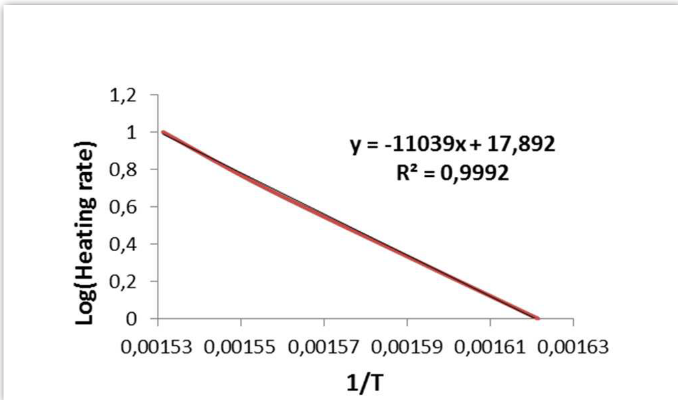


Figure 3 – Log(Heating rate) as a function of 1/T

The value of the slope m was then used to determine the activation energy, following this equation:

$$E = -m\left(\frac{R}{b}\right)$$

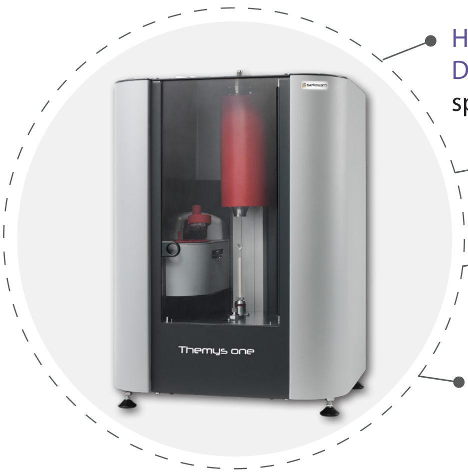
With:
E: the activation energy (J/mol)
R: gas constant (8.314J/mol.K)
b: logarithm of the Doyle approximation (b= 0.457/K for the first iteration)

The results found after calculation of that value and its uncertainty are: **E=200kJ/mol and δE=± 9 kJ/mol.**
It was also possible to determine the pre-exponential factor ln(A) with this method. It was equal to **27.1/min ± 1.3/min.**

Reference: ASTM E1641-13 Standard test method for decomposition kinetics by thermogravimetry using the Ozawa/Flynn/Wallmethod.

INSTRUMENT

THEMYS ONE



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