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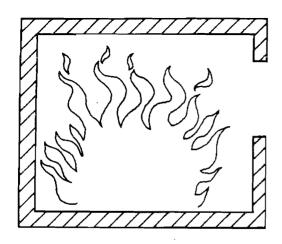
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REPORT NO 79-1



VYTENIS BABRAUSKAS - ULF WICKSTRÖM

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Thermoplastic Pool Compartment Fires

Vytenis Babrauskas - Ulf Wickström



Thermoplastic Pool Compartment Fires

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A numerical investigation is described wherein expected gas temperatures in compartment fires where the fuel consists of a pool of thermoplastic material are determined. Natural ventilation from a single rectangular window is assumed and only steady-state, well-stirred, flashed-over fire is considered. The fuel is assumed to pyrolyze radiatively only. The dominant variable is shown to be the ratio of ventilation parameter to fuel area. A stable higher and an unstable lower solution are obtained for gas temperature. The stable solution corresponds to fuel-rich burning; the unstable solution would indicate fuel-lean burning. For ventilation parameter/fuel area ratio in excess of that at stoichiometry, no real solution is obtained, indicating that a well-stired fire does not occur under this condition. The dependence of gas temperature on the ratio of ventilation parameter to fuel area and window height is developed. Predicted results are compared to experimental data from small-scale fire tests where polyethylene and polymethylmethacrylate were used as fuel and show agreement. The finding that a flashed-over fire does not occur for fuel-lean conditions is verified by this comparison.

1. INTRODUCTION

Thermoplastic fuels tend to melt and burn poollike on the floor of a compartment. The radiative view factor between the pool and the room is thus 1.0 and the self-view factor, zero. The fuel liberation rate for thermoplastic fuel fires depends much more strongly on surrounding gas and wall temperature than it does for conventional wood crib tests [1, 2, 3]. In the latter, the fuel liberation rate is largely self-controlled and variations in external temperature and radiation do not produce marked changes in the rate of burning.

Thus, a numerical investigation undertaken to achieve an understanding of the character of thermoplastic fuel fires is reported here. A single pool of area A_f , located on the floor of a compartment naturally ventilated through a single window of

The ratio of the ventilation parameter $A\sqrt{h}$ to fuel area A_f is shown to be the dominant variable in predicting the behavior of a compartment fire with thermoplastic fuel. A stable higher and an unstable lower solution are found for gas temperature. For a fuel-lean condition, only an unstable solution is obtained, indicating that a well-stirred, flashed-over fire does not occur in this case. The numerical results of this investigation are compared to experimental data. Predicted trends of response and more especially the finding that a flashed-over fire will not occur for a fuel-lean condition are verified.

Bullen [5] performed a numerical calculation

area A, height h, and width b, is considered. Only steady-state, well-stirred, flashed-over fires with no self-viewing fuel surfaces are considered. A flashed-over fire is defined [4] as one in which the average stirred gas temperature in the upper half of the room exceeds 873 K (600°C).

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for a similar problem with liquid fuels. Using the expression for fuel pyrolysis assumed here, he calculated gas temperatures for varying ventilation parameter and heat of vaporization, but did not draw the conclusion that a flashed-over fire cannot occur for a fuel-lean condition. By assuming a single-step Arrhenius reaction rate, Thomas [6] recently demonstrated that heat balance in a compartment can be satisfied at more than one temperature, Takeda and Nakaya [7] conducted an experimental and theoretical study of methanol pool fires and derived a conclusion similar to that of the present study, but from different premises. By considering only convective modes of heat transfer and assuming a single-step Arrhenius reaction rate, they demonstrated that there is an upper and lower limit to the window opening factor $A\sqrt{h}$ at which sustained burning can occur.

2. THEORETICAL CONSIDERATIONS

A solution for the steady-state gas temperature in a burning compartment is sought under the following assumptions:

- a. The gas is well-stirred and its temperature adequately represented by the average value T_f ; the room is flashed-over.
- b. The gas is radiatively gray, a reasonable assumption provided that the fuel is fairly sooty and the compartment sufficiently large.
- c. There is a sufficient supply of fuel to allow for steady-state conditions to occur.
- d. The fuel is a thick thermoplastic pool of area A_f , assumed to pyrolyze solely radiatively according to the equation:

$$\dot{m}_p = A_f \frac{\epsilon \sigma (T_f^4 - T_b^4)}{\Delta h_p} \tag{1}$$

The symbols in this expression are defined in the list of nomenclature. The radiative view factor between the pool and the room is 1.0, the self-view factor zero. Since a steady-state solution is sought, the effect of wall temperature on m_p is small and can be subsumed under ϵ .

e. Reaction rates limit neither gas phase combustion nor fuel pyrolysis.

