DOT/FAA/TC-12/13

Federal Aviation Administration
William J. Hughes Technical Center
Aviation Research Division
Atlantic City International Airport
New Jersey 08405

A PROBABILISTIC ANALYSIS OF PASS/FAIL FIRE TESTS

October 2013

Final Report

U.S. Department of Transportation
Federal Aviation Administration

NOTICE

Technical Report Documentation Page

1. Report No. DOT/FAA/TC-12/13	2. Government Accession No.	3. Recipient's Catalog No.

4. Title and Subtitle

A PROBABILISTIC ANALYSIS OF PASS/FAIL FIRE TESTS

5. Report Date

October 2013

6. Performing Organization Code

7. Author(s)

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8. Performing Organization Report No.

9. Performing Organization Name and Address

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10. Work Unit No. (TRAIS)

11. Contract or Grant No.

12. Sponsoring Agency Name and Address

U.S. Department of Transportation
Federal Aviation Administration
Northwest Mountain Region—Transport Airplane Directorate
1601 Lind Avenue, SW
Renton, WA 98057

13. Type of Report and Period Covered

Final Report

14. Sponsoring Agency Code

ANM-115

15. Supplementary Notes

The Federal Aviation Administration William J. Hughes Technical Center Aviation Research Division COR was Richard E. Lyon.

16. Abstract

Several material fire properties were evaluated as sole explanatory variables for two pass/fail flammability tests using two different probabilistic models. The fire behavior and properties investigated span the range of commercial polymers and flame-retardant plastics. The flammability tests included a fire test used by the Federal Aviation Administration for regulatory purposes and a flame test used by Underwriters Laboratories, Inc., both with categorical outcomes. The probabilistic analysis involved nonlinear least squares regression of the fire test data coded as a binary (pass/fail) outcome on each of the continuous explanatory variables using the logistic response function and a new (phlogistic) response function. The chi-square test showed that both probability models were appropriate for describing the likelihood of passing fire and flame tests using the heat release capacity, heat of combustion, volatile fuel fraction, and heat release parameter as the sole explanatory variable, but neither model was appropriate for thermal decomposition temperature as an explanatory variable. The overall efficacy of the thermal and combustion properties for predicting flammability test results based on the correlation coefficient and mean deviation of the grouped data from the fitted functions is: heat release capacity ≈ heat of combustion > heat release parameter > volatile fuel fraction > thermal decomposition temperature. Both probabilistic models are suitable for determining the likelihood of passing a flammability test using the thermal and combustion properties investigated, but the phlogistic model provides a better fit of the data when the likelihood of passing the test approaches unity.

17. Key Words

Fire test, Flame test, Thermal properties, Combustion properties, Probability, Statistics

18. Distribution Statement

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19. Security Classif. (of this report) Unclassified	20. Security Classif. (of this page) Unclassified	21. No. of Pages 36	22. Price

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LIST OF SYMBOLS AND ACRONYMS

ΔT_p	Temperature interval of pyrolysis
η_c	Heat release capacity of sample
$\bar{\eta}_i$	Mean heat release capacity of sample bin
μ	Pyrolysis residue (mass fraction)
σ_X^2	Variance of independent (explanatory) variable
ϕ	Mass fraction of volatile species
χ	Combustion efficiency of the fuel gases
a	Exponent of logistic response function
b	Exponent of phlogistic response function
B	Number of bins
E_a	Activation energy for pyrolysis
h_c	Heat of combustion of gases
h_g	Heat of gasification
N	Number of samples per bin
N_f	Number of failing results
N_p	Number of passing results
p_{meas}	Probability of passing fire test from measurements
p_{calc}	Calculated probability of passing fire test
Q_∞	Heat of complete combustion of sample gases
R	Gas constant
T_p	Decomposition temperature
X_i	Value of independent (explanatory) variable of sample i
$\bar{X}_i$	Mean value of explanatory variable in sample bin
Y_i	Result of fire test (pass = 1, fail = 0)
$\bar{Y}_i$	Frequency of passing results in sample bin
CFR	Code of Federal Regulations
HR	Heat Release
HRP	Heat Release Parameter
HRR	Heat Release Rate
MCC	Microscale Combustion Calorimeter
PHRR	Peak Heat Release Rate
UL	Underwriters Laboratories, Inc.

EXECUTIVE SUMMARY

Aircraft cabin materials that must meet regulatory requirements for fire safety are produced in large quantities, so multiple fire test specimens requiring several kilograms of material are easily obtained. In contrast, research materials with the potential for improved fire safety are typically produced in gram quantity, which is insufficient for conducting regulatory fire tests. Consequently, a methodology was developed to predict the likelihood of passing kilogram-scale regulatory fire tests using thermal combustion properties of the material measured in a milligram-scale laboratory test. Several thermal and combustion properties were evaluated as explanatory variables for two flammability tests using two different probabilistic models.

The thermal and combustion properties spanned the range of commercial polymers and flame-retardant plastics. The fire tests were a heat release rate test in Title 14 of the Code of Federal Regulations (CFR) 25 and a vertical flame spread test (UL 94 V), both with categorical outcomes. The probabilistic models were the logistic response function and a new (phlogistic) response function. These two models were fit to the frequency (likelihood) of passing results in the two fire tests for each of five explanatory variables: heat release capacity (η_c), heat of combustion (Q_∞), fuel fraction (ϕ), heat release parameter (HRP), and thermal decomposition temperature (T_p).

With suitable explanatory variables, both of the probabilistic models were equivalent in predictive capability when the frequency of passing results was near 50%, but the phlogistic model was much better when the likelihood of passing the test approached 100%, which is the range of greatest interest to regulatory agencies and standards organizations. Using either of these probability models, the predictive capability of the explanatory variables was in the order: $\eta_c \approx Q_\infty > HRP > \phi >> T_p$. This methodology of using the results from milligram scale tests for screening production materials for flammability should be useful for product development and quality control of aircraft cabin materials.

1. INTRODUCTION.

Most flammability tests of materials and products measure, either directly or indirectly, the spread of flame over a solid combustible surface under standardized conditions. These conditions may include a particular sample orientation with respect to gravity, air velocity, ignition source, or imposed heat flux to force the sample to burn. What is measured in the flammability test is the duration, extent, or velocity of burning, or the rate at which heat is released during burning, and a pass/fail rating is assigned to the material based on specified performance criteria [1]. In theory, flame spread or burning rate, and thus the outcome of the flammability test, is a known function of the test conditions and the combustion properties of the specimen [2-4]. In practice, idealized deterministic relationships between fire behavior and combustion properties are rarely obtained because anomalous physical behaviors, such as melting, dripping, swelling, deformation, incomplete combustion, edge effects, and thickness variations, influence the outcomes. Consequently, a methodology for analyzing flammability tests that uses quantitative thermal and combustion properties of the material as explanatory variables, and statistics to account for the influence of physical effects on the variability of test results, may be useful for the development of products that must meet regulatory requirements for fire safety.

Logistic regression models [5 and 6] are commonly used to study the effect of continuous predictor/explanatory variables on categorical outcomes, such as pass/fail results. For example, logistic regression has been used to model the probability of burning nickel alloys as a threshold problem using oxygen pressure as the sole explanatory variable [7]. In the past, logistic regression models have not been applied to pass/fail flammability tests because the environmental variables that would normally be considered independent variables are fixed by the test conditions, and the material combustion properties that are suitable as predictor variables are typically more difficult to measure than the flammability test result itself [8]. Recently, however, a simple laboratory test has become available that measures quantitative thermal combustion properties of materials using milligram samples in a matter of minutes [9 and 10]. These thermal combustion properties are parameters in deterministic models of burning behavior [9 and 10] and have been used to correlate flammability test results [11-13]. In this study, the utility of these thermal combustion properties was examined as explanatory variables for the frequency of passing fire tests, and two statistical models were used to correlate the data.

2. STATISTICAL MODELS.

Consider a fire test with a qualitative pass/fail result, Y_i, that is presumed to be a function of an independent predictor/explanatory variable, X_i. If the response variable, Y_i, is one of two possible outcomes, pass or fail, it may be treated as a Bernoulli random variable with probability distribution, as shown in Table 1.

Table 1. Pass/Fail Probability Distribution

Test Result	Y_i	Probability
Pass	1	$P(Y_i = 1 \mid X_i) \equiv p_i$
Fail	0	$P(Y_i = 0 \mid X_i) \equiv 1\text{-}p_i$

where $P(Y_i = 1 \mid X_i)$ is the probability that $Y_i = 1$ given X_i and $P(Y_i = 0 \mid X_i)$ is the probability that $Y_i = 0$ given X_i. If N_P and N_F represent the number of passing and failing results, respectively, in $N = N_P + N_F$ tests at a particular X_i, then $p_i = N_p/N$, $1\text{-}p_i = N_F/N$ and $N_P/N_F = p_i/(1\text{-}p_i)$ represents the odds of passing the test. If N is large, the mean of Y_i is the expected value $E\{Y_i\} = p_i$. The variance of Y_i, $\sigma^2\{Y_i\} = \sigma_p^2$, is the same as the variance of the error and it is a function of the explanatory variable, X_i, through the probability $p_i = p(X_i)$ [5 and 6]:

$$\sigma_p^2 = \frac{\sum (Y_i - (E\{Y_i\})^2}{N} = \frac{N_P}{N}(1-p_i)^2 + \frac{N_F}{N}(0-p_i)^2 \qquad (1)$$

$$= (p_i)(1-p_i)^2 + (1-p_i)(p_i)^2$$

$$= p_i(1-p_i)$$

2.1 LOGISTIC MODEL.

The task is to find a functional relationship between Y_i and X_i. Fortunately, there is substantial literature on a statistical methodology used to relate dichotomous (pass/fail) response variables to continuous explanatory variables in the medical, mathematical, and social sciences [5 and 6]. The methodology uses a particular model called the logistic response function to relate the independent binary variable, Y_i, and dependent explanatory variable(s), X_i. The logistic response function for explanatory variables, $X_i = X_1, X_2, \cdots X_j$, is the joint probability or likelihood function [5 and 6]:

$$\frac{N_P}{N_F} = \frac{p_i}{1-p_i} = \prod_{i=0}^{j} \exp\left[a_i X_i\right] = \exp\left[a_0 X_0 + a_1 X_1 + a_2 X_2 + \cdots + a_j X_j\right] \qquad (2)$$

Equation 2 represents the odds of passing the fire test in terms of the explanatory variables. The natural logarithm of equation 2 is called the logit and it is used to determine the coefficients, a_j, by the method of maximum likelihood [5 and 6]:

$$\ln\left[\frac{p_i}{1-p_i}\right] = a_0 + a_1 X_i + a_2 X_2 + \cdots + a_j X_j \qquad (3)$$

The logistic model is convenient for statistical analyses because it accommodates multiple, explanatory variables. The simple logistic response function is the probability of equation 2 for a single, continuous explanatory variable X:

$$p = \frac{\exp\left[a_0 - a_1 X\right]}{1 + \exp\left[a_0 - a_1 X\right]} = \frac{1}{1 + \exp\left[-a_0 + a_1 X\right]} \qquad (4)$$

The simple logistic response function (equation 4) plotted in figure 1 was originally proposed to describe population growth [14]. It is an ogive or cumulative probability distribution that is Sshaped (sigmoidal) and is either monotonically increasing or decreasing with X, depending on the signs of a_0 and a_1. The simple logistic response function gradually approaches 0 and 1 in the limits of the X range, which satisfies the constraints on the probability, $0 \leq p \leq 1$.

