Designation: E3007 – 15

Standard Practice for Kinetic Values Used to Evaluate the Study of Decomposition Reactions by Thermogravimetry[1]

This standard is issued under the fixed designation E3007; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 It is the purpose of this practice to provide kinetic parameters for reference material(s) to be used for evaluation of thermogravimetry methods, apparatus, and software where decomposition mass loss and associated temperature are measured. This practice addresses *n*th order reactions.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 There is no International Organization of Standards (ISO) equivalent to this standard.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E473 Terminology Relating to Thermal Analysis and Rheology

E1142 Terminology Relating to Thermophysical Properties

E1641 Test Method for Decomposition Kinetics by Thermogravimetry Using the Ozawa/Flynn/Wall Method

E2958 Test Methods for Kinetic Parameters by Factor Jump/Modulated Thermogravimetry

NOTE 1—Test Methods E1641 and E2958 determine the pre-exponential factor A in units of min^{-1}. These results shall be converted to units of s^{-1} for comparison to values quoted in this practice using:

$$\ln[A,\ s^{-1}] = \ln[A,\ min^{-1}] + \ln[60\ s / min] = \ln[A,\ min^{-1}] + 4.094$$

3. Terminology

3.1 *Definitions*—Specific technical terms used in this practice are defined in Terminologies E473 and E1142, including *Arrhenius equation, derivative, reaction,* and *thermogravimetric analysis*.

3.1.1 *decomposition, n*—the process by which a substance is broken up into constituent parts, elements or simpler compounds.

3.1.2 *kinetics, chemical, n*—the study of the dependence of the chemical reaction rate on temperature and time.

4. Summary of Practice

4.1 Kinetics is the measurement and study of the rate of a chemical reaction to the independent parameters of time and temperature. This relationship is often described using the Arrhenius expression, where:

$$d\alpha/dt = A\, f(\alpha)\, \exp\left[-E/RT\right] \quad (1)$$

and:

α	=	fraction reacted (dimensionless),
$f(\alpha)$	=	some function of α,
E	=	activation energy (J mol^{-1}),
R	=	gas constant (= 8.314 J mol^{-1} K^{-1}),
T	=	absolute temperature (K),
t	=	time (s),
exp	=	natural logarithm base,
$d\alpha/dt$	=	fraction reaction rate (s^{-1}),
A	=	pre-exponential factor (s^{-1}), and
n	=	reaction order.

4.2 The function $f(\alpha)$ is commonly in the form:

$$f(\alpha) = (1 - \alpha)^n \quad (2)$$

and is known as an *n*th order reaction model.

4.3 Eq 1 may be evaluated in either its exponential or logarithmic form:

$$\ln[d\alpha/dt] = \ln[A] + \ln[f(\alpha)] - E/RT \quad (3)$$

4.4 The study of kinetics involves the determination of values of E, A, and n for a given chemical reaction.

NOTE 2—Activation energy and pre-exponential factor are not independent parameters.

NOTE 3—The descriptions provided in Eq 1-3 are only mathematical

[1] This practice is under the jurisdiction of ASTM Committee E37 on Thermal Measurements and is the direct responsibility of Subcommittee E37.02 on Standard Reference Materials.

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.