TABLE I

Values Used in Numerical Calculations

 ϵ , gas emissivity = 0.9 b_p , maximum combustion efficiency = 0.7 A/A_{up} , window/wall area ratio = 0.083

Polyethylene (C2H4)n

 Δh_c , calorific value (lower) = 43.6×10^3 J/g Δh_p , total heat of vaporization = 2400 J/g T_b , vaporization temperature = 663 K r, stoichiometric air-fuel mass ratio = 14.76

Gypsum Wallboard (thickness = 38mm)

ho, density = 790 kg/m³ k, thermal conductivity = 0.17 W/m-K C_p, heat capacity = 0.84 J/g-K

emissivity = 0.5

The analysis of compartment heat balance follows that of Babrauskas and Williamson [8]. The governing equation is:

$$\dot{h}_c = (\dot{m}_{air} + \dot{m}_p) \int_{aaa}^{T_f} C_p dT = \dot{Q}_w + \dot{Q}_r$$
 (2)

where \dot{Q}_{10} and \dot{Q}_{r} are total wall losses and window radiation losses, respectively. Air inflow, \dot{m}_{air} , is given by the Bernoulli equation, and \dot{h}_{c} is equal to the lesser of $(b_{p}\dot{m}_{p}\Delta h_{c})$ and $(b_{p}\dot{m}_{air}\Delta h_{c}/r)$.

3. NUMERICAL CALCULATION

A modified version [9] of the compartment fire algorithm COMPF [10] was used to perform the calculations. The fuel considered was polyethylene; the properties assumed in the analysis are given in Table 1. A gas emissivity of 0.9 was assumed, a reasonable value for full-sized compartments. The heat capacity and molecular weights of the pyrolysates have not yet been successfully determined and were set equal to those of nitrogen. The maximum fraction of pyrolysates burnt (or maximum combustion efficiency), b_p , and the maximum fraction of air utilized for combustion were set equal to 0.7. This value characterizes the

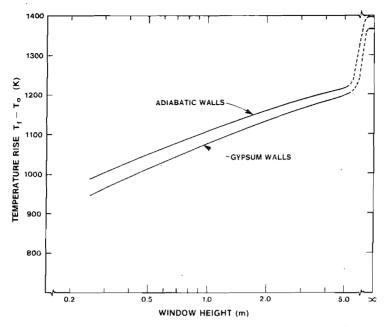


Fig. 1. Effect of wall materials and window height on gas temperatures, $\eta = 1.0$

unmixedness of the compartment. Although direct measurements are not available, b_p can be estimated from its effect on gas temperature. Two wall conditions were considered: adiabatic walls and walls approximating a 38-mm thickness of gypsum wallboard. The window/wall area ratio was taken as 0.083.

Let η be the ratio of air supply to fuel area divided by that same quotient at stoichiometry,

$$\eta = \frac{(A\sqrt{h}/A_f)}{(A\sqrt{h}/A_f)_{\text{ctoich}}} \tag{3}$$

then $\eta=1$ represents a stoichiometric air supply. With η so defined, generalized combustion curves may be readily obtained. To calculate η , $(A\sqrt{h}/A_f)_{\text{stoich}}$ must be determined. A good approximation [8] for \dot{m}_{air} , valid for the realm of flashed-over fires, is

$$\dot{m}_{\rm air} \cong 500 A \sqrt{h} \ (g/s) \tag{4}$$

A stoichiometric air/fuel mass ratio can be defined

as

$$r = \frac{\dot{m}_{\rm air}}{\dot{m}_p} \tag{5}$$

and is a property of the fuel determined by its chemical composition. When combined with the equation for m_p , this gives

$$(A\sqrt{h}/A_f)_{\text{stoich}} = \frac{1}{500} \frac{r}{\Delta h_p} \dot{q}_r''(m^{1/2})$$
 (6)

where $q_r'' = \epsilon \sigma (T_f^4 \cdot T_b^4)$. The window height, h, must also be separately considered, because it influences the relative magnitude of radiation loss through the window.