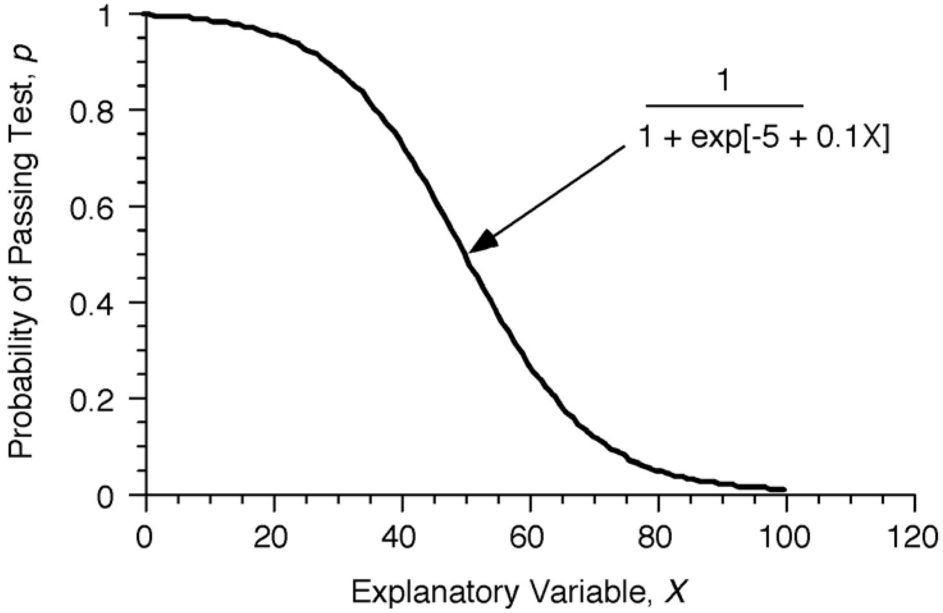


Figure 1. Simple Logistic Response Function (equation 4)

At p_i = 1/2, the coefficients are related, $a_0 = -a_1 X_c = -aX_c$, so the simple logistic response function, equation 4, has the alternative two-parameter (a, X_c) form:

$$p = \frac{\exp\left[-a(X - X_c)\right]}{1 + \exp\left[-a(X - X_c)\right]} = \frac{1}{1 + \exp\left[a(X - X_c)\right]} \tag{5}$$

According to equation 5, a pass or fail result is equally likely, ($p = 1/2$) at $X_i = X_c$, so this is the median of the distribution [7]. The probability density is the derivative of equation 4 and has a maximum value at $X = X_c$, so X_c is also the mode of the logistic distribution. A shortcoming of the logistic response function with regard to the present objective of finding explanatory variables for pass/fail fire tests is the behavior of p at $X = 0$. In particular, $p(0) = 1/(1 + \exp[-aX_c) < 1$ for all finite values of aX_c, regardless of the explanatory power of X. Because the domain $p \rightarrow 1$ is of primary interest to materials developers and regulatory officials concerned with fire test results, a statistical response function that better represents these data is proposed.

2.2 PHLOGISTIC MODEL.

It is easily shown that the simple logistic response function, equation 4, is the solution to the differential equation:

$$\frac{dp}{dX} = -a\,p(1 - p) \tag{6}$$

Where dp is the incremental change in p and dX is the incremental change in X.

The slope of the logistic response function is thus proportional to the variance (equation 1), $\sigma_p^2 = p(1\text{-}p)$, is a maximum at $p = 1/2$, and is zero at $p = 0, 1$. Separating variables

$$\frac{dp}{p(1-p)} = -a\,dX \tag{7}$$

the logistic response function is obtained by integrating equation 7 and the result is a cumulative probability distribution that is log-linear as a consequence of weighting the incremental probability by the inverse of its variance. If the independent/explanatory variable increment is likewise weighted by its inverse variance σ_X^2, equation 7 becomes:

$$\frac{dp}{\sigma_p^2} = -a\frac{dX}{\sigma_X^2}$$

For a one-sided (positive) variable, X, following a Poisson distribution, $\sigma_X^2 = X$, and the explicit relationship between p and X becomes:

$$\frac{dp}{p(1-p)} = -b\frac{dX}{X} \tag{8}$$

The general solution of equation 8 is:

$$\ln\left[\frac{p}{1-p}\right] = c - b\ln[X] \tag{9}$$

Because of the asymptotic limits, the constant of integration, c, is evaluated for the median value of the explanatory variable, $X = X^*$, at $p = 1/2$:

$$\frac{p}{1-p} = \left(\frac{X^*}{X}\right)^b \tag{10}$$

The response function, equation 10, can be extended to multiple explanatory variables, X_1, X_2 … X_j, by writing its joint probability as per equation 2, and performing the logit transformation:

$$\ln\left[\frac{p}{1-p}\right] = -b_0 + b_1\ln[X_1] + b_2\ln[X_2] + \ldots + b_j\ln[X_j] \tag{11}$$

For a single, continuous explanatory variable, X, the cumulative probability distribution is:

$$p = \frac{(X^*/X)^b}{1+(X^*/X)^b} = \frac{1}{1+(X/X^*)^b} \tag{12}$$

Equation 12 is a probabilistic response function that is called phlogistic in this study for its historical significance in fire science [15] and to distinguish it from the more common simple logistic response function (equations 4 and 5). The complementary phlogistic probability is:

$$1-p = \frac{(X/X^*)^b}{1+(X/X^*)^b} \tag{13}$$

Equation 12 and its complement, equation 13, are ogives that, like equations 4 and 5, have asymptotes at $p = 1$ and 0 for all $b > 1$ and, thus, automatically satisfy the constraints on the probability, $0 \le p \le 1$ for the range $X \ge 0$. Unlike equation 5, equation 12 intersects the ordinate at $p = 1$ for $X = 0$. From the perspective of flammability tests, this is a more satisfying and useful result than equations 4 or 5 because it accommodates noncombustible materials (e.g., steel, brick, concrete, etc.) for which $p = 1$ at $X = 0$, by definition.

Equation 12 is plotted in figure 2 for $b = 0, 1, 3, 10$, and 30 over the range $x = 0$ to $x = 2$ of the dimensionless combustion property, $x = X/X^*$.

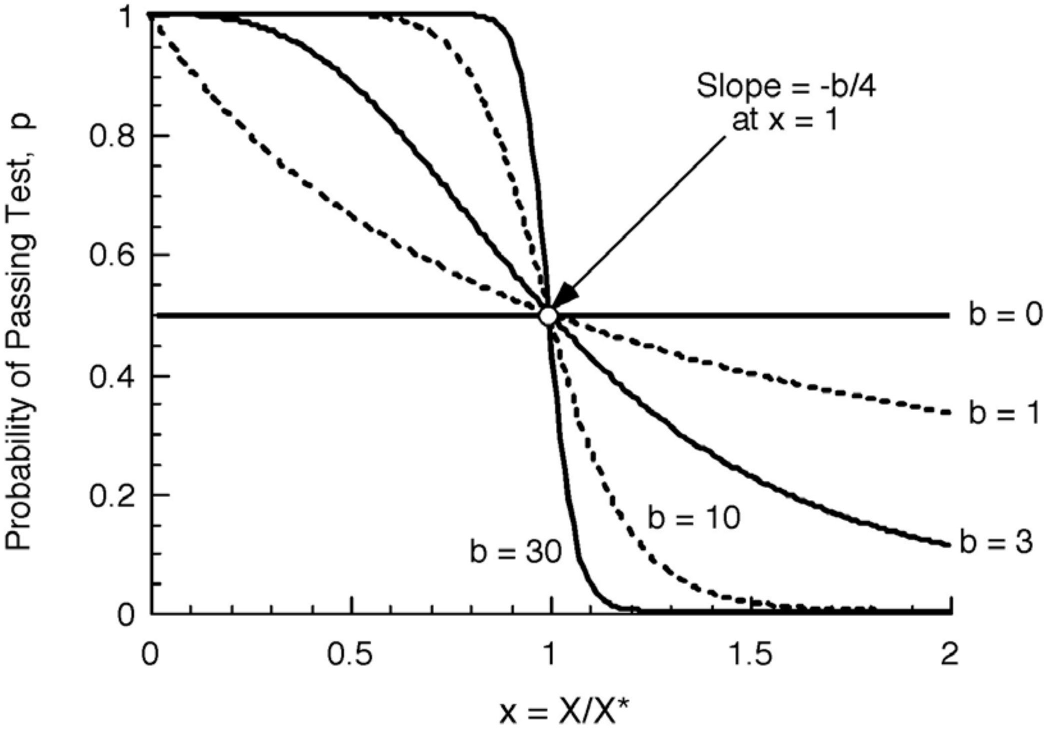


Figure 2. The Simple Phlogistic Response Function (equation 12) Plotted in Reduced Form for Various Values of the Exponent *b*

Equation 12 shows that $X = X_{1/2} = X^*$ is the median of the phlogistic distribution (i.e., the value of X at $p = 1/2$), regardless of the dispersion, $1/b$. The median of the phlogistic distribution in terms of the continuous reduced variable, $x = X/X^*$, is, therefore:

$$x_{1/2} = X_{1/2} / X^* = 1 \tag{14}$$

The phlogistic probability density (frequency distribution) is the derivative of equation 12 with respect to the reduced variable, $x = X/X^*$:

$$p'(x) = -\frac{dp}{dx} = \frac{bx^{b-1}}{\left(1 + x^b\right)^2} \tag{15}$$

The mode of the distribution, $x_{\max}$, is the value of x at which $p'(x)$ is a maximum, and this is obtained by setting the derivative of equation 15 (second derivative of equation 12) equal to zero:

$$x_{\max} = \left[\frac{b-1}{b+1}\right]^{\frac{1}{b}} \tag{16}$$

The mean of the (continuous) phlogistic distribution does not have a simple analytic form, but it is defined as:

$$\bar{x} = \int_0^\infty x\, p'(x)\, dx \tag{17}$$

Figure 3 is a plot of the phlogistic probability density (equation 15) for $b = 3$, showing the relative location of $x_{\max}$, $x_{1/2}$, and $\bar{x}$ (i.e., the mode, median, and mean, respectively, of the phlogistic distribution, with the mean obtained by numerically integrating equation 17).

