Computational Fluid Dynamics Predictions of Thermoplastic Fire Suppression by Water Spray

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ABSTRACT

The effect of thermoplastic fire suppression by water spray is investigated using Computational Fluid Dynamics (CFD) modeling.

Critical water application rate required to extinguish fire is found as a function of a mean droplet diameter in the spray. This dependence may be considered as a fundamental characteristic of the spray suppression capability. Two different regimes of fire suppression, the gas phase and the surface suppression, are observed, and the transition between the two regimes is identified. The semi-analytical approach to the surface extinguishment phenomenon is also considered.

The results of mathematical modeling are compared with the available experimental data and the implications of findings for the optimum fire fighting strategy are discussed.

KEYWORDS: Fire suppression, sprinkler, water spray

NOMENCLATURE

f - Temperature gradient in fuel at the solid-gas interface
h_1 - Heat transfer coefficient between gas and solid
k - Turbulence kinetic energy
k_s - Thermal conductivity of the solid fuel
l - The coordinate of solid-gas interface
L_s - Latent heat of vaporization of PMMA
L_w - Latent heat of water vaporization
m_w - Water application rate
q_{evap} - Heat flux due to droplet evaporation

q_{rad} - Radiative heat flux from flame to surface
Q_s - Heat flux conducted into solid
r - mass loss rate of solid fuel
R_{ebu} - Reaction rate due to Eddy-breakup model
s - Soot conversion factor
t - Time
T - Temperature
T_g - Gas temperature
T_s - Surface temperature
T_0 - Initial solid temperature
u - linear regression rate of the solid phase
x - Cartesian coordinate in the solid phase
Y_F - Fuel mass fraction
Y_o - Oxygen mass fraction

Greek letters
ε - Turbulence dissipation rate
μ - Density of a thermal potential
ρ_s - Solid fuel density
χ - Thermal diffusivity of the solid phase
Ψ - Thermal potential of a single layer
φ - Initial temperature distribution in the solid fuel
ω - Poisson integral

Superscripts
0-steady-state

INTRODUCTION

Experimental and theoretical investigations of fire suppression by sprinkler water sprays has been given increasing attention in the recent years. This activity is underpinned by the present extensive use of sprinkler technology. The wide-spread application of this fire control equipment in the foreseeable future dictates the need for optimization of sprinkler application strategy.

A number of experiments on fire suppression with water sprays were reviewed by Rasbash [1]. Tamanini [2] performed experiments on the extinguishment of vertical wood slabs. Magee and Reitz [3] conducted a similar study on the extinguishment of polymethylmethacrylate (PMMA) slabs. The suppression of propane fire in enclosure was studied by Wighus [4]. A number of experiments (Tamanini [5], Kida [6], Heskestad [7], Takahashi [8]) have been conducted on wood crib extinguishment.

The increasing capability of computational fluid dynamics models has opened the possibility to model two-phase phenomena associated with spray/fire interaction. A number of studies have been reasonably successful in the prediction of fire fighting capabilities of water sprays. Numerical simulations on the Actual Delivered Density (ADD), that is the water density reaching the base of a fire, are reported in [9]. The same model has been used in [10] to model heptane-spray fire scenarios.

The detailed modeling of fire extinguishment has been undertaken in recent studies [11] (for plastic materials) and [12] (for simplified wooden cribs). Fire suppression in the gaseous

phase was modeled in [13].

However, the computational effort has not been sufficient so far to provide a complete picture of fire suppression by sprinklers.

Both experimental and modeling studies reveal a strong effect of the droplet size distribution in the spray on water extinguishment capabilities. For a burning surface fully open to the action of a water spray the major possible mechanisms of fire extinguishment are: 1) diffusion flame suppression in the gaseous phase, and 2) fuel cooling which stops the pyrolysis reaction in the solid phase. One would expect that the primary mechanism for a particular case will depend on the characteristics of the spray. Furthermore, the actual water requirements to extinguish a fire may vary significantly depending on the regime of extinguishment. Despite the obvious importance for fire fighting technology, this effect has not been sufficiently investigated in previous studies.

The extinguishment capability of the spray is naturally described by the critical (minimum) water application rate required to achieve extinguishment. This rate is generally a function of the droplet distribution in the spray. In the present study the spray is characterized, in a first approximation, by a single parameter, that is a mean droplet diameter. We seek, therefore, to establish a general form of critical water flow rate as a function of mean droplet diameter in the spray. We will refer to this function as an *extinguishment curve*.

