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Standard Guide for Obtaining Data for Deterministic Fire Models¹

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1. Scope

- 1.1 This guide describes data required as input for mathematical fire models.
- 1.2 Guidelines are presented on how the data can be obtained.
- 1.3 The emphasis in this guide is on compartment zone fire models.
- 1.4 The values stated in SI units are to be regarded as the standard.
- 1.5 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 Transmisson Properties by Means of the Heat Flow Meter Apparatus²
- C 835 Test Method for Total Hemispherical Emittance of Surfaces from 20 to 1400°C²
- D 2395 Test Methods for Specific Gravity of Wood and Wood-Base Materials³
- D 3286 Test Method for Gross Calorific Value of Coal and Coke by the Isoperibol Bomb Calorimeter⁴
- D 3417 Test Method for Heats of Fusion and Crystallization of Polymers by Thermal Analysis⁵
- E 176 Terminology of Fire Standards⁶
- E 408 Test Methods for Total Normal Emittance of Surfaces Using Inspection-Meter Techniques⁷
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 - ³ Annual Book of ASTM Standards, Vol 04.10.
 - ⁴ Annual Book of ASTM Standards, Vol 05.05.
 - ⁵ Annual Book of ASTM Standards, Vol 08.02.
 - ⁶ Annual Book of ASTM Standards, Vol 04.07.
 - ⁷ Annual Book of ASTM Standards, Vol 15.03.

- E 472 Practice for Reporting Thermoanalytical Data⁸
- E 473 Terminology Relating to Thermal Analysis⁹
- E 537 Test Method for Assessing the Thermal Stability of Chemicals by Methods of Differential Thermal Analysis⁹
- E 603 Guide for Room Fire Experiments⁶
- E 793 Test Method for Heats of Fusion and Crystallization by Differential Scanning Calorimetry⁹
- E 906 Test Method for Heat and Visible Smoke Release Rates for Materials and Products⁶
- E 967 Practice for Temperature Calibration of Differential Scanning Calorimeters and Differential Thermal Analyzers⁹
- E 968 Practice for Heat Flow Calibration of Differential Scanning Calorimeters⁹
- E 1142 Terminology Relating to Thermophysical Properties⁹
- E 1321 Test Method for Determining Material Ignition and Flame Spread Properties⁶
- E 1354 Test Method for Heat and Visible Smoke Release Rates for Materials and Products Using an Oxygen Consumption Calorimeter⁶
- E 1623 Test Method for Determination of Fire and Thermal Parameters of Materials, Products, and Systems Using an Intermediate Scale Calorimeter (ICAL)⁶

3. Terminology

3.1 *Definitions*—For definitions of terms appearing in this guide, refer to Terminology E 176.

4. Significance and Use

- 4.1 This guide is intended primarily for users and developers of mathematical fire models. It is also useful for people conducting fire tests, making them aware of some important applications and uses for small-scale fire test results. The guide thus contributes to increased accuracy in fire model calculations, which depend greatly on the quality of the input data.
- 4.2 The emphasis of this guide is on zone models of compartment fires. However, other types of mathematical fire models need many of the same input variables.

Note 1—Mathematical fire models in this guide are referred to by their acronyms (see 5.4).

⁸ Discontinued; see 1995 Annual Book of ASTM Standards, Vol 14.02.

⁹ Annual Book of ASTM Standards, Vol 14.02.

5. Summary of Guide

- 5.1 This guide provides a compilation of material properties and other data that are needed as input for mathematical fire models. For every input variable, the guide includes a detailed description and information on how it can be obtained.
- 5.2 The following input variables are discussed: 6.1, air/fuel ratio; 6.2, combustion efficiency; 6.3, convective heat transfer coefficient; 6.4, density; 6.5, emissivity; 6.6, entrainment coefficient; 6.7, flame extinction coefficient; 6.8, flame spread parameter; 6.9, heat of combustion; 6.10, heat of gasification; 6.11, heat of pyrolysis; 6.12, rate of heat release; 6.13, ignition temperature; 6.14, mass loss rate; 6.15, production rate of species; 6.16, pyrolysis temperature; 6.17, specific heat; 6.18, thermal conductivity; and 6.19, thermal inertia.
- 5.3 Some guidance is also provided on where to find values for the various input variables.
- 5.4 A general commentary on zone models for compartment fires and a list of acronyms and data requirements for some models are included in Appendix X1.