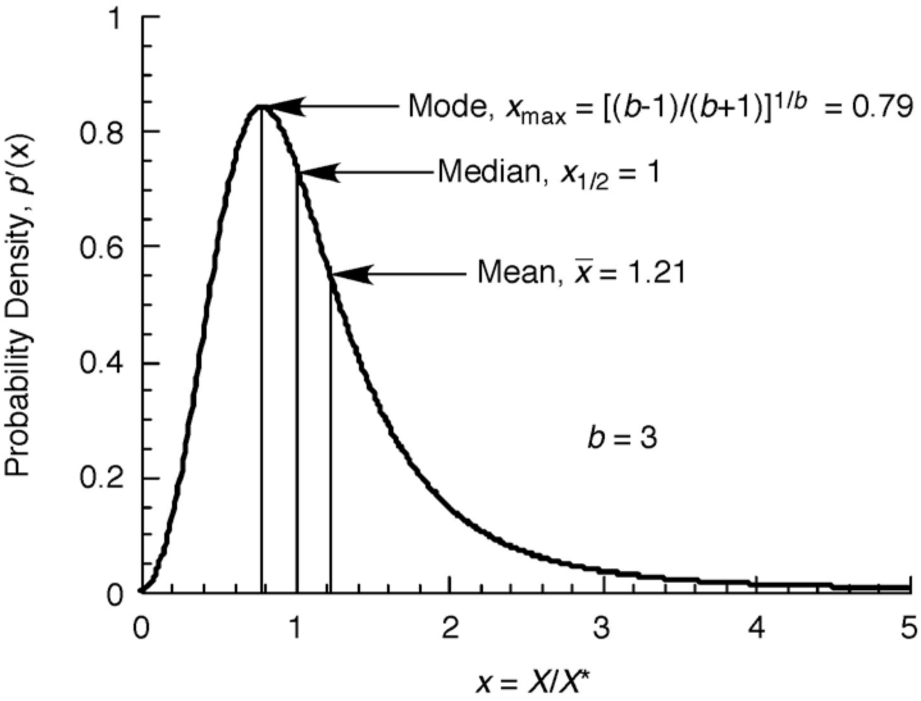


Figure 3. Phlogistic Probability Density for $b = 3$ Showing Location of Mode, Median, and Mean of the Reduced Variable $x = X/X^*$

Figure 3 shows that the phlogistic distribution is not symmetric about x_{max}, while figure 2 shows that the transition from passing results ($p_i = 1$) to failing results ($p_i = 0$) in the cumulative distribution occurs over a narrower range of x as b increases. Thus, for $b > 20$, the simple phlogistic responses (equations 11 and 12) approximate step functions at the median value of the explanatory variable, X^*, which assumes the significance of a threshold parameter. In fire science, threshold parameters, such as critical heat flux [2-4], surface temperature at ignition [16], and HRR at ignition [8, 16, and 17] can often be expressed in terms of the thermal and combustion properties of the material [9-13]. In the following sections, several thermal and combustion properties are examined as explanatory variables for the frequency of passing results in two flammability tests and use the logistic and phlogistic response functions to describe the frequency of passing results, i.e., the likelihood of passing the test.

3. EXPERIMENTAL.

3.1 THERMAL COMBUSTION PROPERTIES.

Thermal properties are condensed phase physical quantities that depend on the temperature history of the material, but do not include chemical reactions, such as the heat of decomposition or combustion. In the present context, the thermal X_i, are the decomposition temperature, T_p (°C), the pyrolysis residue μ (g/g), and the fuel fraction after complete pyrolysis, $\phi = 1-\mu$ (g/g). Thermal properties were measured in triplicate for 235 flame and fire test samples [9-13 and 18-20] by microscale combustion calorimetry (MCC) using 5±2 mg samples at a constant heating rate of 1 K/s according to method A (anaerobic pyrolysis) of a standard procedure [21].

In the present context, the combustion properties, X_i, are the heats of complete combustion of the pyrolysis gases per unit starting mass of material Q_∞ (J/g) measured in triplicate for 235 flame and fire test samples [9-13 and 18-20] by MCC, using 5±2 mg samples at a constant heating rate of 1 K/s according to method A (anaerobic pyrolysis) of a standard procedure [21].

Flammability parameters that combine condensed phase thermal properties and gas phase combustion properties are the ratio of the heat of complete combustion, Q_∞, to the pyrolysis temperature interval ΔT_p, measured by MCC and known as the heat release capacity, $\eta_c = \eta_c / \Delta T_p$ [9-13]. The η_c were measured in triplicate for 235 flame and fire test samples [9-13 and 18-20] by MCC, using 5±2 mg samples at a constant heating rate of 1 K/s according to method A (anaerobic pyrolysis) of a standard procedure [21]. Another thermal combustion property is the dimensionless ratio of the effective heat of flaming combustion to the apparent heat of decomposition/gasification measured in a fire calorimeter and called the heat release parameter (HRP) [3, 4, and 8]. The HRPs were determined for 68 polymers and plastics for which flame test results had also been obtained [19 and 22-25], as the slope of a plot of the peak HRR (PHRR) (W/m^2) versus external heat flux (W/m^2) in a fire calorimeter operating on the oxygen consumption principle according to a standard method [26]. Samples for HRPs were 100-mm square and 3- to 6-mm thick.

Thermal combustion properties T_p, ϕ, Q_∞, η_c, and HRP, are often considered the primary indicators of the burning propensity of the material [3, 4, and 9-13], but they are not independent [8 and 9-11].

$$\eta_c = \frac{\phi h_c}{eRT_p^2 / E_a} = \frac{Q_\infty}{eRT_p^2 / E_a} = \frac{Q_\infty}{\Delta T_p} \tag{18}$$

$$HRP = \chi \frac{h_c}{h_g} = \frac{\chi Q_\infty}{\phi h_g} \tag{19}$$

In equations 18 and 19, E_a is the global activation energy for pyrolysis, $h_c = Q_\infty / \phi$ is the heat of complete combustion of the fuel gases, h_g is the thermal energy required to gasify unit mass of volatile fuel, ΔT_p is the temperature interval over which pyrolysis takes place at a constant heating rate, and χ is the combustion efficiency of the fuel gases in a diffusion flame. All the properties in equations 18 and 19, with the possible exception of χ, are intrinsic properties (i.e., they are independent of the amount of material tested).

3.2 FLAMMABILITY TESTS.

3.2.1 Fire Test.

A 101-sample subset of the 235 polymers, plastics, and fiber-reinforced polymer composites tested for heat release capacity (η_c) were tested for HRR in a fire calorimeter using a thermopile to measure the sensible enthalpy (temperature) rise of the combustion air stream, calibrated to methane, according to a Federal Aviation Administration Title 14 Code of Federal Regulations

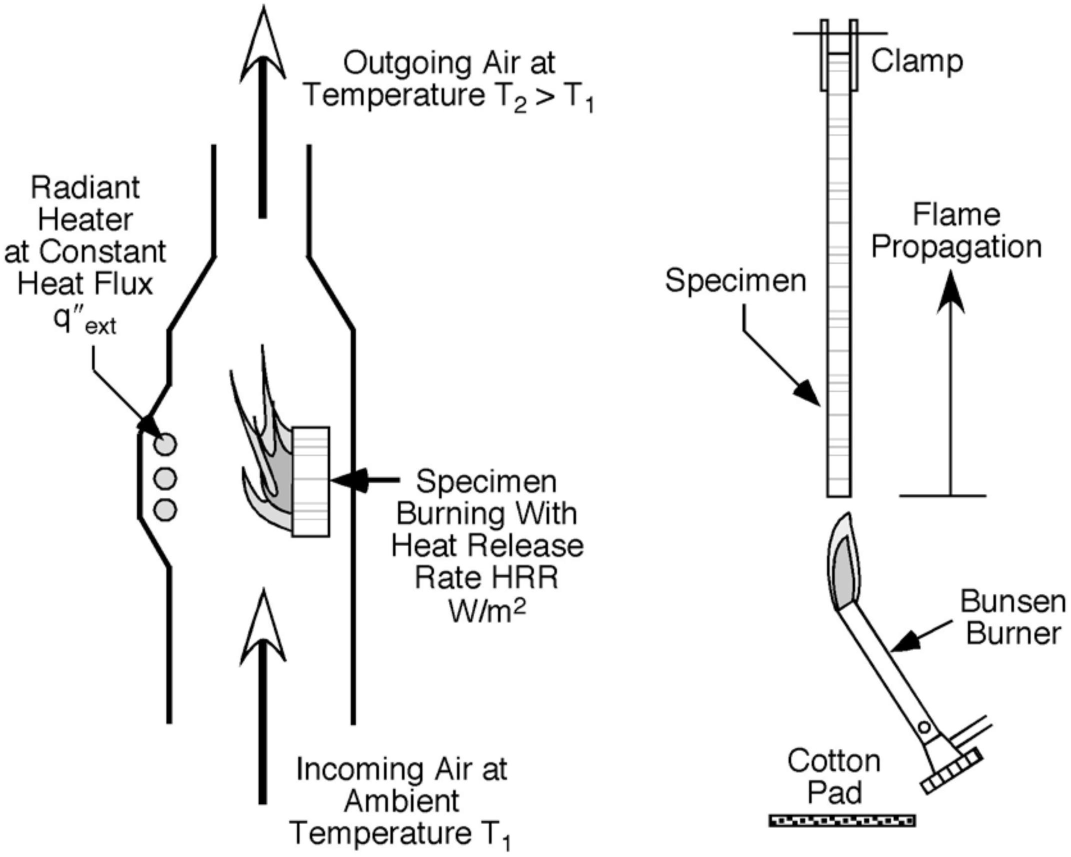
Part 25 (CFR) for the HRR of aircraft cabin materials [27 and 28]. Specimens were 150-mm square and ranged in thickness from 1 mm to 6 mm. The acceptance criteria for the 14 CFR 25.853 HRR test and associated binary outcomes are listed in table 2. The 14 CFR 25 fire test is shown in figure 4.