The extinguishment curve was first simulated by Ball and Pietrzak using a simplified model [14]. For a gaseous flame suppression this curve has a minimum which corresponds to the optimum droplet diameter. For droplets with a diameter smaller than the optimum, the critical water application rate increases as the fine droplets are carried away by hot fire products and cannot evaporate in the flame to bring it to extinguishment. Similarly, large droplets cannot produce the sufficient rate of evaporation as they quickly penetrate to the surface.

However, when surface extinguishment due to fuel cooling is taken into account, the behavior of the extinguishment curve changes dramatically. At some mean droplet diameter a sufficient number of droplets would evaporate on the surface to stop the pyrolysis reaction.

In the present study we expand the study of the extinguishment curve to the case where both flame cooling and solid fuel cooling are taken into account and identify quantitatively different mechanisms of fire suppression.

COMPUTATIONAL ARRANGEMENTS

Three-dimensional fire simulations in a 9.0 m x 9.0 m x 5 m enclosure with side openings (Fig.1) are considered. Polymethylmethacrylate (PMMA) slab of 1.8 m x 1.8 m with 0.05 m thickness is used as a fuel. The size of the slab is chosen to deliver an approximate fire power of 1 MW under steady-state burning conditions. Sprinkler nozzle is located at the center of the ceiling.

MATHEMATICAL MODEL

Gas Flow and Combustion Modeling

The commercial CFD package STAR-CD [15] is used to solve three-dimensional equations for

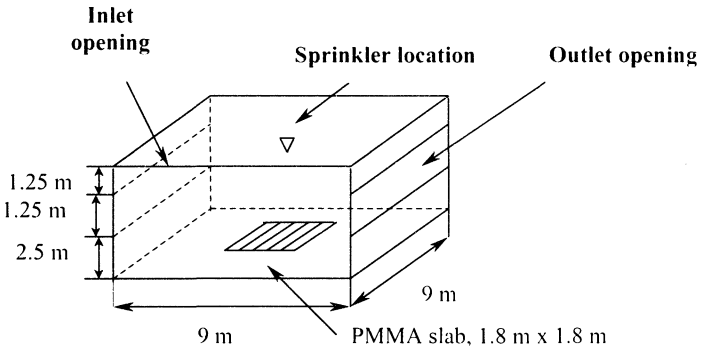

FIGURE 1 A sketch of computational arrangements

turbulent transport of mass, momentum, turbulence energy and dissipation, mixture fraction, fuel mass fraction and enthalpy. The standard k-ε closure for turbulence and the Discrete transfer method for radiation are used. This set of equations is currently widely used in fire modeling, and the details can be found elsewhere, e.g. [11-13].

The following combustion reaction in the gas phase is assumed:

$$C_n H_m + (n - s + m/4)(O_2 + 3.76\, N_2) \rightarrow \\ \rightarrow sC + (n - s)\, CO_2 + m/2\, H_2O + 3.76(n - s + m/4)\, N_2 \qquad (1)$$

where s is a parameter to define the amount of soot produced.

The rate of combustion is modeled using Eddy-Breakup (EBU) approach [16]. In EBU model the conservation equations for both mixture fraction and fuel mass fraction are solved to allow the mass fraction of oxygen and products to be determined. The rate of reaction is then expressed as

where step-function $\Gamma(T)$ is used to cancel the reaction rate for sufficiently low temperature.

$$R_{ebu} = - C_R \rho \varepsilon / k \cdot \min(Y_F, Y_O / S) \cdot \Gamma(T) \\ \Gamma(T) = 1,\ T \geq T_{cxt};\quad \Gamma(T) = 0,\ T \leq T_{cxt} \qquad (2)$$

The local temperature threshold of T_{cxt} = 1600 K is chosen as an extinction criterion for the gaseous flame, which proved to be reasonably accurate in the past studies [13,17].

Spray Model

A conventional Lagrangian approach, widely used in sprinkler modeling [11-13] is adopted to model water spray. Particular heat and mass transfer coefficients, employed by STAR-CD to describe droplet heat-up and evaporation are slightly different from [11-13]. They are based on Ranz-Marshall correlation for Nusselt number, and full details may be found in [15,20]. Complete instantaneous droplet evaporation is assumed once the droplet hits the surface.

