COMPUTER TOOLS TO DETERMINE MATERIAL PROPERTIES FOR FIRE GROWTH MODELING FROM CONE CALORIMETER DATA

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ABSTRACT

A set of computer tools was developed to assist fire protection engineers with the analysis of Cone calorimeter data for modeling. The tools consist of various MS Excel templates and macros. They can be used to determine material properties that are needed as input data for flame spread and fire growth modeling. This paper describes the physical basis for the calculations that are performed by the tools.

INTRODUCTION

The main limitation of current compartment fire models is that they generally are not capable of predicting fire growth, but are only suitable to calculate the consequences of a user-specified fire [1]. An extensive database of fire curves would alleviate this problem, but the development of an exhaustive database of fire curves is not feasible. A more practical approach involves the use of correlations and sub-models, so that fire curves can be constructed for a variety of geometries and configurations on the basis of material properties from small-scale fire test data.

Methods have been developed to predict the heat release rate vs. time of objects that are common in residences such as chairs and TV sets [2-7]; and large objects such as automobiles and railcars [8]. However, the most common geometry for which predictive sub-models have been developed is the room/corner test [9]. Standard room/corner test protocols have been developed domestically (e.g., NFPA 265 and NFPA 286) as well as internationally (ISO 9705).

Many sub-models require that the fire performance of materials be characterized on the basis of a number of fundamental material properties. A set of computer tools was developed to obtain these properties on the basis of Cone calorimeter data (ASTM E 1354 or ISO 5660). The tools consist of various MS Excel templates and macros. This paper describes the physical basis for the calculations that are performed by the tools. Use of the tools to obtain ignition and heat release properties is illustrated for four wood products.

PILOTED IGNITION

Piloted Ignition Properties

Three properties are commonly used to describe the piloted ignition behavior of a material.

- 1. The first property quantifies a critical condition for ignition. Piloted ignition occurs when the lower flammability limit is reached in the fuel-air mixture around the pilot. Consequently, a critical mass flux criterion appears to be logical. This has been proposed [10, 11], but unfortunately it is not very practical. The most common criterion is based on the assumption that ignition occurs when a critical temperature at the surface, T_{ig} , is reached. The surface temperature at ignition of a thermoplastic is reasonably constant and independent of heat flux [12, 13]. The surface temperature at ignition of a charring material such as wood is also reasonable constant when the time to ignition is less than a few minutes, but increases dramatically at heat fluxes below 20-25 kW/m² [14-19].
- 2. The second property is the minimum heat flux for ignition, \dot{q}_{\min} . This heat flux is just sufficient to heat the material surface to T_{ig} for very long exposure times (theoretically ∞). The minimum heat flux is not a true material property, because it depends on the rate of convective cooling from the surface. This, in turn, depends primarily on the orientation, size, and flow field around the exposed surface. Since these are different in a small-scale test vs. a real fire, the minimum heat flux determined based on test data is an approximate value. To make the distinction, it is referred as the critical heat flux for ignition, \dot{q}_{Cr} . The critical heat flux may also vary between different small-scale test apparatuses due to differences in convective cooling. For example, Dietenberger obtained critical heat flux values of 14.3 and 18.8 kW/m² for conditioned redwood in the Cone calorimeter and LIFT apparatus (ASTM E 1321) respectively [20].
- 3. The third property is a measure of how fast the surface temperature of a material rises when exposed to heat. This property is usually referred to as the thermal inertia, kpc. A material with lower kpc will ignite faster than a material with higher kpc and the same T_{ig} exposed to the same heat flux.

Procedures to Obtain Ignition Properties

Ignition properties can be determined by direct measurements. T_{ig} can be measured with fine thermocouples attached to the exposed surface of ignition test specimens, or by using an optical pyrometer. \dot{q}'_{Cr} can be determined by bracketing, i.e., by conducting experiments at incrementally decreasing heat flux levels until ignition does not occur within a specified period (usually 10 or 20 min). *kpc* can be determined by measuring thermal conductivity, density, and specific heat separately. However, since **k** and *c* are temperature-dependent measurements at elevated temperature are needed.

Because it is very tedious to measure T_{ig} and **kpc** directly, it is much more common to determine ignition properties on the basis of an analysis of time-to-ignition data obtained over a range of heat fluxes. The analysis is usually based on a simple heat conduction model, which assumes that the solid is inert (negligible pyrolysis prior to ignition) and thermally thick (heat wave does not reach the back surface prior to ignition). Some procedures have been expanded to account for specimen thickness effects. It is important to understand that properties obtained from such analyses are model parameters, which are not necessarily a good estimate of the real values. An overview of different procedures that are included in the computer tools are briefly discussed below.