Table 2. Acceptance Criteria for 14 CFR 25.853 HRR Test for Cabin Materials

Criteria (≥3 specimens)	Accept/Pass	Reject/Fail
Average maximum HRR during the 5-min test (PHRR)	≤65 kW/m^2	>65 kW/m^2
Average total heat released during the first 2 min of test (HR)	≤65 kW-min/m^2	>65 kW-min/m^2
Y_i	1	0

3.2.2 Flame Test.

A 134-sample subset of the 235 polymers and plastics tested for thermal combustion properties were tested for flame resistance according to the Underwriters Laboratories, Inc. (UL) vertical test for flammability of plastics standard procedure [29 and 30]. The 134 samples included flame retardant polymer formulations (plastics) containing bromine and phosphorus compounds, inert/mineral fillers, and char-swelling (intumescent) compounds. Flame test results were measured in our laboratory or obtained from the literature [18-24] on rectangular bars 125-mm long, 13-mm wide, and 1.6- to 3.2-mm thick. A diagram of the UL 94 vertical flame test is shown in figure 4. During the test, the specimens were held lengthwise in a vertical orientation and the lower 10 mm of the specimen was subjected to two consecutive 10-second exposures to a 20-mm-high, premixed, methane burner flame. The duration of flaming (burn time) after each of the two applications of the burner, t_1 and t_2, are recorded, as is the extent of burning and whether flaming drops ignited an underlying cotton pad. Five specimens were tested and evaluated according to the criteria in table 3. The Y_i assigned to each classification are shown in the last row.



a. 14 CFR 25 HRR Test b. UL 94 V Flame Test

Figure 4. Diagrams of (a) 14 CFR 25 HRR Test and (b) UL 94 Vertical Flame Test

Table 3. Material Classifications in UL 94 Vertical Flammability Test

Criteria Conditions (5 specimens)	V-0	V-1	V-2	No Rating (NR)
Individual Burn Time (t_1 or t_2)	≤10 s	≤30 s	≤30 s	>30 s
Total Burn Time (5 Specimens, $t_1 + t_2$)	≤50 s	≤250 s	≤250 s	>250 s
Individual Glowing Time	≤30 s	≤60 s	≤60 s	>60 s
Burns up to Holding Clamp (Any Specimen)	No	No	No	Yes
Cotton Indicator Ignited by Flaming Drops	No	No	Yes	Yes
Y_i	1	0	0	0

The test results in sections 3.2.1 and 3.2.2 are extrinsic quantities (i.e., they depend on the amount or thickness of the material tested). Sample thickness was not strictly controlled in this study, so it is a source of variability in the pass/fail results that cannot be accounted for by the intrinsic (thermal combustion) properties.

4. STATISTICAL ANALYSIS.

4.1 NONLINEAR LEAST SQUARES REGRESSION OF PROBABILITY FUNCTIONS ON BINARY DATA.

The acceptance criteria in tables 2 and 3 were applied to the quantitative results of the 14 CFR 25 fire test (PHRR, HR) and the qualitative results of the UL 94 vertical flame test (V-0, V-1, V-2, NR) to generate the binary outcomes shown in the last row of tables 3 and 4. The logistic and phlogistic response functions, equations 5 and 12, respectively, were fit to the (Y_i, X_i) data by nonlinear least-squares regression using a Levenberg-Marquardt algorithm in a scientific graphing and analysis program, KaleidaGraph® (Synergy Software) running on an iMac® personal computer (Apple®). Logistic regression of the Y_i on X_i yielded the logistic (a, X_c) and phlogistic (b, X^*) response function parameters for each of the candidate explanatory variables, $X_i = \eta_c$, Q_∞, ϕ, T_p, and HRP. Identical results for the parameters were obtained using an EXCEL® spreadsheet (Microsoft®) and computational software, MATLAB® (MathWorks®).

4.2 GROUPING/BINNING DATA TO COMPUTE PASSING FREQUENCY.

The relationship between the fire test results for each of the candidate explanatory variables (4 thermal combustion properties and the heat release parameter) was obtained by ranking the (Y_i, X_i) data pairs in ascending order by the explanatory variable X_i and grouping these data into $B = S/N$ bins containing an equal number of samples ranging from $N = 10$ to $N = \sqrt{S}$ for each of the sample populations, $S = 68$, 101, and 134. For each fire and flame (flammability) test the frequency of passing results in each bin, $\overline{Y_i} = (\Sigma Y_i)/N$ was calculated for the N explanatory variables X_i having mean value $\overline{X}_i = (\Sigma X_i)/N$. This binning/grouping procedure produces a histogram of the relative frequency of passing results for a particular fire test $\overline{Y_i}$ versus the average value of the explanatory variable for the bin $\overline{X}_i$, as shown in figure 5, where the $\overline{X}_i$ are indicated by tic marks at the top of the bars. If the bin size is large, the frequency of passing results in the flammability test approaches the probability of passing the test, i.e., $\overline{Y_i} \to p$ as $N \to \infty$. Unfortunately, the choice of bin size is a compromise between the true probability p of a particular pass/fail test result (large N) and having a sufficient number of ($\overline{Y_i}, \overline{X}_i$) pairs to reveal trends in the data with respect to the explanatory variable (small N). Since the number of samples used to compute $\overline{Y_i}$ was not large in this study ($N \leq 12$), the passing frequency in the flammability test is not a true probability of passing.

However, the logistic (equation 5) and phlogistic (equation 12) probability functions were evaluated with regard to their ability to describe the frequency of passing results for each flammability test using the candidate explanatory variables. The regression coefficients obtained from the fit of the binary data (section 4.1) were used to generate the probability distributions and these were compared to the grouped (binned) experimental data by inspection and by the chi square (χ^2) test as described in standard texts [5, 6, and 31].

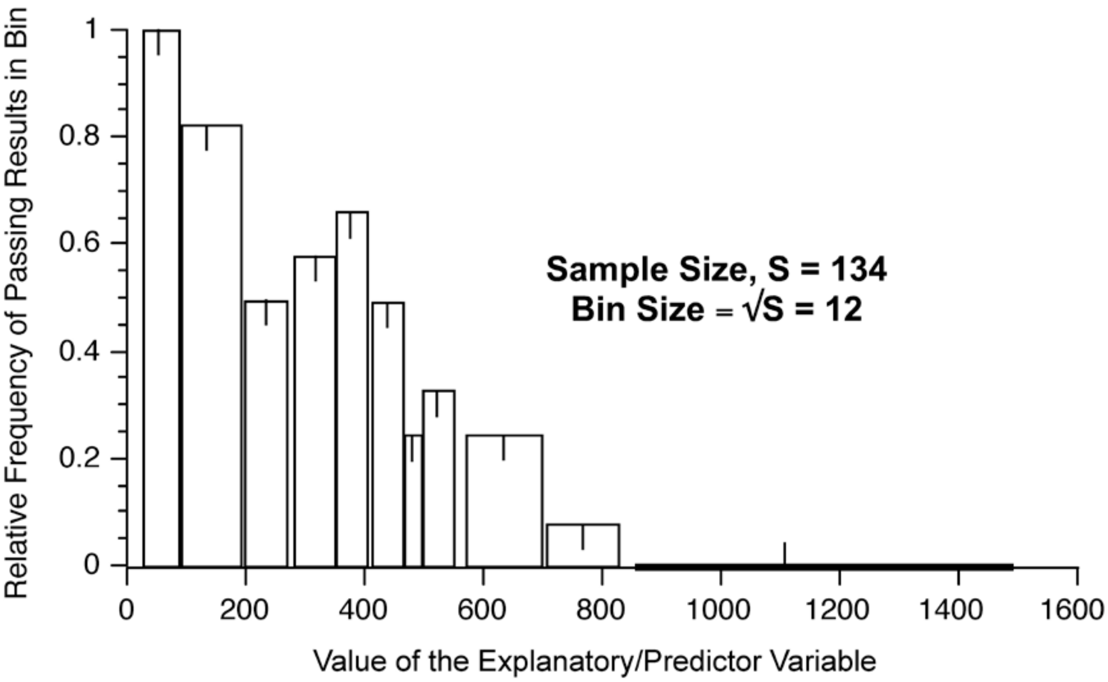


Figure 5. Binning Process Used to Generate the Probability Distribution (The variable range of the explanatory variable is a consequence of the fixed bin size *N*.)

4.3 REGRESSION DIAGNOSTICS.

The continuous probability distributions $p(\overline{X}_i)$ were computed by the logistic and phlogistic response function and compared to the passing frequency distribution using the Pearson chi square statistic for binary data [5 and 6],

$$X^2 = B\sum_{j=1}^{B}\frac{\left(\overline{Y}_i - p\right)^2}{p} + \frac{\left(\overline{Y}_i - p\right)^2}{1-p} \tag{20}$$

If the statistical response function is appropriate, X^2 follows approximately a χ^2 distribution for the ν = B-2 degrees of freedom and $X^2 < \chi^2(s;\nu)$ for a level of significance *s*.

The correlation between each of the logistic and phlogistic response functions and the grouped data was estimated using Pearson's R, using the mean value of the passing frequency, $\langle\overline{Y}_i\rangle$

$$R = \sqrt{1 - \frac{\sum_B(\overline{Y}_i - p)^2}{\sum_B(\overline{Y}_i - \langle\overline{Y}_i\rangle)^2}} \tag{21}$$

The mean deviation of logistic and phlogistic probabilities *p* and passing frequency $\overline{Y}_i$ was computed for each of the explanatory variables

$$\mathit{Mean\ Deviation}\ (MD) = \frac{\sum_{B} |p - \bar{Y}_i| / B}{\sum_{B} \bar{Y}_i / B} = \frac{\sum_{B} |p - \bar{Y}_i|}{\sum_{B} \bar{Y}_i} \tag{22}$$

5. RESULTS.

5.1 THE 14 CFR 25 HRR OF AIRCRAFT CABIN MATERIALS AND HEAT RELEASE CAPACITY.

Every material that passed the PHRR requirement also passed the HR requirement in table 2, although the converse was not true (i.e., samples that passed HR would sometimes fail PHRR). Consequently, PHRR is the more discriminating response variable for 14 CFR 25, so the following discussion is limited to Y_i computed from PHRR and $X_i = \eta_c$. Table 4 contains all 101 of the (Y_i, η_i) pairs and PHRR for 14 CFR 25 as well as the mean of these data for each of the $B = 10$ bins. Figure 6 is a plot of the 101 (Y_i, η_i) pairs shown as open circles and the fit of these data using nonlinear regression of the logistic (dashed line) and phlogistic (solid line) response functions. The best-fit parameters and the quality of the fits are listed in tables 10 and 11, respectively. The mean values $\bar{Y}_i$ and $\bar{\eta}_i$ for each of the $B = 10$ bins are also plotted in figure 6 as solid circles. Note that the standard deviation σ of the $\bar{Y}_i$, computed from the grouped Y_i in table 4, is the square root of the variance of equation 1. Figure 6 clearly shows that both the phlogistic and logistic models capture the overall trend in the frequency data, but only the phlogistic model intersects the ordinate at $p = 1$ for $\eta_c = 0$. The chi-square test shows that both models are appropriate, with the phlogistic model having $X^2 = 7.9$, which is much less than the required $\chi^2 = 15.5$ for the $\nu = B - 2 = 8$ degrees of freedom at the $s = 0.95$ significance level.

Table 4. Heat Release Capacity η_c, PHRR in 14 CFR 25.853, and Pass/Fail Rating ($Y_i = 1/0$).