6. Data for Zone Fire Models

- 6.1 Air/Fuel Ratio:
- 6.1.1 Introduction:
- 6.1.1.1 Flames can be characterized as being either premixed or diffusion. Premixed flames can be defined as those flames that result from the ignition of intimately mixed fuels and oxidizers. Diffusion flames can be defined as those flames that result from the ignition of the fuel within the region in which the originally separate fuel and oxidizer meet and mix. Diffusion flames are by far the more common type of flame to be encountered in hostile fire situations. A burning upholstered furniture item is an example of diffusion flame burning.
- 6.1.1.2 The source of the oxidizer in most fires is the oxygen contained in normal air. If a flame receives insufficient oxygen to burn all of the fuel vapors present completely, the flame is considered to be "oxygen limited" or "oxygen starved." Stoichiometric burning refers to conditions in which the amount of oxygen available in the combustion region exactly equals the amount required for complete combustion. A fuel-limited flame is one for which the amount of oxygen available is greater than that required for complete combustion of the available fuel vapors. Fuel-limited flame is sometimes also referred to as "free burn fire."
- 6.1.1.3 The air/fuel ratio, γ , of a fuel is a measure of the mass of air required per unit mass of fuel being burned. The effective air/fuel ratio required in some mathematical fire models is greater than or equal to the stoichiometric air/fuel ratio since it reflects the excessive air entrainment associated with free burning fires.
- 6.1.1.4 The air/fuel ratio is used in the fire models to calculate mass burning rates and hence heat release rate. The air/fuel ratio is unique to each fuel and is dimensionless [that is, mass/mass].
 - 6.1.2 Procedures to Obtain Air/Fuel Ratios:
- 6.1.2.1 As mentioned above, the stoichiometric air/fuel ratio is derived easily from the chemical balance equation describing the complete combustion of the fuel in normal air. For example, consider the burning of propane (C_3H_{\circ}) gas in air.

Here, air is described simply as containing oxygen and nitrogen.

air
$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3 CO_2 + 4H_2O + 18.8N_2$$
reactants products (1)

The mass ratio of air to fuel is found to be 686.4/44 = 15.6. Thus, the stoichiometric air to fuel ratio, γ_s , for propane is found to be 15.6.

- 6.1.2.2 Some models use an "effective" air/fuel ratio; for example, see Ref (1). ¹⁰ The main purpose of using an effective ratio different from the stoichiometric ratio is to prevent full utilization of oxygen entrained from the lower layer. However, this ad hoc approach is not generally accepted and validated. A physically correct method of preventing full utilization of the entrained oxygen requires the inclusion of an oxygen mass balance in the set of model conservation equations. Only the stoichiometric air/fuel ratio is needed in this case, while the combustion submodel accounts for the effects of vitiation and oxygen starvation.
- 6.1.3 Apparatus to Be Used—There is no direct need for an apparatus to determine the stoichiometric air/fuel ratio. The ratio can be calculated from the stoichiometry of the combustion reactions, but this is often not possible since the elemental composition of the fuel is seldom known. The most common way of determining the stoichiometric air/fuel ratio in actual fires or experiments is by calculating the ratio between the amount of energy released by combustion per mass unit of air fully depleted of its oxygen and the heat of combustion. The former is nearly identical for a wide range of materials and equal to 3 MJ/kg of air \pm 5%. Methods of determining the latter are discussed in 6.9.
 - 6.2 Combustion Efficiency:
- 6.2.1 Introduction—The effective heat of combustion in fires is smaller than the net heat of combustion because of the incomplete combustion of fuel vapors. The combustion efficiency, χ , accounts for incomplete combustion.
- 6.2.2 Procedures to Obtain Combustion Efficiency—The ratio between the effective heat of combustion and net heat of combustion is the combustion efficiency. Thus,

$$\chi = \frac{\Delta h_{c,eff}}{\Delta h_{net}} \tag{2}$$

where:

 $\Delta h_{c,eff}$ = effective heat of combustion, kJ/kg, and $\Delta h_{c,net}$ = net heat of combustion, kJ/kg.

The combustion efficiency for most hydrocarbons ranges from 0.4 to 0.9.