Quintiere

Quintiere et al. developed a practical procedure for analyzing ignition data obtained with the Lateral Ignition and Flame spread Test or LIFT apparatus [21]. The apparatus and procedure are described in detail in ASTM E 1321. The LIFT is primarily a flame spread apparatus. But as the heat flux is fairly uniform over

the first 100 to 150 mm near the hot end of the specimen, the apparatus can also be used for ignition tests. In that case 155 mm × 155 mm samples are exposed in the vertical orientation to the heat of a radiant gas panel (280 mm **x 483** mm). A premixed acetylene pilot is located in the boundary layer above the sample.

The first step in Quintiere's procedure consists of running ignition tests starting at an irradiance level near the maximum for the apparatus ($60-65 \text{ kW/m}^2$). Time to ignition is obtained at heat flux levels in descending order at intervals of 5 to 10kWAm², preferably with some replicates. When ignition time becomes sufficiently long (say about 10 minutes), data is obtained at heat flux levels more closely together (1.5 to 2 kW/m^2 intervals). At a certain level, ignition will no longer occur within the (arbitrary) maximum test duration of 20 minutes. The critical heat flux is taken to be slightly above this level. Usually, a few more tests are conducted around this level to confirm its value. Once the critical heat flux is known, T_{ig} can be calculated from a heat balance at the surface (see Figure 1) after very long exposure, since heat conduction into the specimen then becomes negligible

$$\alpha \dot{q}_{cr}^{"} \approx \varepsilon \dot{q}_{cr}^{"} = h_c (T_{ig} - T_{\infty}) + \varepsilon \sigma (T_{ig}^4 - T_{\infty}^4) \equiv h_{ig} (T_{ig} - T_{\infty})$$
(1)

where a = surface absorptivity

E = surface emissivity

 $h_{\rm c}$ = convection coefficient (kW/m²·K)

- $T_{ig} = surface temperature at ignition (K)$ $<math>T_{\infty} = surface temperature at ignition (K)$
- σ = Boltzmann constant (5.67 kW/K⁴·m²)
- h_{ig} = total heat transfer coefficient at ignition (kW/m²·K)

Surface temperature measurements under steady state conditions for a number of inert materials and some combustible materials resulted in the following fit:

$$\dot{q}_{CF}^{"} = 0.015(T_{ig} - T_{\infty}) + \sigma(T_{ig}^{4} - T_{\infty}^{4}) = h_{ig}(T_{ig} - T_{\infty})$$

$$(2)$$

$$P + LOT FLAME$$

$$(1 - \varepsilon) q^{"} t h_{c}(T - T_{c}) e^{-\varepsilon} e^{-\varepsilon$$

Figure 1. Surfaceheat balance of a specimen exposed in a piloted ignition test

Thus, if specimens are heated for a sufficiently long time in the LIFT apparatus, it may be assumed that $\alpha = \varepsilon = 1$ and that $h_c = 15 \text{ W/m}^2 \cdot \text{K}$. Once T_{ig} is calculated from the empirical value for \dot{q}'_{cr} via Eq. (2), a total heat transfer coefficient fkom the surface at ignition can be obtained by rearranging Eq. (2)

$$h_{ig} = \frac{\dot{q}_{cr}^{''}}{T_{ig} - T_{\infty}} = 0.015 + \sigma \frac{T_{ig}^4 - T_{\infty}^4}{T_{ig} - T_{\infty}}$$
(3)

In analogy with results obtained by Simms [22], surface temperature at igntion for exposure to a constant irradiance is written as

$$T_{ig} = T_{\infty} + \frac{\dot{q}''_e}{h_{ig}} \mathbf{F}(t_{ig})$$
(4)

where t_{ig} = time to ignition (s) \dot{q}''_{e} = incident heat flux (kW/m²)

For a semi-infinite solid, based on solutions for linearized surface heat losses, F(t) is approximated as

$$F(t) = \begin{cases} \frac{2 h_{ig} \sqrt{t}}{\sqrt{\pi k \rho c}} & \text{small} \\ 1 & \text{large } t \end{cases}$$
(5)