Each spray with a particular mean diameter D_m has been statistically represented by 10 groups of droplets, their diameters being uniformly distributed from 0.5 D_m to 1.5 D_m. Equal mass fractions of *0.1* were given to each group.

PMMA Burning Model

PMMA volatiles are released into the gas phase as a result of a volatilization process which is modeled as a phase change at a constant surface temperature. In the solid phase, the one-dimensional heat transfer equation

$$\frac{\partial T}{\partial t} = \chi \frac{\partial^2 T}{\partial x^2} \quad ; \quad -\infty < x < l(t) = \int_0^t u(t)dt \tag{3}$$

is solved where u is a surface regression rate which needs to be taken into account to accurately represent rapid surface extinguishment process, and $l(t)$ represents the position of the moving PMMA surface. Therefore, the heat transfer equation must be solved in the region with the moving boundary. The slab behaves as a thermally thick solid which allows the solution in the semi-infinite region to be considered.

The boundary conditions at the front surface in contact with the gas phase are taken as

$$T = T_s \quad ; \quad k_s \frac{\partial T}{\partial x} - \rho_s L_s u = h_l (T_g - T_s) + q_{rad} - q_{evap} \tag{4}$$

Here, q_{rad} is calculated from the radiation model. Heat flux due to water evaporation q_{evap} is obtained using spray submodel for water droplet tracking. The value h_l is calculated using the conventional log-law boundary conditions.

Instead of solving a partial differential equation in the region with unknown moving boundary, a novel approach is taken here, which represents the solution in the form of a thermal potential:

$$T(x,t) = \Psi(x,t,l(t),\mu(t)) + \omega(x,t) \tag{5}$$

where

$$\Psi(x,t,l(t),\mu(t)) = \frac{1}{2\pi^{1/2}} \chi^{1/2} \int_0^t \frac{\mu(\tau)}{(t-\tau)^{1/2}} \exp\left[-\frac{(x-l(\tau))^2}{(4\chi(t-\tau)}\right] d\tau \tag{6}$$

is a thermal potential of a single layer (function $\mu(t)$ is called *density* of a thermal potential) and

$$\omega(x,t) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \frac{\varphi(s)}{(\chi t)^{1/2}} \exp\left(\frac{-(x-s)^2}{4\chi t}\right) ds \qquad (7)$$

is a solution (Poisson integral) of heat transfer equation in the region $-\infty < x < \infty$ with the initial distribution $\varphi(s)$.

The thermal potential is known to satisfy thermal conduction equation (3) for $-\infty < x < l(t)$. Using (5-7), boundary conditions (4) may be written a system of integro-differential equations for the two unknown functions $\mu(t)$ and $l(t)$, which allows effective numerical solution. Details are provided in [18].

Note that this approach eliminates the need to compute temperature distribution in the solid phase, which is usually not needed, and explicitly provides the required value of the burning rate $u=l(t)$.

No extinguishment criterion is needed for surface extinguishment as the burning rate turns into zero when the total heat flux to the surface equals to the heat conducted into the solid.

NUMERICAL SOLUTION PROCEDURE

The simulations are carried out on a mesh which has 50 cells along, 50 cells across the room and 30 cells in vertical direction. The mesh is refined in the vicinity of the burning region. A steady-state solution in the absence of the spray is obtained first. To achieve a full coupling between solid and gas phases, at each time step several iterations are carried out in both phases to achieve a converged burning rate which satisfies (4).

Then a spray is released into the computational domain and steady-state solution is obtained once again to examine if extinguishment has actually happened. The initial angles of the droplets were distributed so that the spray covered the whole fuel area in the absence of fire. The mean droplet diameter in the spray has been varied from 100 μm to 1400 μm. Water application rates were in the range from $0.025\ l/(m^2 s)$ to $0.1\ l/(m^2 s)$.

Different computational time steps are employed for burning and extinguishment stages. A time step of 1 s was used during free burn of the fuel. To model the extinguishment, the time step was set to 0.01 s. A total of 10000 droplets were tracked to represent water spray.

RESULTS AND DISCUSSION

The Extinguishment Curve

The simulations of a developed PMMA fire are illustrated in Fig. 2, where the predicted temperature and velocity fields are shown.

The computed extinguishment curve is shown in Fig. 3 by solid line. At a given mean droplet diameter, water application rate above the curve extinguish fire, while for the application rate below the curve fire is not extinguished.