- 6.2.3 Apparatus to Be Used:
- 6.2.3.1 Test Method D 3286 for $\Delta h_{\rm c,net}$ (with adjustment for water vapor; see 6.9); and
- 6.2.3.2 Cone Calorimeter (Test Method E 1354), ICAL Apparatus (Test Method E 1623), or the Factory Mutual Small Scale Flammability Apparatus (2) for $\Delta h_{c,eff}$ (see 6.9).
 - 6.3 Convective Heat Transfer Coefficient:
 - 6.3.1 Introduction:

 $^{^{\}rm 10}$ The boldface numbers in parentheses refer to the list of references at the end of this standard.

6.3.1.1 Convective heat transfer refers to the movement of heat (energy) between a solid surface and a contacting fluid due to a temperature difference between the two. The modeling of convective heat transfer requires the use of a convective heat transfer coefficient, commonly referred to as h, which can be defined as follows:

$$h \equiv \frac{\dot{q}''}{\Lambda T} \tag{3}$$

 \dot{q}'' = energy transferred per unit area, W/m², and

= temperature difference between the surface and moving fluid, K.

- 6.3.1.2 The convective heat transfer coefficient commonly has SI units of W/m²·K; it is a function of the fluid properties (thermal conductivity, density, and viscosity), nature of the fluid flow (velocity and turbulence), and geometry of the solid surface.
- 6.3.2 Procedures to Obtain the Convective Heat Transfer Coefficient:
 - 6.3.2.1 General Method:
- (1) The selection of a proper heat transfer coefficient can be difficult due to the extremely large number of variables that must be included in its derivation, even for the relatively small number of practical situations encountered in mathematical fire modeling.
- (2) One wishing to obtain values for heat transfer coefficients generally searches compilations of previously derived values for those that best apply to a problem or situation. Examples of these sources include heat transfer texts (for example, see Ref (3)). The situation can be further simplified when the fluid is air, which of course is the situation generally encountered in fire modeling. Most fire models assume that smoke behaves like and has physical characteristics similar to those of air.
- (3) For example, the convective heat transfer coefficient for exchange between a turbulent air flow and a vertical plane can be approximated as follows:

$$h = 0.95(\Delta T)^{1/3} \tag{4}$$

where:

= W/m²·K, and

 ΔT = temperature difference between the vertical surface and the air, K.

6.3.2.2 Default Values in Some Existing Fire Models:

- (1) Some models currently have fixed heat transfer coefficients. Regardless of the conditions within the hot layer, the coefficient is set at a constant value of approximately 10 $W/m^2 \cdot K$.
- (2) Other models, such as CFC V (4) and FIRST (5) use a slightly more complex approach wherein the heat transfer coefficient is expressed as a function of the hot layer temperature. A lower limit of 5 W/m²·K and an upper limit of 50 W/m²·K were selected in this approach. The expression for calculating h in this method is as follows:

$$h = \text{minimum of } 50 \text{ W/m}^2 \text{K and } 5 + 0.45(T_1 - T_w)$$
 (5)

where:

 T_1 = layer temperature, K, and

 T_w = wall temperature, K.

(3) Finally, some models (6,7) use an even more complex approach in which the heat transfer coefficient is calculated from the Nusselt Number (Nu), which is a function of the Grashof Number (Gr) and the Prandtl number (Pr) in the familiar form:

$$Nu = \frac{hl}{k} = C_1 \text{ (GrPr)}^y$$
 (6)

where:

convective heat transfer coefficient, W/m²·K,

characteristic length of surface, m,

= thermal conductivity of the fluid, W/m·K,

 C_1 = a constant, and

= a constant.

(4) The equation implies that heat transfer is dominated by natural convection. This is not always true and not everywhere the case in room fires. For example, plume and vent flows generate significant velocities that drive heat transfer. Since the velocity is generated external to the heat transfer process, the convection heat transfer between walls or objects and these flows is forced rather than natural. For forced convection, the following equation for the Nusselt Number as a function of the Reynolds Number (Re) and the Prandtl number shall be used:

$$Nu = \frac{hl}{k} = C_2 \operatorname{Re}^{x} \operatorname{Pr}^{y}$$
 (7)

where:

where: $C_2 = a \text{ constant, and}$

= a constant.

6.3.3 Apparatus to Be Used—Unless there is a need (and availability) of a heat transfer coefficient for a specific situation, sufficient accuracy should be provided by selecting a value (or deriving one) judiciously from tabular data (and formulas). If experimental data are desired, the apparatus required may vary depending on the problem being explored.