With (3) and (4) this leads to the following expression for correlation of piloted ignition data:

$$\frac{\dot{q}_{cr}}{\dot{q}_{e}''} = \mathbf{F}(t_{ig}) = \begin{cases} \frac{2 h_{ig} \sqrt{t_{ig}}}{\sqrt{\pi k \rho c}} & t_{ig} \leq t^{*} \\ \frac{1}{\sqrt{\pi k \rho c}} & t_{ig} > t^{*} \end{cases}$$
(6)

where $t^* = \text{time to reach steady conditions (s)}$

Thus, all data is plotted in a graph of $\dot{q}''_{Cr}/\dot{q}''_{e}$ versus $\sqrt{t_{ig}}$. An "apparent" value for kpc can be calculated from the slope of the line through zero that best fits the data. This line crosses $\dot{q}_{cr}'/\dot{q}_{e}'' = 1$ at t*, the time needed to reach "steady-state" conditions. The functional form of (6) at small times is identical to that of the solution of the one-dimensional heat conduction equation for a semi-infinite solid exposed to a heat flux without heat losses from the surface. Consequently, $k\rho c$ values obtained with this procedure are higher than actual average values. The same procedure can be used to analyze piloted ignition data obtained with the Cone calorimeter, provided an adjustment is made to h_c to account for the differences in convective cooling conditions. Since specimen size (100 × 100 mm) is smaller than in the LIFT apparatus, subsequent studies by Quintiere et al. used an estimated lower value of $h_c = 10 \text{ W/m}^2 \text{ K}$ for the Cone calorimeter [23, 24].

Mikkola

Mikkola and Wichman analyzed a thermal ignition model in two ways [23-25]:

- 1. Exact solution via Laplace transforms of the linearized heat conduction problem with constant *k* and *c* for thermally thick and thermally **thin** samples.
- 2. Approximate integral solution of the problem with non-linear heat losses for thermally thick, thermally thin and thermally intermediate specimens.

Both approaches resulted in the recommendation to correlate $(1/t_{ig})^n$ with \dot{q}_e , where n = 0.5 for thermally thick materials, n = 1 for thermally thin materials and n = 2/3 for thicknesses in between. Mikkola and Wichman also provided some guidance for estimating thermal thickness from physical thickness of wood products. Thermally thick samples are over 15-20mm, thermally thin samples are thinner than 1-2mm, while n = 2/3 corresponds to a thickness around 5 mm. Practical application of this procedure was illustrated for some data from previous investigators **and** new data obtained for some wood products and PMMA.

Delichatsios

Delichatsios et al. considered the heat conduction equation for a semi-infinite solid with constant thermal properties together with the following more general boundary condition at the exposed side [26]:

$$-k \left. \frac{\partial T}{\partial x} \right|_{x=0} = \dot{q}_{net}^{"} \left(T_s(t), t \right)$$
(7)

where **k**

k = thermal conductivity (kW/m·K) T = temperature (K) x = length coordinate and distance from exposed surface (m) $\dot{q}''_{net} = \text{net heat flux into the solid (kW/m²)}$ $T_{s} = \text{surface temperature (K)}$

Applying Duhamel's theorem leads to the following integral equation for surface temperature:

$$T_{s}(t) = T_{\infty} + \sqrt{\frac{1}{\pi k\rho c}} \int_{0}^{t} \frac{\dot{q}_{net}^{"}(\tau)}{\sqrt{t-\tau}} d\tau$$
(8)

The net heat flux $\dot{q}_{net}^{"}$ is equal to the difference between the absorbed irradiance and the heat losses from the surface. Delichatsios solved Eq. (8) numerically for the case of surface heat losses only due to reradiation (no convection) via a continuation method. The form of the solution was too complex for correlation of experimental data. However, it was used to validate other asymptotic and approximate solutions, simple enough for correlation of experimental data. Two such asymptotic solutions were obtained and validated: one for small times and one for large times. Both were linear relationships between $1/\sqrt{t_{ig}}$ and $\dot{q}_e^{"}$, but with different slopes and intercepts. The critical heat flux from extrapolation of high-flux data was found to be approximately **64%** of the intercept with the abscissa and the linear fit through the low-flux data. Piloted ignition data obtained for PMMA correlated well according to the asymptotic solutions.