A range of $0.005 \le \eta \le 1.2$ and $0.25 \le h \le 5$ m was used in the analyses of the adiabatic and gypsum wallboard cases. The rise in gas temperature, $T_f - T_0$, is shown in Fig. 1 for $\eta = 1$. When the window height was decreased while the window area was held constant, the flow rate decreased but

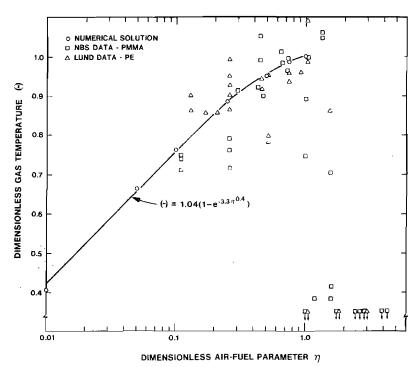


Fig. 2. Measured and calculated values of dimensionless gas temperatures

window radiation losses were unchanged. The relative magnitude of radiation loss was therefore greater in this case and the gas temperature decreased.

For other values of η , a dimensionless gas temperature defined by

$$\theta = \frac{(T_f - T_0)}{(T_f - T_0)_{n=1}} \tag{7}$$

can be represented as a universal curve dependent only on η . The computed values are shown in Fig. 2. The results can be fit to within 4% over the range $0.01 \le \eta \le 1$ by the expression

$$\theta = 1.04\{1 - \exp(-3.3\eta^{0.4})\}$$
 (8)

4. THE SOLUTION

Heat balance exists only at those temperatures where the residual of the heat balance equation equals zero:

$$f_1 = \dot{h}_c - (\dot{m}_{air} + \dot{m}_p) \int_{298}^{T_f} C_p \, dT - \dot{Q}_w - \dot{Q}_r$$
(9)

In Fig. 3, the temperature dependence of f_1 (the residual of the heat balance equation), h_c (heat generated), and $(h_c - f_1)$ (heat losses) is illustrated for two values of η . The heat release curve, h_c , begins at zero at the fuel surface temperature — 663 K in this case — rises to a peak, and then gradually diminishes. The losses begin at the virtu-

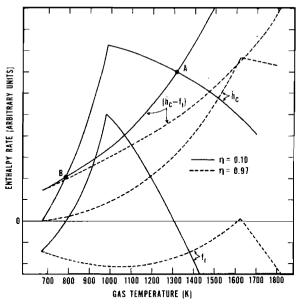


Fig. 3. Heat balance for two values of η

al origin of $T_f = T_0$ and increase monotonically with temperature. The peak of the \dot{h}_c curve represents stoichiometric conditions. However, burning can take place stoichiometrically only if $\eta \equiv 1$. For other values of η , stoichiometric burning is not possible because heat balance does not occur. At peak gas temperature, irradiation to the fuel surface is approximately proportional to η . Thus, the peak of the $\eta = 0.1$ curve in Fig. 3 falls at:

$$\frac{0.1}{1.0} \approx \frac{978^4 - 663^4}{1633^4 - 663^4} \tag{10}$$

The relationship is not exact because the weak dependence of m_{air} on T_f is not accounted for.

For all η less than 1.0 and greater than approximately 0.004, there are two solutions for T_f . Consider the upper solution, point A for $\eta = 0.1$. This is a stable solution since, for a slight increase in temperature, losses increase and heat gain decreases. The temperature will therefore return to that at point A. It can also be seen that this upper solution represents fuel-rich burning. Point B can

be shown to be unstable by a similar argument. For a slight increase in temperature, both heat gain and losses increase; the heat gain is, however, greater than the losses, resulting in a further increase in temperature until the heat balance equilibrium at point A is reached. A temperature decrease at point B, on the other hand, leads to extinction. Point B, being to the left of the peak on the \dot{h}_c curve, would represent fuel-lean burning.

For $\eta > 1.0$ there is no real solution in the physical domain. A well-stirred, flashed-over fire thus cannot occur for this condition. Burning is, of course, possible, but will be localized with significant temperature gradients in the fire compartment.

If wall properties or window area A are varied without changing the ventilation parameter $A\sqrt{h}$ or any other variable, only the terms Q_w and Q_r in the heat balance equation are affected. The value of $(A\sqrt{h}/A_f)_{\text{stoich}}$ increases as losses decrease (Fig. 3). A compartment fire may not be flashed over for a considerable period of time while the wall surfaces are cold and wall losses Q_w great.