6.4 Density:

6.4.1 Introduction:

- 6.4.1.1 The density of a material is the mass of material per unit volume. In fire models, density is usually expressed as kg/m .
- 6.4.1.2 There are two reasons for density to change as a material is heated: volatile (flammable or nonflammable, or both) may be lost and dimensional changes (expansion or contraction) may occur. Although corrections for temperature dependence can be made (8), many models use constant (room) temperature values.
 - 6.4.2 Procedures to Obtain Density:
- 6.4.2.1 The density of a material is determined by measuring the mass and physical dimensions (volume) of a sample of the material. There are detailed ASTM guidelines for certain types of building materials, for example, Test Methods D 2395 for wood and wood-base materials.
- 6.4.2.2 When the temperature dependence of density is sought, changes in mass with temperature can be determined using thermogravimetric analysis and changes in dimensions with temperature using dilatometric analysis (8,9).
 - 6.4.3 Apparatus to Be Used:
 - 6.4.3.1 Mass Balance (or equivalent).

6.4.3.2 Caliper, Ruler (or equivalent).

6.4.3.3 Dilatometric Apparatus.

6.4.3.4 Thermogravimetric Analyzer.

6.5 *Emissivity*:

6.5.1 *Introduction*—The emissivity of a material is the ratio of the power per unit area radiated from its surface to that radiated from a black body at the same temperature. A material's emissivity represents its thermal radiative behavior integrated over all wavelengths. Emissivity is a dimensionless quantity with an upper limit of unity for a black body.

6.5.2 Procedures to Obtain Emissivity— Several standard test methods have been developed to measure the emissivity of materials. A specimen of the material is usually placed in an evacuated chamber and heated (often with an electric current) to the temperature of interest. The power dissipated by the material is determined and equated to the radiative heat transfer to the surroundings. The emissivity of the material is computed using this power and the Stefan-Boltzman equation.

6.5.3 Apparatus to Be Used:

6.5.3.1 Vacuum Emittance Test Apparatus (Test Method C 835).

6.5.3.2 Inspection Meter (Test Methods E 408).

6.6 Entrainment Coefficient:

6.6.1 Introduction—Mass flow rates in flames and plumes are typically calculated in compartment zone fire models via empirical equations that are derived from entrainment theory. The latter is based on the assumption that the amount of air entrained into the flame or plume at a certain height is proportional to its (center-line) velocity at that height. The entrainment coefficient is defined as the constant of proportionality between both velocities or flow rates. The coefficient is dimensionless.

6.6.2 Procedures to Obtain Entrainment Coefficient:

6.6.2.1 For models that predict flame and plume flows via empirical equations, the entrainment coefficient is embedded into these equations. The equations are based on correlations of experimental data, and they are often hard-wired into the model code so that the user cannot change them. Some models account for a reduction in entrainment for flames and plumes against a wall or in a corner of walls. This is usually done automatically on the basis of the location of the fire, and the user is not allowed to change the entrainment coefficient explicitly.

6.6.2.2 Some models, such as the OSU room fire model (10), do not use empirical flame and plume equations. Alternatively, they include a numerical solution of the conservation equations in the flame and plume region. The entrainment coefficient shows up explicitly in the conservation equations, and the user is allowed to specify its value. The selection of a value for the coefficient is guided by experience and fine-tuned to optimize agreement between model predictions and experimental data.

6.6.3 Apparatus to Be Used—A standardized apparatus to measure the entrainment coefficient is not available. However, numerous experimental arrangements have been used to analyze diffusion flames and plumes. One approach to determine

entrainment consists of detailed velocity, temperature, and composition mapping of the flame or plume (11,12). However, such measurements are very tedious and time-consuming, and the flow rates that are obtained from integration of the measured profiles are prone to errors. The only practical method of measuring entrainment and hence the entrainment constant is the layer method used by Beyler, Zukoski, and others (13,14).