Janssens

Janssens' extensive numerical calculations showed that the following expression is suitable for correlating piloted ignition data of thermally thick solids [27].

$$\dot{q}_{e}'' = \dot{q}_{cr}'' \left[1 + 0.73 \left(\frac{k \rho c}{h_{ig}^{2} t_{ig}} \right)^{0.55} \right]$$
(9)

The practical significance of Equation (9) is that for a thick material, ignition data points plotted as $(1/t_{ig})^{0.55}$ versus $\dot{q}_e^{"}$ should fall on a straight line. The intercept of the line with the abscissa is $\dot{q}_{cr}^{"}$. Once $\dot{q}_{cr}^{"}$ is found, T_{ig} and h_{ig} can be obtained by solving Eq. (2) with $h_c = 13.5 \text{ W/m}^2$ ·K for the Cone calorimeter in the vertical orientation [18]. Finally, $k\rho c$ can be calculated from the slope of the line. Actual ignition data usually show some scatter, but the linear trend in a plot of $(1/t_{ig})^{0.55}$ versus $\dot{q}_e^{"}$ remains apparent, provided the material is thermally **thick.** A linear regression analysis is performed to find the best-fitting straight line through the data. The intercept and slope of the line are used to obtain the best estimates for \dot{q}_{cr} (and consequently T_{ig} and h_{ig}) and kpc.

For materials that do not behave as a semi-infinite solid at low irradiance levels, it is proposed to concentrate measurements in the region where the material appears to behave as a thermally thick solid [28]. In this case \dot{q}_{cr} is found by correlating t_{ig} and \dot{q}_{e}'' according to the following power law relationship first suggest by Smith et al. [29]:

$$(\dot{q}_e^{"} - \dot{q}_{cr}^{"})t^n = C \tag{10}$$

where n = exponent to be determined as fitting parameter C = constant to be determined as fitting parameter

Dietenberger

Dietenberger developed the following interpolation formula for finitely thick materials with convective cooling and radiative heating on the exposed side and insulation on the unexposed side [20]:

$$\frac{\dot{q}_{e}^{"}}{\dot{q}_{cr}^{"}} = 1 + \frac{1}{\left(F_{thick}^{n} + F_{thin}^{n}\right)^{n}}$$
(11)

where \dot{q}_{cr} and h,, are related to T_{ig} according to Eq. (2) and

$$n = \frac{2.68 \pm 0.4Bi}{1\pm Bi} \tag{12}$$

$$F_{thick} = \sqrt{\frac{4}{\pi} B i^2 F o}$$
(13)

$$F_{thin} = \exp\left(\frac{BiFo}{1+0.254Bi}\right) - 1$$

$$Bi = \text{Biot number } (h_{ig}L/k)$$

$$Fo = \text{Fourier number } (kt_{ig}/\rho cL^2)$$

$$L = \text{specimen thickness } (m)$$

$$\rho = \text{density } (kg/m^3)$$

$$c = \text{specific heat } (kJ/kg\cdot K)$$

$$(14)$$

A non-linear parameter estimation program is used to determine the values for T_{ig} , k, and kpc that result in the best agreement between Eq. (12) and the experimental data. Dietenberger found that the convection coefficient (kW/m²·K) in the Cone calorimeter varies with heat flux (kW/m²) according to the following relationship:

$$h_c = 0.01433 + 1.33 \cdot 10^{-4} \dot{q}_e^{"} \tag{15}$$

Shields

Analogous to **Smith's** approach Shields et al. correlated piloted igntion data according to **Eq.** (10) with C defined as the flux-time-product or *FTP* [30].

Tewarson

Tewarson correlates piloted ignition data obtained in the Fire Propagation Apparatus (ASTM E 2058) by plotting $1/\sqrt{t_{ig}}$ as a function of \dot{q}''_{e} [31]. The intercept with the abscissa of a straight-line fit through the data is defined as the critical heat flux. The reciprocal of the slope of the line is referred to as the thermal response parameter (TRP).

Hopkins

Hopluns et al. also proposed plotting $1/\sqrt{t_{ig}}$ as a function of \dot{q}_e'' [24]. The critical **flux** is obtained as the intercept of a straight-line fit and the abscissa. T_{ig} is calculated from \dot{q}_{cr}' according to Eq. (2) with $h_c = 10$ W/m²·K for the Cone calorimeter in the horizontal orientation. Thermal inertia is calculated from the following equation, which was derived from an integral solution of the heat conduction problem:

$$k\rho c = \frac{3}{2} \left(\frac{\varepsilon}{S(T_{ig} - T_{\infty})} \right)^2$$
(16)