TABLE 2	
Small-Scale Test Conditio	ns

	NBS	LUND
Fuel type	PMMA	PE
r	8.27	14.76
Δh_n	1630 J/g	2400 J/g
Compartment size $(H \times W \times D)$	$0.30 \times 0.30 \times 0.56 \text{ m}$	$0.75 \times 0.75 \times 0.75 \text{ m}$
Compartment walls	25 mm ceramic fiber block	1.5 mm steel, $\rho = 7770 \text{ kg/m}^3$
	(Kaowool, Babcock & Wilcox Co.) $\rho = 250 \text{ kg/m}^3$	10 mm asbestos, $\rho = 1020 \text{ kg/m}^3$
η	0.11 - 9.84	0.13 - 3.01
h	0.225 m	$0.34 - 0.68 \mathrm{m}$
A_f	$0.0025 - 0.0225 \text{ m}^2$	$0.0784 - 0.3136 \mathrm{m}^2$
q_r (measured: $\eta \cong 1$)	$1.20 \times 10^5 \mathrm{W/m^2}$	$1.32 \times 10^5 \text{W/m}^2$
$(A\sqrt{h}/A_f)_{\text{stoich}}$	1.22 m ^{1/2}	1.68 m ^{1/2}
ϵ (from radiometer	0.74	0.64
measurement)	$(T_f = 1303 \text{ K})$	$(T_f = 1383 \text{ K})$
\dot{m}_{n} (measured: $\eta \approx 1$)	52 g/s-m ²	65 g/s-m ²
$\epsilon \text{ (from } \dot{m}_{p}\text{''})$	0.74	0.51

 $(A\sqrt{h}/A_f)_{\text{stoich}}$ may then be less than the actual value of $(A\sqrt{h}/A_f)$ of the compartment, making η greater than 1. A local pool fire may, however, increase the wall temperature, leading to a lower value of Q_w and a higher value of $(A\sqrt{h}/A_f)_{\text{stoich}}$. If η then becomes less than 1, a flashed-over fire develops and gas temperature rises rapidly.

5. COMPARISON TO EXPERIMENTAL DATA

Analytical predictions were compared to two sets of experimental data from small-scale tests. Quintiere et al. [11] at the National Bureau of Standards (NBS) measured polymethyl-methacrylate (PMMA) fuel fires, and Kristiansson and Lidgren [12] at the Lund Institute of Technology burned polyethylene (PE) fuel. Values for the experimental conditions are given in Table 2. The Lund tests consisted of twenty-three experiments covering a range of 0.13 $\leq \eta \leq$ 3.01 calculated using measured \dot{q}_r ". The average upper gas space temperatures at peak burning rate are given in Fig. 2. In most but not all cases these correspond to a steady-state condition. Window heights covered the range of $0.34 \le h \le 0.68$ m. T_f at $\eta = 1$, adjusted to a constant value of h = 1.0 m according to Fig. 1, was taken as 1368 K. The values of

 $(A\sqrt{h}/A_f)_{\text{stoich}}$ in Table 2 were calculated using Eq. 6 and the measured maximum values for q_r'' . Test data from forty tests in the NBS series were available in the range $0.11 \le \eta \le 9.84$. Values for tests where $\eta > 5$ are not shown in Fig. 2; θ was less than 0.2 for all tests in this range. Six tests at the smallest window width, b = 0.015 m, were excluded since results were erratic. For the NBS tests, T_f at $\eta = 1$ was taken as 1243 K. Values of Δh_p were taken from Tewarson and Pion's [13] tabulation.

The data generally follow the curve in Fig. 2, although there is considerable scatter. The scatter can in many instances be attributed to a failure to reach steady-state burning. The prediction of the discontinuous behavior at $\eta=1$ is, however, strikingly accurate. Within the range $\eta=0.9$ to 1.6, the θ values jump from 1.0 to less than 0.4. Experimental observations indicate that at approximately the same point, the character of burning changes from that of a general room fire to that of a localized fire plume. Thus, the prediction that a flashed-over fire for $\eta>1$ does not occur was verified by the results of the small-scale tests.