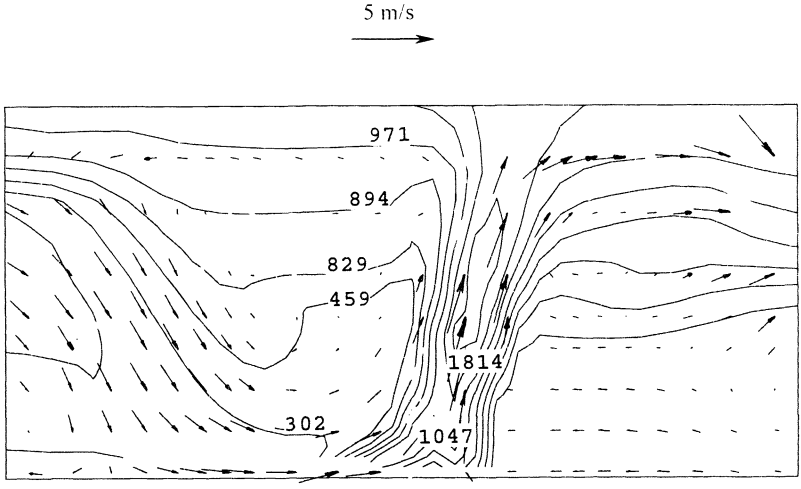

FIGURE 2 Temperature (° K) and velocity fields (presentation grid) through the symmetry plane of the computational region (Figure 1). Steady-state fire without water suppression.

Two different regimes of fire suppression are evident from Fig. 3. For small droplets, carried away from fire by upward air motion (mean diameter < 200 μm) flame suppression occurs in the gas phase. Critical water application rate rises sharply as the mean droplet diameter decreases. This regime corresponds to complete evaporation of the spray (Fig. 3) in the flame region. Heat extraction from the gaseous phase is, therefore, the dominant fire suppression mechanism in this case.

For mean droplet diameters over ~ 250 μm the critical rate remains essentially constant as the spray hits the surface. This range of diameters corresponds to the surface extinguishment regime. Solid fuel cooling by evaporating water droplets is a primary suppression mechanism for this regime.

The sharp transition between the two regimes occurs over a narrow range of mean droplet diameters between approximately 200 μm and 250 μm. Generally both mechanisms of suppression are involved in this transition region.

For comparison, an extinguishment curve for the pure gaseous suppression is shown by dashed line and reproduces the results [13]. This curve has a minimum at some optimum mean droplet diameter and then the critical water application rate starts to rise. The transition to surface extinguishment starts before that minimum is reached so that the extinguishment curve for the case where both phases are involved is monotonic.

The monotonic shape of the curve conforms with the results of Ball and Pietrzak [14] who also found the extinguishment curve to be monotonically decreasing. Also, likewise in [14], the departure of the curves which correspond to gaseous and surface extinguishment happens just near the minimum of the gaseous extinguishment curve. The mean droplet diameter at which the transition between the two mechanisms occurs is also reasonably close to that obtained in [14].

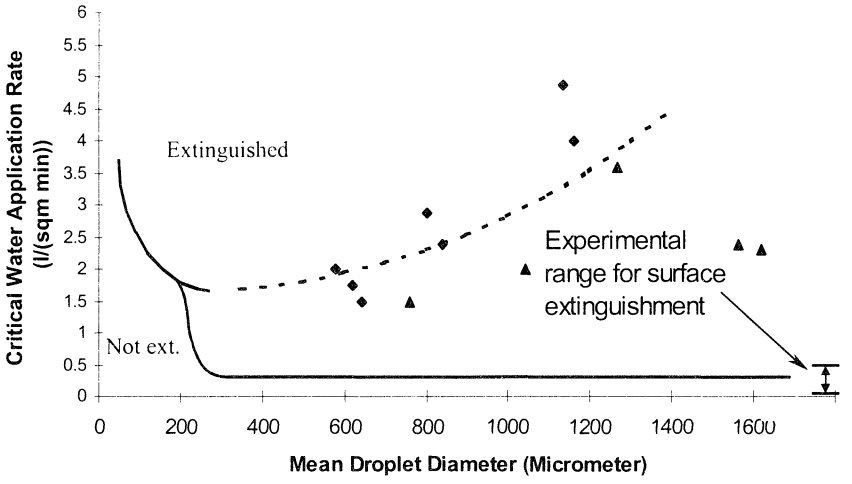

FIGURE 3 Critical water application rate as a function of a mean droplet diameter
———— - both solid and gas phase involved
---------- - gas extinguishment only
▲ - not extinguished, experimental data [4]
◆ - extinguished, experimental data [4]