Moghtaderi

Moghtaderi et al. proposed a procedure to analyze ignition data of wood that is very similar to that developed by Hopluns et al. [32]. It was demonstrated that the proposed procedure is consistent with surface temperature measurements, which indicate that T_{ig} increases at decreasing heat fluxes. $h_c = 11$ W/m²·K and $\varepsilon = 1$ were used for the Cone calorimeter in the horizontal orientation and **charred** wood

respectively. Thermal inertia is calculated from the following equation, which was also derived from an integral solution of the heat conduction problem:

$$k\rho c = \frac{4}{3} \left(\frac{l}{0.7071S(T_{cr} - T_{\infty})} \right)^2 = \frac{8}{3} \left(\frac{1}{S(T_{cr} - T_{\infty})} \right)^2$$
(17)

where $T_{cr} = T_{ig} \operatorname{at} \dot{q}''_{e}$ equal to \dot{q}''_{Cr} (K)

Spearpoint

Finally, Spearpoint et al. also used an integral model to develop a procedure for analyzing piloted ignition data of wood [33]. It is proposed to plot $1/\sqrt{t_{ig}}$ as a function of $\dot{q}_e^{"}$. The intercept of a straight-line-fit through high-flux data points ($\dot{q}_e^{"} \ge 20 \text{ kW/m}^2$) and the abscissa is approximately 76% of the critical heat flux. T_{ig} is calculated from $\dot{q}_{cr}^{"}$ according to Eq. (2), with $h_c = 18 \text{ W/m}^2 \text{ K}$ for the Cone calorimeter and $\mathbf{z} = 1$ for charred wood. Thermal inertia is again calculated from the slope of the regression line.

HEAT RELEASE RATE

Heat Release Rate Properties

The two properties that are related to heat release rate are the effective heat of combustion, ΔH_c , and the heat of gasification, *L*. Both are expressed in MJ/kg. The effective heat of combustion is the ratio of heat release rate to mass loss rate measured in a small-scale calorimeter:

$$\Delta H_c \equiv \underbrace{\Theta''}_{m''} \tag{18}$$

where $\dot{Q}'' =$ heat release rate per unit exposed area (kW/m²) $\dot{m}'' =$ mass loss rate per unit exposed area (g/m²As)

The heat of gasification is defined as the net heat flow into the material required to convert one mass unit of solid material to volatiles. The net heat flux into the material can be obtained from an energy balance at the surface of the specimen. Typically, a sample exposed in a bench-scale calorimeter is heated by external heaters and by its own flame. Heat is lost from the surface in the form of radiation. Due to the small sample size, the flame flux is primarily convective, and flame absorption of external heater and specimen surface radiation can be neglected. Hence, L can be defined as

$$L = \frac{\dot{q}_{net}}{\dot{m}''} = \frac{\dot{q}_{e}'' + \dot{q}_{f}'' - \dot{q}_{l}''}{\dot{m}''}$$
(19)

where $\dot{q}_{e}^{"}$ = heat flux from external sources (kW/m²) $\dot{q}_{f}^{"}$ = heat flux from the flame (kW/m²) $\dot{q}_{l}^{"}$ = heat losses from the exposed surface (kW/m²)

Procedures to Obtain Heat Release Properties

Dillon et al. proposed three methods to calculate the effective heat of combustion [23]. The first value is equal to the ratio of first peak heat release rate and mass loss rate at the same time. The second value is obtained as the ratio of the average heat release rate over the peak burning period and the mass loss rate over the same period. The peak burning period is defined as the period around the first peak heat release rate during which the heat release rate is at least 80% of the first peak heat release rate. The third value is equal to the ratio of total heat released and total mass loss over the entire flaming period.

Similarly, Dillon et al. proposed six methods to calculate the heat of gasification [23]. The first three values are derived from Eq. (19), and are equal to the reciprocal of the slope of a linear fit through data points of peak mass loss rate, average mass loss rate over the peak burning period and average mass loss rate over the entire flaming period respectively plotted as a function of heat flux. The other three values are equal to the appropriate heat of combustion times the reciprocal of the slope of a linear fit through data points of first peak heat release rate, average heat release rate over the peak burning period and average mass loss rate over the entire flaming period respectively plotted as a function of heat flux.

Janssens demonstrated that the values based on peak or average mass loss rates are too high for wood, and suggested a method to determine L as a function of char depth [34]. This method is based on an integral model for the heat conduction through the char layer, assumes that wood converts to char at T_{ig} , and uses literature values for the specific heat and thermal diffusivity of wood char. Janssens' results are consistent with a theoretical analysis [35] and calculated L values based on measured surface temperatures [36].

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