6.7 Flame Extinction Coefficient:

6.7.1 *Introduction*—The flame extinction coefficient interrelates average radiation parameters such as emissivity, flame intensity, and temperature over the entire spectrum of wavelengths. It is used in the following equation to calculate the emissive power of a flame:

$$\dot{E} = A\sigma_f^A \left(1 - e^{-kl}\right) \tag{8}$$

where:

E = emissive power of the flame, W,

 $A = \text{enveloping area of the flame, m}^2$,

 $\sigma = \text{Boltzman constant}, 5.67 \cdot 10^{-8} \text{ W/m}^2 \cdot \text{K}^4$

 T_f = flame temperature, K,

 \vec{k} = flame extinction coefficient, m⁻¹, and

l = path length, m.

k is also called the absorption coefficient, absorptionemission coefficient, or effective emission coefficient.

6.7.2 Procedures to Obtain Flame Extinction Coefficient—The coefficient k can be estimated from measurement of the emissivity ϵ and path length l, assuming emissivity can be expressed as $\epsilon = 1 - e^{-kl}$.

6.7.3 Apparatus to Be Used—There is no apparatus for measuring the flame extinction coefficient. The extinction coefficient can be determined by measuring all flame parameters in the equation for E except k. Fire models include many of such empirical equations, but the documentation usually does not specify what the parameters mean and how they are to be determined. It must be stressed that the equation for E is highly empirical. This makes it essential that the flame area, flame temperature, and extinction coefficient be determined in a self-consistent manner.

6.8 Flame Spread Parameter:

6.8.1 Introduction:

6.8.1.1 The opposed-flow (against the direction of the surrounding flow or against gravity) flame spread rate over a surface can be predicted via the equation originally developed by deRis (15):

$$V_p = \frac{\Phi}{k\rho c (T_{ig} - T_s)^2} \tag{9}$$

where:

 V_n = flame travel rate, m/s,

 ϕ^p = flame spread parameter, W²/m³,

 $k = \text{thermal conductivity, W/m} \cdot K$,

 ρ = density, kg/m³,

e = heat capacity, J/kg·K,

 T_{ig} = surface temperature at ignition, K, and

 T_s = surface temperature just prior to arrival of the flame front, K.

6.8.1.2 The flame spread parameter, ϕ , for specific orientations and in standard air environments is a characteristic for the heat transfer from the flame to the fuel ahead of the flame front in the vicinity of the flame foot. It is a material property expressed in W^2/m^3 .

6.8.2 Procedures to Obtain the Flame Spread Parameter—The flame spread parameter can be obtained from a correlation of opposed-flow flame spread data, that is, flame spread rate over a range of irradiance levels (or surface temperatures). The test method described in Test Method E 1321 was developed specifically to measure the flame spread parameter. It must be stressed that the equation for V_p is highly empirical. This makes it essential that V_p , $k\rho$ c, and T_{ig} be determined in a self-consistent manner. Further details on consistent methods to determine T_{ig} and $k\rho c$ can be found in 6.13 and 6.19, respectively.

6.8.3 Apparatus to Be Used:

6.8.3.1 LIFT Apparatus (Test Method E 1321).

6.9 Heat of Combustion:

6.9.1 Introduction—All combustion reactions generate energy, which may be expressed as heat. The heat of combustion is defined as the amount of heat generated when a unit quantity of fuel is oxidized completely. SI units for heat of combustion, $\Delta h_{\ c}$, is kJ/kg.

6.9.2 Procedures to Obtain Heat of Combustion:

6.9.2.1 Heats of combustion are measured by combustion bomb calorimetry. A known mass of fuel is burned completely in an adiabatic apparatus containing pure oxygen. This method yields the gross heat of combustion. The net heat of combustion can be determined by subtracting the latent heat of evaporation (2.26 kJ/kg of water) from the gross heat of combustion.

6.9.2.2 An effective heat of combustion can also be obtained from other tests that use oxygen calorimetry. For example, the cone calorimeter (Test Method E 1354) measures the mass loss rate and heat release rate. Incomplete combustion may occur in this environment. The effective heat of combustion, $\Delta h_{c,eff}$, is the ratio between heat release rate and mass loss rate.

$$\Delta h_{c,eff} = \frac{\dot{q}}{\dot{m}} \tag{10}$$

where:

 \dot{q} = heat release rate, kW, and

 \dot{m} = mass loss rate of the sample, kg/s.