No systematic study of thermoplastic pool fires in full-size rooms is available for comparison. Exploratory measurements by Anderson [14] of *n*-heptane pool fires in a full-size room indicate behavior similar to that seen in the small-scale tests. At $\eta = 0.92$, the fire covered large areas of the room, at $\eta = 1.2$ the fire was smaller and oscillatory, and at $\eta = 2.0$ and 3.0 only a localized pan fire still burned.

6. DISCUSSION

Steady-state compartment fire temperature solutions were obtained for a range of practical controlling variable values. Heat balance for the compartment and the fuel surface was calculated assuming that reaction rates limit neither combustion nor pyrolysis. Two solutions, one stable and the other unstable, resulted for $0.005 < \eta < 1.0$. For $\eta = 1.0$, one solution was obtained, and for $\eta > 1.0$, none. At approximately $\eta = 0.004$ the two solutions collapse to a single, trivial value, $T_f = T_b$.

By including a single-step Arrhenius reaction rate in gas phase both Thomas [6] and Takeda and Nakaya [7] demonstrated that effectively η must be restricted to a value above a lower bound set by the reaction rate. Values for reaction rate constants for use in that type of model have not been investigated. An empirical lower limit on η may, however, be estimated from the findings of Jansson and Onnermark [4]. Their experimental results indicate that the minimum gas temperature necessary for a compartment to be flashed over is 873 K (600°C). This value does not appear to be sensitive to variations in fuel type or ventilation. but the relation is not understood in detail. In none of the small-scale tests were η values sufficiently low to verify the lower limit.

The effect of varying h and η on steady-state temperature is illustrated in Figs. 1 and 2, respectively. Since in full-scale buildings only a modest range of wall loss values is found, the gypsum wall-board case analyzed here can be assumed typical. The weak dependence of the present solution on wall losses suggests that the common practice of using $(A\sqrt{h}/A_{10})$ to characterize compartment fires is inadvisable. Furthermore, the method presented here allows the adiabatic case to be treated naturally.

Heats of combustion for most thermoplastics

vary over a range of approximately 3:1. For fixed r, gas temperature would in theory rise markedly with increasing Δh_c . In practice, however, the ratio $\Delta h_c/r$ is by far the more important variable for heat balance, and since for most plastics $\Delta h_c/r$ varies only by approximately \pm 20% from the value for polyethylene [15], it cannot significantly affect gas temperature in most thermoplastic fuel fires

The effect of variations in the heat of vaporization, Δh_p , is largely accounted for by the nondimensional variable η . At $\eta=1$, Δh_p does not affect temperature. For lower values of η , temperature decreases slightly when Δh_p is raised, due to extra losses absorbed in pyrolyzing the unburnt fuel fraction. When Δh_p is doubled or halved, temperature is affected by a maximum of approximately 8% at $\eta=0.05$. Changes in the surface temperature of the fuel, T_b , do not affect gas temperature significantly except as T_t approaches T_b .

Effective emissivities, including the wall effect, for small-scale test conditions were in the range 0.51 to 0.74 (Table 2). Emissivity increases with scale and a value of 0.9 were chosen as typifying a full-scale fire for calculating the curves in Fig. 1. That value and the value of 0.7 assumed for b_p are speculative and may have to be changed considerably in practice.

Flashover may well occur for $\eta > 1$ for fuels that exhibit surface reactions or are self-viewing. In such cases, and in the case of mixed fuels, it may not be prudent to assume that flashover can be prevented simply by letting η exceed unity.

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NOMENCLATURE

A window area (m^2) A_f fuel pool area (m^2)

 A_w wall area (m2) b window width (m) b_p combustion efficiency (--) C_{p} heat capacity (J/g - K)h window height (m) h_c combustion enthalpy rate (W) $\dot{m}_{\rm air}$ air inflow rate (g/s) fuel pyrolysis rate (g/s) \dot{m}_{p} \dot{q}_r fuel irradiance (W/m²) Q_w wall losses (W) Ò٠ window radiation loss (W) stoichiometric air-fuel mass ratio (--) I T_b fuel vaporization temperature (K) compartment gas temperature (K) T_f T_0 ambient temperature (298 K) Δh_r heat of combustion (J/g) heat of vaporization (J/g) Δh_p emissivity (--) Ē compartment equivalence ratio (--) η θ nondimensional gas temperature (--) Stefan-Boltzmann constant $(W/m^2 - K^4)$ σ

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