No.	η_c (J/g-K)	PHRR (kW/m^2)	Y_i		No.	η_c (J/g-K)	PHRR (kW/m^2)	Y_i
1	1	8	1		51	214	80	0
2	9	25	1		52	215	150	0
3	10	59	1		53	215	213	0
4	13	13	1		54	230	97	0
5	15	66	0		55	235	258	0
6	22	31	1		56	248	55	1
7	29	55	1		57	253	145	0
8	50	30	1		58	261	44	1
9	83	59	1		59	265	188	0
10	105	54	1		60	276	199	0
B1	34 ±35	40 ±21	0.9 ±0.3		B6	241 ±23	143 ±72	0.2 ±0.4
11	108	92	0		61	288	82	0
12	115	61	1		62	295	93	0

Table 4. Heat Release Capacity η_c, PHRR in 14 CFR 25.853, and Pass/Fail Rating (Y_i = 1/0) (Continued)

No.	η_c (J/g-K)	PHRR (kW/m^2)	Y_i		No.	η_c (J/g-K)	PHRR (kW/m^2)	Y_i
13	120	49	1		63	298	211	0
14	120	123	0		64	301	232	0
15	121	60	1		65	316	166	0
16	121	52	1		66	345	115	0
17	127	109	0		67	349	207	0
18	129	66	0		68	351	141	0
19	134	66	0		69	359	119	0
20	136	65	1		70	359	90	0
B2	123 ±9	74 ±25	0.5 ±0.5		B7	326 ±29	146 ±55	0.0 ±0.0
21	140	69	0		71	360	171	0
22	141	110	0		72	376	246	0
23	144	44	1		73	384	148	0
24	152	63	1		74	390	150	0
25	152	51	1		75	394	110	0
26	152	90	0		76	395	160	0
27	153	30	1		77	402	142	0
28	155	85	0		78	409	250	0
29	156	45	1		79	413	116	0
30	159	72	0		80	427	117	0
B3	150 ±6	66 ±24	0.5 ±0.5		B8	395 ±19	161 ±50	0.0 ±0.0
31	160	43	1		81	437	183	0
32	164	69	0		82	441	78	0
33	165	34	1		83	458	97	0
34	171	53	1		84	473	134	0
35	173	106	0		85	476	149	0
36	174	80	0		86	487	50	1
37	182	40	1		87	504	181	0
38	183	110	0		88	520	119	0
39	184	75	0		89	537	198	0
40	185	72	0		90	540	137	0
B4	174 ±9	68 ±26	0.4 ±0.5		B9	487 ±37	133 ±48	0.1 ±0.3
41	192	36	1		91	552	213	0
42	192	89	0		92	563	137	0
43	196	32	1		93	577	70	0
44	196	97	0		94	579	90	0
45	197	86	0		95	610	190	0
46	198	76	0		96	636	98	0
47	201	74	0		97	641	82	0
48	203	65	1		98	655	144	0
49	206	83	0		99	669	300	0
50	209	58	1		100	833	109	0
B5	199 ±6	70 ±22	0.4 ±0.5		101	858	71	0
					B10	652 ±103	137 ±72	0.0 ±0.0

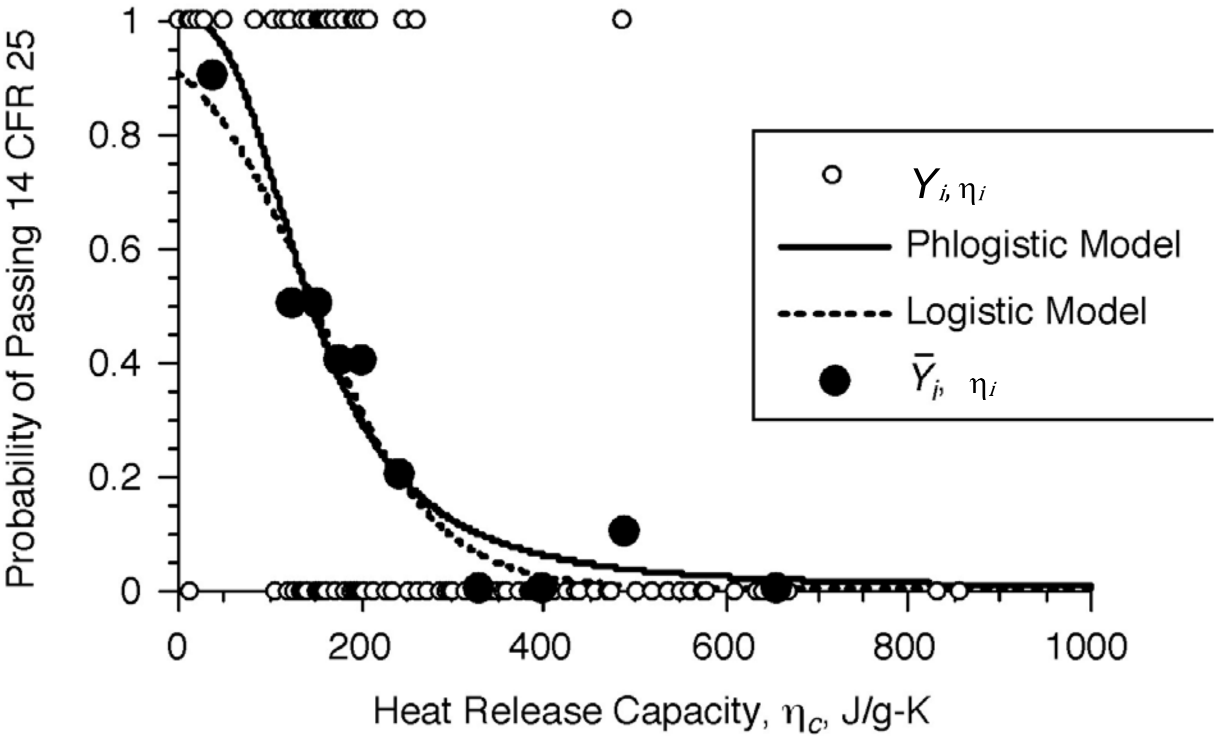


Figure 6. Probability of Passing 14 CFR 25 HRR vs. Heat Release Capacity

5.2 THE UL 94 VERTICAL TEST FOR FLAME RESISTANCE AND HEAT RELEASE CAPACITY.

Table 5 contains the 134 (Y_i, η_i) pairs for the UL 94 vertical flame test ranked by η_c. Figure 7 is a plot of the (Y_i, η_i) pairs shown as open circles and the fit of these data using nonlinear least-squares regression of the logistic (dashed line) and phlogistic (solid line) response functions. The bin size was set at $N = \sqrt{134} = 12$ samples and the mean values $\bar{Y}_i$ and $\bar{\eta}_i$ for each of the $B = 134/12 = 11$ bins are also plotted in figure 7 as solid circles. Figure 7 clearly shows that both the phlogistic and logistic models capture the overall trend in the frequency of passing results in the flame test using η_c as the explanatory variable, but only the phlogistic model intersects the ordinate at $p = 1$ for $\eta_c = 0$. The chi-square test shows that both models are appropriate, with the phlogistic model having $X^2 = 7.0$, which is much less than the required $\chi^2 = 16.9$ for the $\nu = B - 2 = 9$ degrees of freedom at the $s = 0.95$ significance level.

Table 5. Pass/Fail (Y_i = 1/0) Results in UL 94 Flammability Test Ranked by Heat Release Capacity of Sample η_c

η_c	Y_i	η_c	Y_i	η_c	Y_i	η_c	Y_i	η_c	Y_i	η_c	Y_i	η_c	Y_i	η_c	Y_i
J/g-K		J/g-K		J/g-K		J/g-K		J/g-K		J/g-K		J/g-K		J/g-K	
25	1	120	1	257	1	364	1	461	1	501	0	646	0	825	0
33	1	121	1	270	0	365	0	463	1	507	0	646	0	860	0
42	1	162	1	278	1	366	1	463	1	507	0	666	1	895	0
43	1	164	1	291	0	366	1	468	1	516	1	667	0	933	0
52	1	168	0	297	1	380	1	468	0	518	1	669	0	959	0
53	1	189	0	302	1	389	0	469	0	521	0	691	1	967	0
65	1	198	1	306	0	396	0	473	0	522	0	707	0	1002	0
65	1	199	0	309	0	399	1	473	0	526	1	713	0	1024	0
65	1	206	0	310	0	403	1	475	0	526	0	719	0	1100	0
72	1	207	1	332	1	416	1	479	1	541	0	720	0	1120	0
72	1	215	1	333	0	416	0	480	0	546	1	743	0	1163	0
78	1	221	1	343	1	416	0	482	1	575	0	781	0	1183	0
79	1	233	0	343	1	421	0	483	1	581	0	785	0	1400	0
89	1	234	1	345	1	432	0	490	0	599	0	790	0	1401	0
93	1	246	0	353	1	436	1	495	0	608	0	796	1	1488	0
99	1	253	1	359	1	437	0	496	0	616	0	806	0		
115	1	254	0	362	0	441	0	500	0	620	1	823	0		

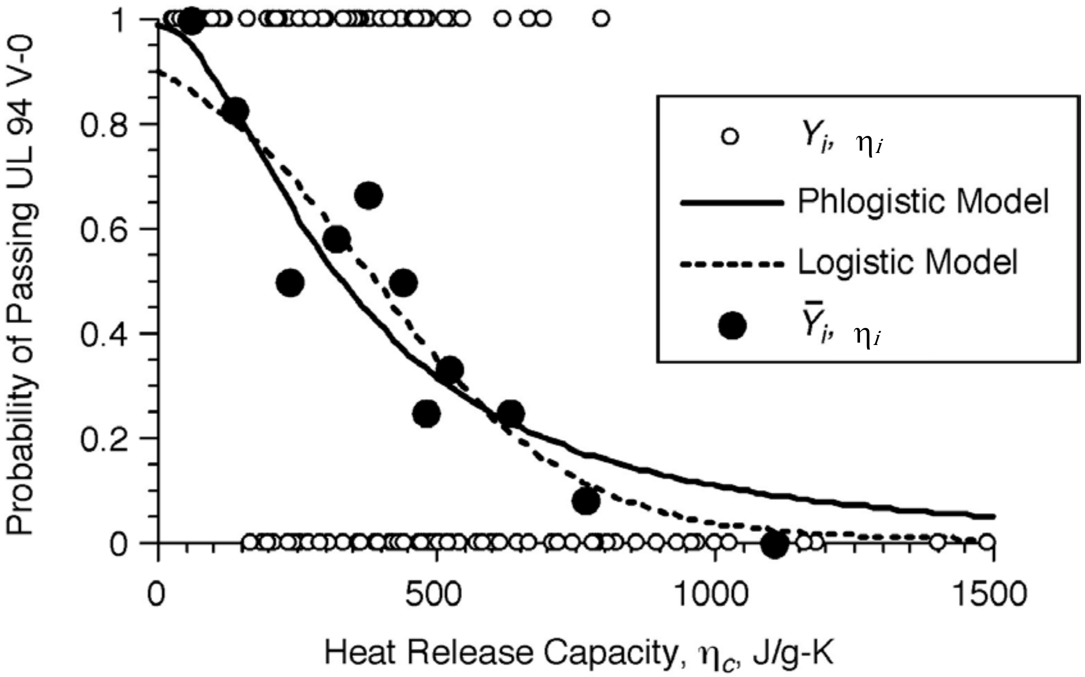


Figure 7. Probability of a V-0 Classification in the UL 94 Test vs. Heat Release Capacity

5.3 THE UL 94 VERTICAL TEST FOR FLAME RESISTANCE AND HEAT OF COMBUSTION.

Table 6 contains the 134 (Y_i, Q_∞) pairs for the UL 94 vertical flame test ranked by Q_∞. Figure 8 is a plot of the (Y_i, Q_∞) pairs shown as open circles and the fit of these data using nonlinear least-squares regression of the logistic (dashed line) and phlogistic (solid line) response functions. The best-fit parameters and the quality of the fits are given in tables 10 and 11, respectively. The bin size was set at $N = \sqrt{134} = 12$ samples and the mean values $\overline{Y_i}$ and $\overline{Q_i}$ for each of the $B = 134/12 = 11$ bins are also plotted in figure 8 as solid circles. Figure 8 clearly shows that both the phlogistic and logistic models capture the overall trend in the frequency of passing results in the flame test using Q_∞ as the explanatory variable, but the phlogistic model intersects the ordinate at $p = 1$ for $\eta_c = 0$. The chi-square test shows that both models are appropriate, with the phlogistic model having $X^2 = 7.3$, which is much less than the required $\chi^2 = 16.9$ for the $\nu = B - 2 = 9$ degrees of freedom at the $s = 0.95$ significance level.

Table 6. Pass/Fail ($Y_i = 1/0$) Results in UL 94 Flammability Test Ranked by Heat of Combustion of Sample Q_∞

Q_∞ kJ/g	Y_i	Q_∞ kJ/g	Y_i	Q_∞ kJ/g	Y_i	Q_∞ kJ/g	Y_i	Q_∞ kJ/g	Y_i	Q_∞ kJ/g	Y_i	Q_∞ kJ/g	Y_i	Q_∞ kJ/g	Y_i
2.70	1	9.60	1	14.3	1	17.3	0	20.0	1	23.5	0	26.9	0	36.5	0
2.70	1	9.70	1	14.5	1	17.5	1	20.0	0	24.0	0	27.0	0	36.7	0
2.80	1	9.90	1	15.0	0	17.7	1	20.4	1	24.3	0	28.0	0	37.0	0
4.20	1	10.3	1	15.4	0	18.1	1	20.8	0	24.4	0	28.4	0	37.1	0
4.80	1	10.7	1	15.4	1	18.2	0	20.9	1	24.5	1	28.4	0	37.1	0
6.20	1	11.1	1	15.7	0	18.4	1	20.9	0	24.6	0	28.8	0	38.0	0
6.60	1	11.4	1	15.9	0	18.5	1	21.1	0	24.7	1	29.0	0	38.6	0
6.90	1	12.0	0	15.9	0	18.6	0	21.2	0	24.9	0	29.0	1	38.7	0
7.10	1	12.3	1	16.0	1	18.6	0	21.2	0	25.2	0	29.0	0	38.8	0
7.20	1	12.6	1	16.1	0	18.9	1	21.3	0	25.3	1	29.5	0	38.8	0
7.30	1	12.9	1	16.3	1	19.5	0	21.4	1	25.7	0	30.6	0	41.0	0
8.10	1	12.9	0	16.3	0	19.5	1	21.4	1	26.0	0	30.8	0	42.1	0
8.50	1	13.0	1	16.6	1	19.7	0	21.5	1	26.1	0	31.6	0	42.9	0
8.60	1	13.2	0	16.6	1	19.8	1	22.4	0	26.2	1	32.0	0	43.0	0
9.10	1	13.8	1	16.7	1	19.8	0	22.5	0	26.5	0	33.2	0	44.4	0
9.30	1	14.1	0	17.2	1	19.9	0	23.1	0	26.5	1	35.0	0		
9.40	1	14.1	0	17.2	1	19.9	1	23.2	0	26.6	0	35.7	0		

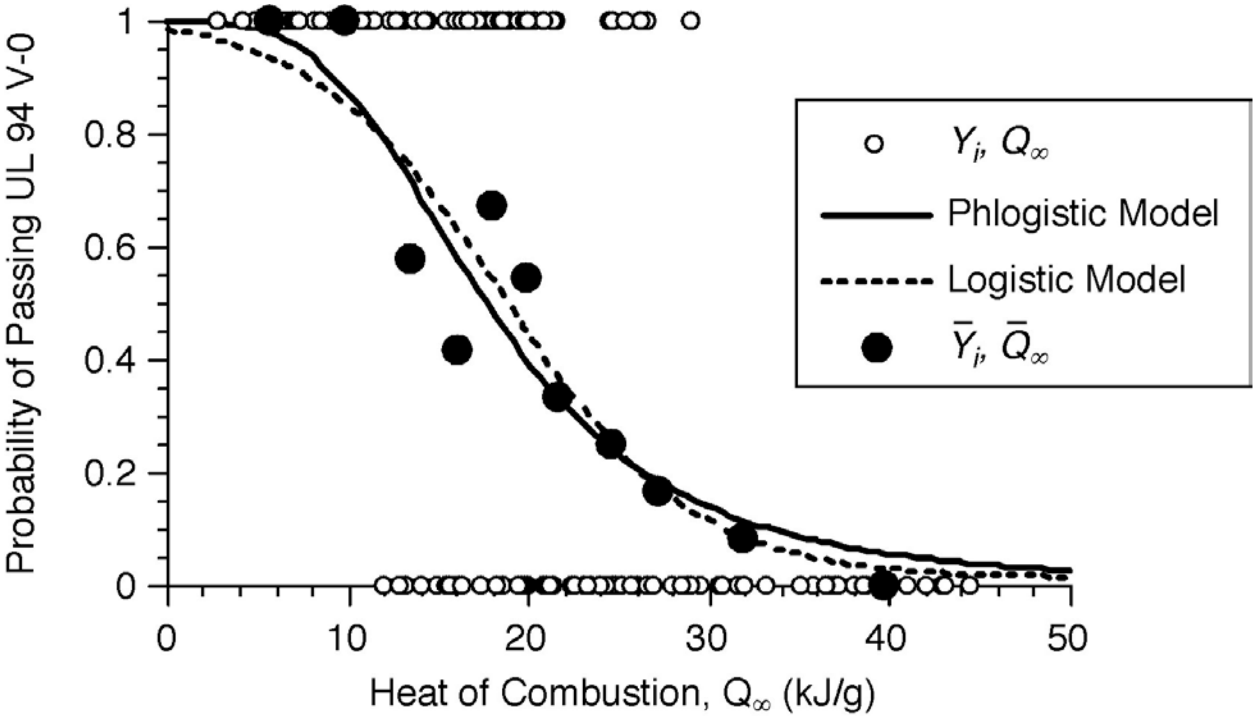


Figure 8. Probability of a V-0 Classification in the UL 94 Test vs. the Heat of Combustion

5.4 THE UL 94 VERTICAL TEST FOR FLAME RESISTANCE AND VOLATILE FUEL FRACTION.

Table 7 contains the 134 (Y_i, ϕ) pairs for the UL 94 vertical flame test ranked by the volatile fuel fraction of the sample ϕ. Figure 9 is a plot of the (Y_i, ϕ) pairs shown as open circles and the fit of these data using nonlinear regression of the logistic (dashed line) and phlogistic (solid line) response functions. The best-fit parameters and the quality of the fits are given in tables 10 and 11, respectively. The bin size was set at $N \approx \sqrt{134} = 12$ samples and the mean values $\overline{Y_i}$ and $\overline{\phi_i}$ for each of the $B = 134/12 = 11$ bins are also plotted in figure 9 as solid circles. Figure 9 clearly shows that both the phlogistic and logistic models captured the overall trend in the frequency of passing results in the flame test using ϕ as the explanatory variable. Both models intersected the ordinate at $p = 1$ for $\phi = 0$; and the chi-square test shows that both models are appropriate, with the phlogistic model having $X^2 = 8.3$, which is much less than the required $\chi^2 = 16.9$ for the $\nu = B - 2 = 9$ degrees of freedom at the $s = 0.95$ significance level. However, the predictive quality of ϕ as an explanatory variable is highly sensitive to the test population used for the regression analysis because the heat generated by combustion of the volatile fuel is not considered. For example, the addition of any number of fluoropolymers (e.g., fluorinated ethylene-propylene) to the test population will add as many $Y_i = 1$ at $\phi = 1$, because the fluorpolymer pyrolysis products resist combustion in the gas phase/flame.

Table 7. Pass/Fail (Y_i = 1/0) Results in UL 94 Flammability Test Ranked by Volatile Fuel Fraction of Sample ϕ

ϕ	Y_i	ϕ	Y_i	ϕ	Y_i	ϕ	Y_i	ϕ	Y_i	ϕ	Y_i	ϕ	Y_i	ϕ	Y_i
g/g		g/g		g/g		g/g		g/g		g/g		g/g		g/g	
0.24	1	0.50	1	0.65	1	0.74	0	0.79	0	0.90	0	0.96	1	1.00	0
0.26	1	0.50	1	0.65	1	0.75	0	0.79	1	0.91	0	0.96	1	1.00	1
0.27	1	0.51	1	0.66	1	0.75	0	0.80	1	0.92	0	0.98	0	1.00	0
0.30	1	0.52	1	0.66	0	0.76	1	0.80	0	0.92	1	0.98	0	1.00	0
0.32	1	0.53	0	0.67	0	0.76	1	0.80	1	0.93	0	0.98	0	1.00	0
0.33	1	0.53	1	0.67	0	0.76	0	0.81	0	0.93	0	0.98	0	1.00	0
0.36	1	0.55	1	0.68	0	0.77	0	0.81	1	0.93	0	0.99	1	1.00	0
0.40	1	0.55	1	0.68	0	0.77	0	0.81	0	0.93	0	0.99	0	1.00	0
0.41	1	0.55	1	0.68	1	0.77	0	0.81	0	0.94	0	0.99	0	1.00	0
0.42	1	0.55	1	0.69	0	0.78	1	0.82	0	0.94	1	0.99	0	1.00	0
0.46	1	0.56	1	0.69	0	0.78	0	0.85	1	0.94	0	1.00	0	1.00	0
0.46	1	0.61	0	0.70	1	0.78	0	0.86	0	0.94	0	1.00	0	1.00	0
0.46	1	0.62	1	0.72	0	0.79	1	0.86	1	0.95	0	1.00	0	1.00	0
0.48	1	0.63	1	0.72	1	0.79	1	0.87	0	0.95	0	1.00	0	1.00	0
0.48	1	0.63	0	0.73	1	0.79	1	0.87	0	0.95	0	1.00	1	1.00	0
0.49	1	0.64	0	0.74	0	0.79	1	0.88	0	0.96	0	1.00	0		
0.49	1	0.64	1	0.74	1	0.79	1	0.90	1	0.96	0	1.00	0		

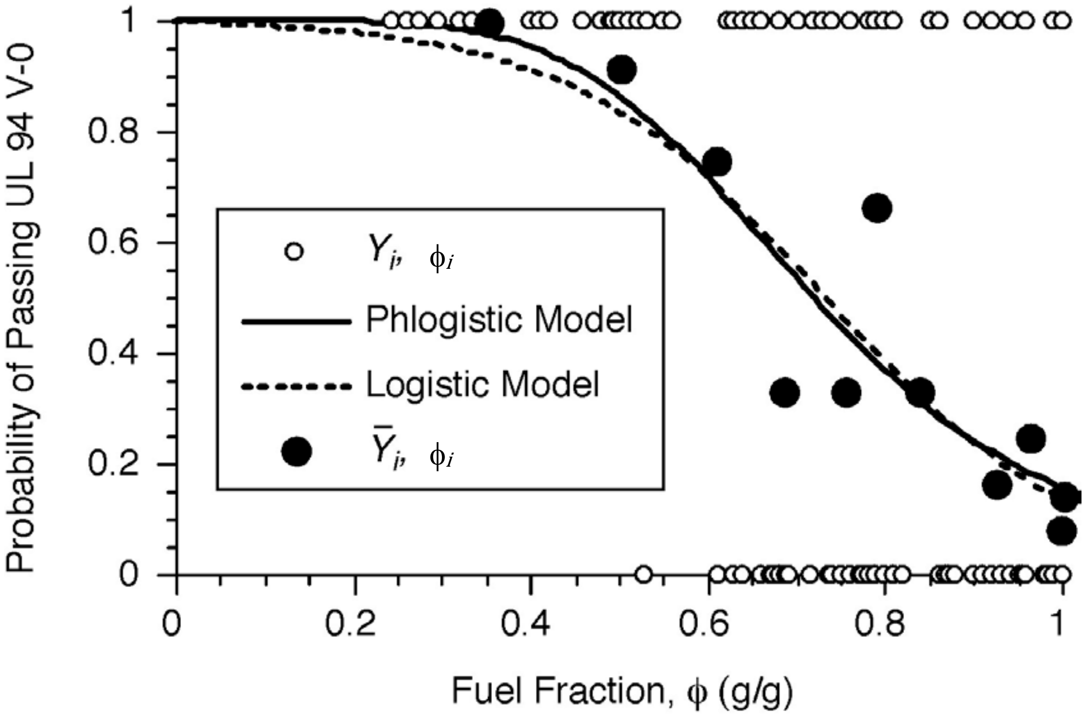


Figure 9. Probability of a V-0 Classification in the UL 94 Test vs. the Volatile Fuel Fraction ϕ

5.5 THE UL 94 VERTICAL TEST FOR FLAME RESISTANCE AND THERMAL DECOMPOSITION TEMPERATURE.

Table 8 contains the 81 (Y_i, T_p) pairs for the UL 94 vertical flame test ranked by the thermal decomposition temperature of the sample T_p. Figure 10 is a plot of the (Y_i, T_p) pairs shown as open circles and the fit of these data using nonlinear regression of the logistic (dashed line) and phlogistic (solid line) response functions. The best-fit parameters and the quality of the fits are given in tables 10 and 11, respectively. The bin size was set at $N = 10$ samples, and the mean values $\overline{Y}_i$ and $\overline{T}_i$ for each of the $B = 81/10 = 8$ bins are also plotted in figure 10 as solid circles. Figure 10 shows that both the phlogistic and logistic models capture the overall trend in the frequency of passing results for the flame test equally well. However, the chi-square test shows that neither model is appropriate for the binary UL 94 pass/fail results using T_p as the sole explanatory variable. The Pearson statistic for the phlogistic model, $X^2 = 43.6$, was much greater than the maximum allowable $\chi^2 = 12.6$ for the $\nu = B - 2 = 6$ degrees of freedom at the $s = 0.95$ significance level. The coefficients of the phlogistic regression for T_p are highly sensitive to test population because plastics with low thermal decomposition temperatures can be formulated to achieve a UL 94 V-0 classification with the addition of halogen-containing flame retardants that act in the gas phase/flame to resist combustion.

Table 8. Pass/Fail (Y_i = 1/0) Results in UL 94 Flammability Test Ranked by Thermal Decomposition Temperature, T_p

T_p	Y_i	T_p	Y_i	T_p	Y_i	T_p	Y_i	T_p	Y_i	T_p	Y_i	T_p	Y_i	T_p	Y_i
°C		°C		°C		°C		°C		°C		°C		°C	
297	1	429	0	472	0	489	0	533	0	555	1	573	1	627	1
341	1	445	0	472	0	490	0	544	1	555	0	576	1	629	1
356	0	446	0	473	1	491	0	546	1	556	0	583	1	645	1
373	0	446	0	473	0	495	0	547	0	557	1	590	1	789	1
376	0	456	0	480	0	495	1	548	1	558	0	605	1		
395	0	459	0	482	1	496	0	551	1	558	0	605	1		
397	0	462	0	482	0	500	0	552	0	559	1	607	1		
403	0	463	0	482	1	509	0	553	0	560	1	611	1		
405	0	467	1	483	0	510	0	553	0	562	1	612	1		
411	0	468	1	487	0	513	0	553	1	565	1	612	1		
411	0	468	0	488	0	518	1	554	1	573	1	619	1		

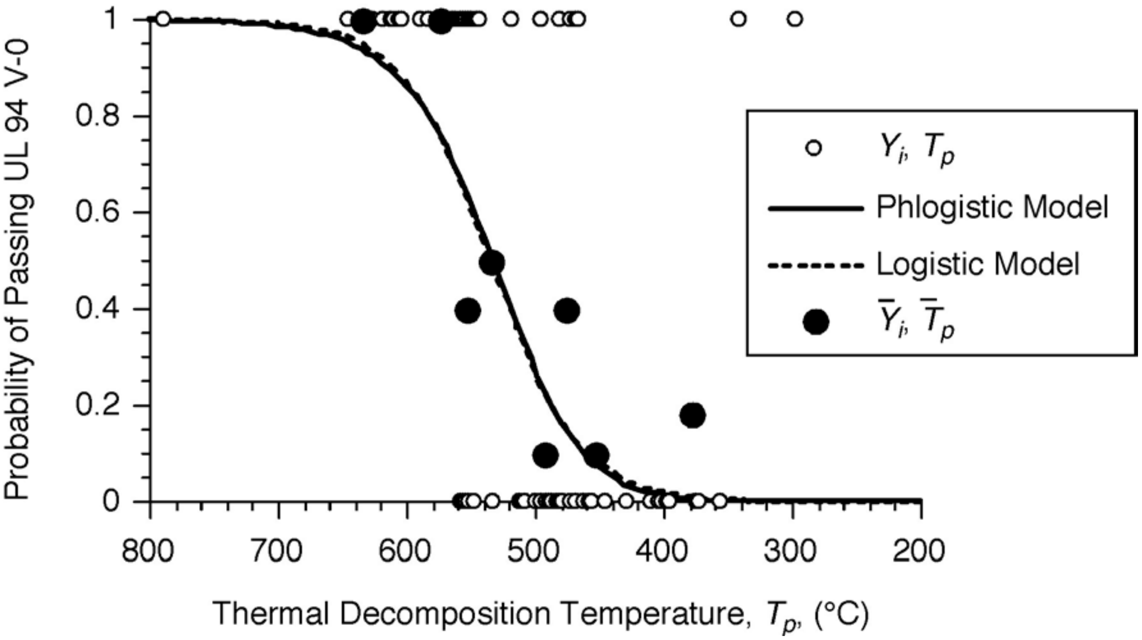


Figure 10. Probability of a V-0 Classification in the UL 94 Test vs. the Thermal Decomposition Temperature T_p

5.6 THE UL 94 VERTICAL TEST FOR FLAME RESISTANCE AND HRP.

Table 9 contains the 68 (Y_i, HRP) pairs for the UL 94 vertical flame test ranked by the HRP.

Table 9. Pass/Fail (Y_i = 1/0) Results in UL 94 Flammability Test Ranked by HRP

HRP	Y_i	HRP	Y_i	HRP	Y_i	HRP	Y_i	HRP	Y_i	HRP	Y_i	HRP	Y_i	HRP	Y_i
J/J		J/J		J/J		J/J		J/J		J/J		J/J		J/J	
0.70	1	2.4	1	3.2	0	4.0	1	5.0	0	6.7	0	13	0	18	0
0.80	1	2.5	0	3.2	1	4.0	1	5.5	1	7.0	0	13	0	18	0
1.7	1	2.6	0	3.3	1	4.0	1	5.5	1	8.0	0	13	0	18	0
1.9	1	2.9	1	3.3	1	4.5	0	5.6	0	8.0	1	14	0	20	0
2.0	1	2.9	0	3.5	0	4.6	0	5.7	0	8.8	0	14	0	22	0
2.0	1	3.0	1	3.6	1	4.7	0	6.0	1	9.0	0	15	0		
2.1	0	3.0	1	3.7	0	4.9	0	6.0	1	11	0	16	0		
2.3	1	3.0	1	4.0	1	5.0	0	6.0	0	13	0	16	0		
2.3	0	3.1	0	4.0	0	5.0	0	6.0	0	13	0	16	0		

Figure 11 is a plot of the (Y_i, HRP) pairs shown as open circles and the fit of these data using nonlinear regression of the logistic (dashed line) and phlogistic (solid line) response functions. The best-fit parameters and the quality of the fits are given in tables 10 and 11, respectively. The bin size was set at N = 10 samples, and the mean values $\bar{Y}_i$ and $\overline{\text{HRP}}_i$ for each of the B = 68/10 = 7 bins are also plotted in figure 11 as solid circles. Figure 11 shows that both the phlogistic and logistic models capture the overall trend in the frequency of passing results in the flame test equally well. The chi-square test shows that both models were appropriate for the binary UL 94 pass/fail results using HRP as the sole explanatory variable. The Pearson statistic for the phlogistic model, $X^2 = 3.4$, was much less than the maximum allowable $\chi^2 = 11.1$ for the $\nu = B - 2 = 5$ degrees of freedom at the $s = 0.95$ significance level. It was observed that HRP, which is measured in flaming combustion and thus includes the effects of incomplete combustion typically associated with halogen-containing polymers and flame retardants, is no better at predicting the UL 94 V-0 test outcome as the sole explanatory variable than is the condensed phase thermal combustion properties η_c, Q_∞, $1-\mu$ and T_p from MCC. This probably reflects the greater uncertainty in HRP (≈ 20%) compared to the thermal and combustion properties (≈ 5%).

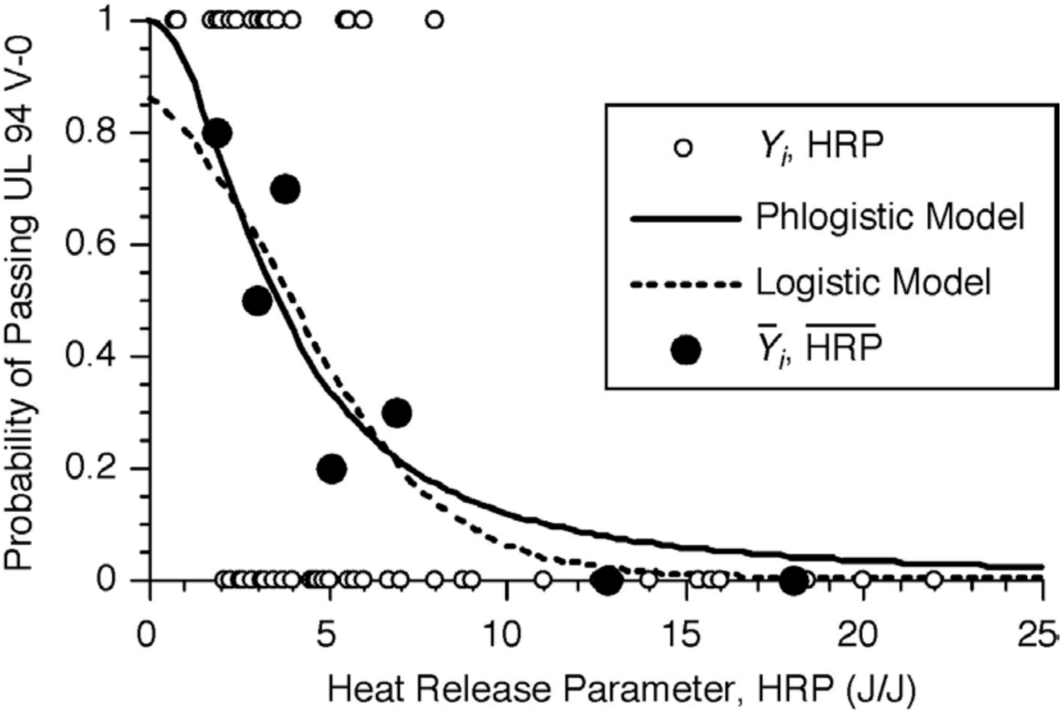


Figure 11. Probability of a V-0 Classification in the UL 94 Test vs. the HRP

Table 10. Nonlinear Least-Squares Regression Coefficients

		Logistic Response Function (equation 5)		Phlogistic Response Function (equation 12)	
Flammability Test	Predictor Variable	X_c	$-a$	X^*	b
14 CFR 25 HRR	η_c	149 J/g-K	2.24	145 J/g-K	2.74
UL 94 V-0	η_c	385 J/g-K	2.31	340 J/g-K	1.84
UL 94 V-0	Q_∞	18.6 kJ/g	3.55	17.8 kJ/g	3.43
UL 94 V-0	ϕ	0.733	5.11	0.717	5.09
UL 94 V-0	HRP	3.91	1.80	3.61	1.96
UL 94 V-0	T_p	535°C	-15.50	533°C	-15.40

Table 11. Quality of Response Functions for Fitting *B* Pairs of Grouped/Binned Data Using Model Parameters of Table 9

			Logistic Response Function (Equation 5)			Phlogistic Response Function (Equation 12)		
Flammability Test	Predictor Variable	B	R	MD (%)	$p(0)$	R	MD (%)	$p(0)$
14 CFR 25 HRR	η_c	10	0.98	14.1	0.90	0.97	19.4	1.00
UL 94 V-0	η_c	11	0.94	16.5	0.90	0.94	19.0	1.00
UL 94 V-0	Q_∞	11	0.94	17.8	0.97	0.95	17.7	1.00
UL 94 V-0	ϕ	11	0.91	19.8	0.99	0.92	19.5	1.00
UL 94 V-0	HRP	7	0.92	26.0	0.88	0.92	26.5	1.00
UL 94 V-0	T_p	8	0.78	29.4	1.00	0.93	30.3	1.00

6. DISCUSSION.

The general utility of the simple logistic and phlogistic models for predicting the likelihood (frequency) of a passing result in a flame and fire test using a single thermal or combustion property as the explanatory variable was demonstrated for specific pass/fail criteria and a particular, wide ranging set of material compositions. Table 9 and figures 6 through 11 show that the median values of the explanatory variables X_c and X^* are similar for both models, as are the dispersion parameters a and b. The quality-of-fit parameters in table 10 show that the grouped data is highly correlated (R >0.9) by both the logistic and phlogistic response functions for η_c, Q_∞, HRP, and ϕ, but not for T_p, which is consistent with the rejection of T_p as a suitable explanatory variable by the chi-square test. For both models, the mean deviation of the predicted and grouped data is generally less than 20% for combustion properties η_c, Q_∞, and HRP, but is greater than 20% for the thermal properties ϕ and T_p. Consequently, the logistic and phlogistic models are equivalent from the perspective of a regression analysis of these binary flammability test data against a single explanatory variable. However, only the phlogistic model gives a value of $p_i = 1$ at $X_i = 0$ in accord with the definition of a noncombustible material as deduced from its thermal or combustion properties. It is understood that the regression parameters in table 9 and their predictive capability in table 10 are unique to the tests, criteria, and sample population of this study.

Multivariate probabilistic analyses using equations 2 and 11 with various combinations of flammability properties were conducted, but these showed no significant improvement in predictive capability for either model compared to the univariate analyses using η_c, Q_∞ as the sole explanatory variable (see tables 6 and 11). The reason that the multivariate analyses did not improve the predictive capability of the models is that the fire parameters chosen as explanatory variables for this study are not independent as shown by equations 18 and 19. The large scatter of the binary and grouped data around the predicted values in the univariate case is because no single explanatory variable is sufficient to describe the fire behavior in these tests. A first-order approximation of how each explanatory variable relates to the outcome of the 14 CFR 25 fire test is to write the steady HRR as an inequality in terms of the criterion for passing the test, HRR ≤ 65 kW/m^2:

$$HRR = HRP\left(q''_{ext} + q''_{flame} - \sigma T_p^4\right) \leq 65\,\text{kW/m}^2 \tag{23}$$

$$HRP = \chi \frac{\eta_c}{h_g / \Delta T_p} = \frac{\chi}{\phi}\frac{Q_\infty}{h_g}$$

In equation 23, q''_{ext} is the externally applied heat flux from a burner flame or heater, q''_{flame} is the heat flux to the sample from its attached flame, χ is the combustion efficiency of the fuel gases in the sample diffusion flame, h_g is the energy required to thermally decompose unit mass of solid to volatile fuel (heat of gasification), and σ is the Boltzmann radiation constant. The HRR criterion (equation 23) is satisfied by a wide range of values for the thermal/combustion properties and no single thermal/combustion property or test parameter will determine the outcome of the 14 CFR 25 fire test because the remaining properties/parameters vary from material to material.

In the UL 94 vertical flame test, HRR ≈ 65 kW/m^2 at extinction/V-0 [17 and 19], so the same inequality (equation 23) applies with $q''_{ext} = 0$ after the Bunsen burner is removed.

$$HRP\left(q''_{flame} - \sigma T_p^4\right) \leq 65\,\text{kW/m}^2 \tag{24}$$

Consequently, the V-0 criterion can be satisfied by larger values of the thermal combustion properties (compare η_c for 14 CFR 25 and UL 94 V-0 in table 9) because the external heat flux (burner) is removed at the start of the burn time measurements.

Entirely absent from this qualitative analysis of the effect of intrinsic (thermal combustion) properties on fire test results is the effect of the extrinsic/physical processes of melting and dripping; swelling and intumescence; gas phase inhibition; barrier formation; and sample thickness that can significantly influence the outcome of these fire tests. Consequently, individual thermal combustion properties can influence, but not determine, the outcomes of 14 CFR 25, UL 94, and other fire tests, and this is reflected in the broad cumulative probability distributions in figures 6 through 11. Given the importance of extrinsic factors and the multi-parametric nature of HRR in these tests, it is remarkable that a statistical (probabilistic) analysis using a single explanatory variable provides a reasonable correlation of fire test results with only two adjustable parameters (e.g., X^* and b). This is undoubtedly due to the wide range of values of the explanatory variables examined in the study and their interdependence (e.g., high char yield/low fuel fraction is often associated with high decomposition temperature and low heat of combustion, all of which contribute to a passing result, as shown in equations 23 and 24).

A practical use of the results of this study would be to make a decision about scaling up a particular flame-retardant plastic formulation for commercial production using only a small (gram-sized) research sample. The end-use application is assumed to be an electrical component that requires a UL 94 V-0 rated plastic. Choosing η_c as the sole explanatory variable, and measuring η_c = 175 J/g-K for the research plastic in a laboratory test, the likelihood of passing the UL 94 V-0 test is estimated from equation 5 or equation 12 and the regression parameters in table 9. The result is $p = 0.77$ (phlogistic) or $p = 0.74$ (logistic), so the research plastic will have about a 75% chance of achieving a V-0 classification in the UL 94 vertical flame test.

7. CONCLUSIONS.

Several thermal and combustion properties were evaluated as sole explanatory variables for two pass/fail flammability tests using two different probabilistic models. The thermal and combustion properties spanned the range of commercial polymers and flame-retardant plastics. The flammability tests were a fire test in Title 14 of the Code of Federal Regulations (CFR) 25 and a vertical flame test (UL 94 V) with categorical outcomes. The probabilistic analysis involved nonlinear least squares regression of the frequency of passing results for each of the continuous explanatory variables using the logistic and phlogistic response functions with two adjustable parameters. The chi-square test showed that the logistic and phlogistic probability models were appropriate for describing the 14 CFR 25 and UL 94 V results, using η_c, Q_∞, ϕ, and HRP as the sole explanatory variable, but these models were not appropriate for T_p as an explanatory variable. Moreover, the combustion properties η_c, Q_∞, and HRP that combine condensed phase (T_p h_g, ϕ) and gas phase (h_c) properties are more reliable predictors of pass/fail flammability test results than the thermal properties of the condensed phase alone. The overall efficacy of the thermal and combustion properties for predicting flammability test results based on the correlation coefficient and mean deviation of the grouped (binned) data from the fitted response functions is:

$$\eta_c \approx Q_\infty > HRP > \phi > T_p$$

Both of the probabilistic models are suitable in the vicinity of the median explanatory variable (X^* or X_c), but the logistic model provides a better fit at $X > X_c$ and the phlogistic model provides a better fit at $X < X^*$, particularly at $X = 0$.

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