



Designation: E 1231 – 96a

Standard Practice for Calculation of Hazard Potential Figures-of-Merit for Thermally Unstable Materials¹

This standard is issued under the fixed designation E 1231; 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 This practice covers the calculation of hazard potential figures-of-merit for exothermic reactions, including:

- (1) Time-to-thermal-runaway,
- (2) Critical half thickness,
- (3) Critical temperature, and
- (4) Adiabatic decomposition temperature rise.

1.2 The kinetic parameters needed in this calculation may be obtained from differential scanning calorimetry (DSC) curves by methods described in other documents.

1.3 This technique is the best applicable to simple, single reactions whose behavior can be described by the Arrhenius equation and the general rate law. For reactions which do not meet these conditions, this technique may, with caution, serve as an approximation.

1.4 The calculations and results of this practice might be used to estimate the relative degree of hazard for experimental and research quantities of thermally unstable materials for which little experience and few data are available. Comparable calculations and results performed with data developed for well characterized materials in identical equipment, environment, and geometry are key to the ability to estimate relative hazard.

1.5 The figures-of-merit calculated as described in this practice are intended to be used only as a guide for the estimation of the relative thermal hazard potential of a system (materials, container, and surroundings). They are not intended to predict actual thermokinetic performance. The calculated errors for these parameters are an intimate part of this practice and must be provided to stress this. It is strongly recommended that those using the data provided by this practice seek the consultation of qualified personnel for proper interpretation.

1.6 *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:

- C 177 Test Method for Steady-State Heat Flux Measurements and Thermal Transmission Properties by Means of the Guarded Hot Plate Apparatus²
- C 518 Test Method for Steady-State Heat Flux Measurements and Thermal Transmission Properties by Means of the Heat Flow Meter Apparatus²
- D 4351 Test Method for Measuring the Thermal Conductivity of Plastics by the Evaporation-Calorimetric Method³
- E 473 Terminology Relating to Thermal Analysis⁴
- E 698 Test Method for Arrhenius Kinetic Constants for Thermally Unstable Materials⁴
- E 793 Test Method for Heats of Fusion and Crystallization by Differential Scanning Calorimetry⁴

3. Terminology

3.1 Definitions:

3.1.1 The definitions relating to thermal analysis appearing in Terminology E 473 shall be considered applicable to this practice.

3.2 Definitions of Terms Specific to This Standard:

3.2.1 *time-to-thermal-runaway*, t_c —an estimation of the time required for an exothermic reaction, in an adiabatic container, (that is, no heat gain or loss to the environment), to reach the point of thermal runaway, expressed by Eq 1.

3.2.2 *critical half thickness*, a —an estimation of the half thickness of a sample in an *unstirred container*, in which the heat losses to the environment are less than the retained heat. This buildup of internal temperature leads to a thermal-runaway reaction, expressed by Eq 2.

NOTE 1—This description assumes perfect heat removal at the reaction boundary. This condition is not met if the reaction takes place in an insulated container such as when several containers are stacked together or when a container is boxed for shipment. These figures-of-merit underestimate the hazard as a result of this underestimation of thermal conductivity.

3.2.3 *critical temperature*, T_c —an estimation of the lowest temperature of an *unstirred container* at which the heat losses

¹ This practice is under the jurisdiction of ASTM Committee E-27 on Hazard Potential of Chemicals and is the direct responsibility of Subcommittee E27.02 on Thermal Stability.

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² *Annual Book of ASTM Standards*, Vol 04.06.

³ *Annual Book of ASTM Standards*, Vol 08.03.

⁴ *Annual Book of ASTM Standards*, Vol 14.02.