6.9.3 Apparatus to Be Used:

6.9.3.1 Oxygen Bomb Calorimetry (Test Method D 3286).

6.9.3.2 Cone Calorimeter (Test Method E 1354).

6.9.3.3 ICAL Apparatus (Test Method E 1623).

6.9.3.4 Furniture calorimeter.

6.10 Heat of Gasification:

6.10.1 *Introduction*—The heat of gasification of a material is equal to the net amount of heat that must be supplied through its exposed surface to convert a mass unit to gaseous volatiles.

$$\Delta h_g = \frac{\dot{q}''_{net}}{\dot{m}''} \tag{11}$$

where:

 \dot{q}''_{net} = net heat flux into the material, kW/m², and \dot{m}'' = mass loss rate of the material, kg/m²·s.

The unit of Δh_g is kJ/kg.

6.10.2 Procedures to Obtain Heat of Gasification:

6.10.2.1 For a flaming sample, the net heat flux conducted into the material is equal to the sum of radiation and convection from the flame and the external heat flux (from the radiant heater in a small-scale test), minus the (radiant) heat losses from the surface. The flame flux and heat losses depend on the surface temperature, which is very difficult to measure. The cone calorimeter (Test Method E 1354) has been used, in conjunction with surface temperature measurements, to determine Δh_p for wood products and PMMA.

6.10.2.2 For some materials, the surface temperature is reasonably constant and independent of exposure conditions. A plot of (mean or peak) mass loss rates as a function of external irradiance yields a fairly linear relationship for such materials. Values of Δ h_g can then be estimated from the inverse of the slope of the regression line through the data points. Tewarson and Petrella have used this technique to obtain Δh_g values for a wide range of plastics (2,16).

6.10.2.3 Unfortunately, surface temperatures are not constant for many materials, in particular charring materials and materials with a high smoke yield. The method by Tewarson and Petrella can still be used, but it yields results that have little physical meaning. Various investigators have used the version of the equation for Δh_g and have obtained a time-dependent heat of gasification curve instead of a single value (17,19)

6.10.3 Apparatus to Be Used:

6.10.3.1 Cone Calorimeter (Test Method E 1354).

6.10.3.2 ICAL Apparatus (Test Method E 1623).

6.10.3.3 Factory Mutual Small Scale Flammability Apparatus (2).

6.11 Heat of Pyrolysis (Heat of Reaction):

6.11.1 Introduction:

6.11.1.1 Chemical reactions generally involve the generation or absorption of energy. The heat of pyrolysis is the energy emitted or lost during the pyrolysis or thermal degradation of material. It is also defined as the difference between the enthalpy of the virgin material and the enthalpy of the products. In calculation of the heat of reaction, the products are assumed to be at the pyrolysis temperature, and the virgin material is assumed to be at the ambient temperature. SI units of the heat of pyrolysis are J/kg. It is sometimes expressed in J/m³ or J/s·m³ in models.

6.11.1.2 Bench scale tests generally measure the heat of pyrolysis of a small sample exposed to well-prescribed thermal conditions. Heat of pyrolysis or the corresponding change in enthalpy is usually an input parameter in the energy balance equation for a solid material undergoing thermal degradation.

6.11.1.3 The heat of pyrolysis is generally found in models that calculate the temperature profile within a solid material as it is being heated. The internal energy generation term can be represented in several different ways depending on model. One common way is to multiply the heat of pyrolysis Q (in kJ/kg) by the local rate of decomposition (in kg/m³·s) to obtain the energy generation term. An alternative is simply to use an

energy generation term dE/dt (in kW/m³). An alternative for Q is to input the specific heat capacities and enthalpies of formation and have the computer program calculate the enthalpies and corresponding heat of pyrolysis Q. Some models will not have a heat of pyrolysis term since the net energy change is assumed to be zero. The energy generation term may also include sensible energy as well as energy change due to pyrolysis.

6.11.2 Procedures to Obtain Heat of Pyrolysis:

6.11.2.1 The most common experimental procedure to measure the heat of pyrolysis is differential scanning calorimetry (DSC). A small quantity (a few mg) of sample is placed in the apparatus. Thermal degradation is obtained using a specified time-temperature exposure. Heat is added to the sample and an inert reference compound so the two materials are maintained at identical temperatures. The added heat is recorded and is assumed to equal the energy lost or gained as a result of the endothermic or exothermic reaction. The sample environment is purged with nitrogen or another inert gas when oxidation reactions are not to be considered. DSC results are affected by such factors as particle size and heating rate. Because of these factors, it can be argued that the DSC results for such small samples are not representative of the behavior of the material in practice. DSC procedures are also used to measure the enthalpy gain or loss associated with physical processes such as vaporization and desorption, as well as the specific heat capacity of a material.