However, there are significant differences in the two studies. The curve for the surface extinguishment in [14] falls much more slowly as the droplets are getting bigger. In contrast, in the present study the sharp transition is observed. It is believed to be the result of differences in the extinguishment criteria between [14] and the present study. In [14] a surface temperature threshold of 200 ^{0} C, averaged over the whole interior surface (not just fuel surface), is used as a criterion for fire knockdown due to fuel cooling. This criterion allowed the authors to get universal dependencies for compartments of different sizes, however, it is obvious that such a procedure highly overestimates the critical water flux. In the present study the surface extinguishment is modeled in a physically consistent way with no need for arbitrary extinguishment criterion.

Unfortunately there is a lack of experimental data on the transition between different types of extinguishment. However, some comparisons with experimental data can be made. The available data corresponds to the gaseous extinguishment at relatively large medium droplet diameters and surface extinguishment (both shown in Fig. 3).

The data on gas phase extinguishment is taken from study by Wighus [4] on water suppression of 1 MW fire. The computed extinguishment curve for pure gas extinguishment (dashed line, Fig. 3) reasonably well reproduces this set of data. The discrepancies between the simulations and experiments (particularly for coarse spray with mean droplet diameter of around 1.5 mm, Fig. 3) may be attributed to different droplet size distributions in the spray. The detailed distribution was not measured in [4].

Surface extinguishment data [1,3] suggests critical water fluxes which are about two times

smaller than found in the present study (1.3 g/(m^2 s) - 1.8 g/(m^2 s) compared to 2.8 g/(m^2 s)). It should be noted, however, that in the present study fire power was set to 1 MW for consistence with the experiments [4]. The fire powers in [1,3] were lower, which increased penetration capability of the droplets. It is important, however, that this comparison is put into the perspective of the general fire extinguishment picture. The present study confirms that the change in fire suppression regimes results in a significant (~10 times) drop in a required water flow rate. This indicates that large droplets are much more effective for fire suppression on open surfaces. It is this difference which is of real importance for design of fire suppression systems. The prediction error of ~ 1-2 g/(m^2 s) for the surface extinguishment should, therefore, be considered small compared with the difference in water requirements between the major extinguishment mechanisms.

To examine the sensitivity of simulations to different parameters, two additional sets of calculations were performed.

In the first, the extinction temperature was varied from 1500 K to 1700 K. The numerical experiments showed rather weak dependence of results on this parameter. The difference in the predicted critical flow rate was about 20 % and was approximately the same over the entire range of mean droplet diameters.

To examine the sensitivity to the droplet distribution in the spray, the distribution was made wider with the droplet diameters from 0.1 D_m to 2.0 D_m. The effect of this change was mostly observed for relatively fine sprays (D_m < 1.0 mm) and was about 30 % in terms of the critical water application rate, while for a more coarse spray (D_m ~ 1.3 mm) it was significantly lower (around 10%). Therefore, the model predictions appear to be reasonably insensitive to the uncertainty in the governing parameters.

Steady-state Limit for Surface Extinguishment

In this section we briefly discuss a semi-analytical approach for surface extinguishment modeling. This method gives reasonably accurate representation for a plateau on extinguishment curve (Fig. 3, mean droplet diameter > 250 μm).

The extinguishment curve has been obtained by computations of non-steady extinguishment process. However, a steady-state considerations may be successfully used to explain surface extinguishment phenomenon. In a steady-state approach we consider extinguishment as a non-existence of a steady-state balance between flame heat feedback to the burning surface and the burning rate of solid fuel.

Consider the rate of PMMA burning first. If surface temperature remain constant then a steady-state temperature distribution in the solid phase (Mikhelson profile) is given by

$$T^0(x) = T_0 + (T_s^0 - T_0)\exp(u^0 x/\chi); \quad f^0 = u^0(T_s^0 - T_0)/\chi \tag{8}$$

and the relationship between heat flux to the surface and burning rate is

$$Q_s = \frac{k_s r^0}{\chi \rho_s}(T_s - T_0) \tag{9}$$

When water flux m_w, applied to the burning surface, is less than critical then a new

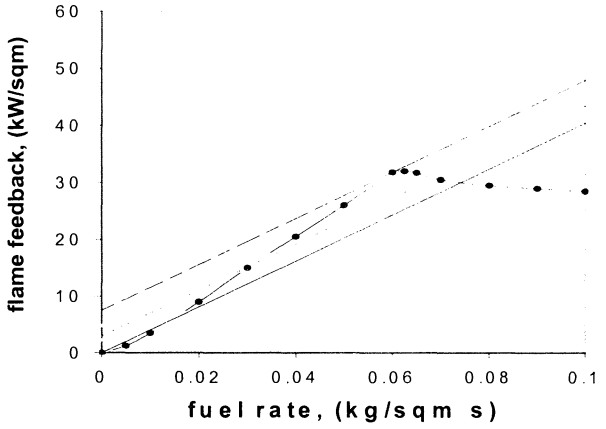

FIGURE 4 *Burning rate – flame feedback* diagram for PMMA
● - flame feedback $Q_s^{'}(r'')$; ——— - $Q_s(r'')$, m_w=0.0 g/(m^2 s); ..... - $Q_s(r'')$, m_w=1.28 g/(m^2 s); – – – – - m_w=3.2 g/(m^2 s)

steady-state burning rate is possible, which is given by

$$Q_s = \frac{k_s r''}{\chi \rho_s}(T_s - T_0) + L_w m_w \qquad (10)$$

On the other hand, if flammable volatiles are released into the gas phase at the rate $r''=\rho_s u''$ then flame feedback to the surface is a function of r'', $Q_s^{'} = Q_s^{'}(r'')$ and this function may be obtained as, for example, a result of CFD simulations

For steady-state solution to exist, an intersection of the curves $Q_s(r'')$ and $Q_s^{'}(r'')$ is required. Fig. 4 shows both curves for different values of water application rate. The flame feedback $Q_s^{'}(r'')$ is obtained from CFD simulations [19]. Clearly, as the water application rate increases, a steady-state solution is not possible after some critical water flow rate has been reached. This value may be considered as the critical water application rate required for extinguishment. This approach gives for the case of thermally thick PMMA slab a critical value of 3.2 g/(m^2 s) which is very close to the results of numerical simulations.

Table 1 compares steady-state approach predictions with different experiments as well as computations made in the present study.

It should be pointed out that the steady-state approach generally overestimates water requirements. Indeed, the extinguishment happens generally as a non-steady process, the governing parameters being in the region where a steady-state solution may still be possible theoretically. Therefore, the steady-state approach considers the most strict conditions for extinguishment and correspondingly overestimates critical water application rate. However, the accuracy of the method is sufficient for practical applications.

TABLE 1. Comparison of steady-state predictions for critical water application rate with experimental data and computational results.

Reference	Material	Critical water flux, g/(m^2 s)
Magee and Reitz [3]	PMMA	1.8
Rashbash [1]	PMMA	1.3 – 1.7
Mapping method, present study	**PMMA**	**3.2**
Unsteady numerical simulations, present study	**PMMA**	**2.8**
Wighus [4]	Flame extinguishment in gas phase, different droplet sizes	33.3 – 75.0

CONCLUSIONS

Numerical modeling of plastic (PMMA) fire suppression by water spray has been performed using commercial CFD package STAR-CD. Spray has been modeled using conventional Lagrangian formulation. A novel effective approach involving integro-differential equations has been taken to model PMMA burning process with surface regression.

The results indicate the presence of the two different fire suppression mechanisms - gas phase and solid phase extinguishment. A sharp transition has been observed between the two mechanisms. It would be interested to obtain the similar curve for charring materials. Earlier results [13] on extinguishment times for wood suggest more smooth transition than for plastics.

It has been shown that the extinguishment due to surface cooling requires approximately ten times less water than fire suppression in a gas phase. Therefore, coarse sprays are more effective on open surfaces, fully accessible to water droplets. These results are in good agreement with the available experimental data.

A semi-analytical approach to the solid phase extinguishment has also been discussed. The method reasonably accurately predicts critical water flow rate required to extinguish burning solid fuel. The predictions of the method are also in agreement with the numerical simulations.

The present study provide an insight into different fire suppression mechanisms and may be used to assess practical water requirements for plastic fire suppression.

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