6.11.2.2 The heat of pyrolysis (Δh_p) is generally considered negative for exothermic reactions and positive for endothermic reactions. DSC results are usually presented as a curve, with the energy input on the ordinate with upward deflection reflecting an exothermic reaction and time or temperature on the abscissa increasing from left to right. Standard practices for reporting thermoanalytical data are given in Practice E 472.

6.11.2.3 An alternative thermal analysis is differential thermal analysis (DTA). The temperature difference between the sample and the reference material is measured in DTA as a function of temperature. Quantitative results for the heat of pyrolysis can be calculated from DTA results. Thermogravimetry (TGA) can be used to measure the mass loss as a function of temperature.

6.11.2.4 Estimates for heat of pyrolysis have also been calculated from other measurements. One alternative to measuring the heat of reaction is to add the enthalpies of the products and subtract them from the enthalpy of the virgin material. Another procedure that has been used is to develop a transient heat balance model that has the heat of pyrolysis as the unknown. The energy balance equation is solved for the heat of pyrolysis based on experimentally obtained temperature profile data.

6.11.2.5 The methods mentioned above are not suitable for layered composite materials.

6.11.3 Apparatus to Be Used:

6.11.3.1 Several commercial instruments are available and are generally designed to perform other types of thermal analysis as well as DSC. The basic components of the DSC are the sample containers, heating unit, programmable temperature controller, inert reference material, and measuring and recording devices.

6.11.3.2 DSC procedures and apparatuses are discussed in Test Methods D 3417, E 537, and E 793. Power-compensation DSC and heat-flux DSC are two types of apparatuses. Calibration of DSC equipment is discussed in Practices E 967 and E 968.

6.12 Rate of Heat Release:

6.12.1 Introduction—A realistic calculation of the effects of fire requires knowledge of the burning rate. The burning rate can be expressed as the mass generation rate of fuel volatile or as a rate of heat release, \dot{q} . The units of heat release rate are W or kW.

6.12.2 Procedures to Obtain Rate of Heat Release:

6.12.2.1 The rate of heat release cannot be predicted from basic measurements of material properties; it is a function of the thermal environment, fuel volatilization, and efficiency of volatile combustion. The heat release rate and mass loss rate are related by the following equation:

$$\dot{q} = \dot{m}\chi \Delta h_{c,net} \tag{12}$$

where:

 $\Delta h_{c,net}$ = net heat of combustion of the volatile, kJ/kg,

= combustion efficiency, and = mass loss rate of fuel, kg/s.

6.12.2.2 The heat release rate can also be estimated by assuming that heat is generated by a reaction in which only H₂O, CO₂, and CO are produced, and O₂ is depleted (20, chapter 3). The heat release rate, \dot{q} , can be calculated from the following equations (21):

$$\dot{q}'' = k_{O_2} \dot{D}_{O_2}^{"} \tag{13}$$

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$$\dot{q}'' = \frac{\Delta h_{c,net}}{k_{CO}} \dot{G}_{CO_2}'' + \frac{\Delta h_{c,net} - \Delta h_{CO}}{k_{CO}} \dot{G}_{CO}''$$
(14)

where:

= heat release rate per unit area, kW/m²,

= net heat of complete combustion of the material,

= heat of combustion of CO, kJ/kg,

 $\dot{\Delta}h_{CO}$ \dot{D}''_{O_2} = depletion rate of oxygen per unit surface area,

kg/m ·s,

= mass oxygen-to-fuel stoichiometric ratio, kg/kg,

 k_{O_2} k_{CO_2} maximum possible yield of CO₂, kg/kg, k_{CO} G''_{CO_2} G''_{CO} maximum possible yield of CO, kg/kg, generation rate of CO₂, kg/m²·s, and = generation rate of CO, $kg/m^2 \cdot s$.

6.12.3 Apparatus to Be Used:

6.12.3.1 The heat release rate can be estimated by measuring the sensible enthalpy of the fire gas outflow. The Ohio State University apparatus (Test Method E 906) applies this principle, but it has proven difficult and generally inaccurate. Most heat release rate measurement devices currently use the oxygen calorimetry principle (22) as implemented in the cone calorimeter (Test Method E 1354). One can use the following for small-scale measurements: