Simplified Methodology to Predict Polyurethane Foam Mass Loss Rate in the Cone Calorimeter

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ABSTRACT

The work presented here is the first step of a larger study aiming at improving the description of fuel mass loss rate (MLR) in fire simulations, through multi-scale experimentation and model development. The final model, based on cone calorimeter scale measurements and on heat transfer modelling, is developed to predict full-scale fire spread over polyurethane foam slabs. In the present paper, small-scale tests performed in cone calorimeter are described, as well as a model predicting the material mass loss rate as a function of heat flux from the cone heater.

Several irradiance levels were tested (from 20 to 70 kW/m^2), and two simple mathematical functions were chosen to describe experimental curves of mass loss rate. Correlations between the functions parameters and cone calorimeter heat fluxes were computed, thus producing a model able to predict MLR as a function of time and irradiance level. The numerical results are in accordance with experimental data for intermediate heat fluxes (approximately 40 to 70 kW/m^2). For lower heat fluxes, the model fails (by construction) to reproduce the combustion decay. This is not considered to be a problem, as the range of heat fluxes for which the correlations are valid can be easily estimated from the results. In conclusion, the proposed methodology allows to predict MLR results in cone calorimeter conditions (e.g. only for 5 cm-thick samples) for various heat fluxes. After adding other sub-routines, it will be coupled to a heat transfer model in order to predict fire spread over polyurethane foam slabs.

KEYWORDS: Cone calorimeter, fire testing, modelling.

NOMENCLATURE

a	coefficient in the hyperbolic tangent function (s^{-1})
MLR	mass loss rate (kg/s)
t	time (s)

Greek

ϕ	incident heat flux (kW/m^2)
σ	standard deviation (s)

Subscripts

1/3	time when one third of the mass has been burned
end	time of flame out
first	for the first stage of MLR
ign	time of ignition
max	maximum value of MLR

INTRODUCTION

Numerical simulations are now a major tool for fire engineers and investigators. They can produce valuable results, provided appropriate data and models are used. Among these, fuel mass loss rate

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(MLR) is particularly important. This is usually done by prescribing a time dependent MLR (based on full-scale tests or engineering calculations), or by modelling pyrolysis (based on material properties and dedicated matter scale models). The first approach is often used for its simplicity, but is limited by the fact that experimental data may not be fully representative of the scenario being investigated. The second approach is more versatile (MLR is calculated based on the conditions in the simulation), but requires extensive input data, model calibration and computational resources. As long as pyrolysis models are not usable for engineering applications, an alternative seems necessary. The approach proposed here is to adapt fuel mass loss rate to the changes in heat flux during the simulation. This would be done using bench-scale MLR experimental data, thus avoiding the complexity of modelling chemical reactions in the condensed phase. This compromise would thus require a heat transfer model and a MLR model (to predict mass loss based on irradiance level, a so-called "thermal model" [1]). The work presented here focuses on the later, by describing a simplified approach to predict MLR at various heat fluxes at cone calorimeter scale.

The fuel chosen to illustrate this modelling approach is polyurethane (PU) foam, as it is widely used in upholstered furniture, and is involved in many residential fires. Its burning behaviour is thus crucial to understand and model, for fire safety engineering but also for fire investigation. Upholstered furniture and PU foams have long been studied [2–6]. Although numerous models are available [4, 7–10], none of them suited the purpose described earlier. New data were thus acquired through an extensive cone calorimeter experimental campaign, as described in the next section, and used to build a model to predict MLR as a function of time and irradiance level.

EXPERIMENTAL STUDY

Experimental setup

The polyurethane foam used here had a density of 30 kg/m^3 (water blown, 2/3 polyol and 1/3 toluene diisocyanate). Tests were performed in the cone calorimeter according to the ISO 5660 standard [11] (5 cm thick samples), except for the specimen holder. For the latter, three setups from the literature were tested:

1. Aluminium foil with steel frame [11, 12];
2. Aluminium only, on all sides [12];
3. Aluminium only, on the back and bottom centimetre of the sides [6].

The second one was chosen because it showed the highest repeatability, was more convenient to use (compared to the first configuration), and did not allow for side burning (as opposed to the third configuration). In addition to the aluminium foil, samples laid on a 1 cm thick gypsum substrate to protect the load cell.

Heat release rates and mass loss rates were measured, and all the experiments were videotaped. For the tests used here, irradiance levels ranged from 20 to 70 kW/m^2, and experiments were repeated at least three times.

Results

Only mass loss rate measurements will be presented here, as it was chosen to focus on the prediction of MLR (rather than heat release rate [HRR]). Indeed, the objective is to provide a fire spread model based on heat transfers: it seems a reasonable approximation to consider that mass loss mainly depends on heat transfers (and chemistry for material decomposition), whereas it is not for heat release, which can be more strongly affected by oxygen concentration for example. Moreover, mass loss is easier to measure than energy release, especially at larger scales. Similarly, the MLR is calculated with less parameters than the HRR [11]. Consequently, with measuring devices of equivalent precision, the uncertainties on HRR are higher than on MLR.

MLR were post-processed using a low frequency filter defined as

$$MLR_{filtered}(t) = 0.8MLR_{raw}(t-1) + 0.2MLR_{raw}(t) \quad (1)$$

The filter had to be efficient enough to soften the fluctuations of the signal without losing information such as the maximum value of MLR. This post-processing step is illustrated in Fig. 1.

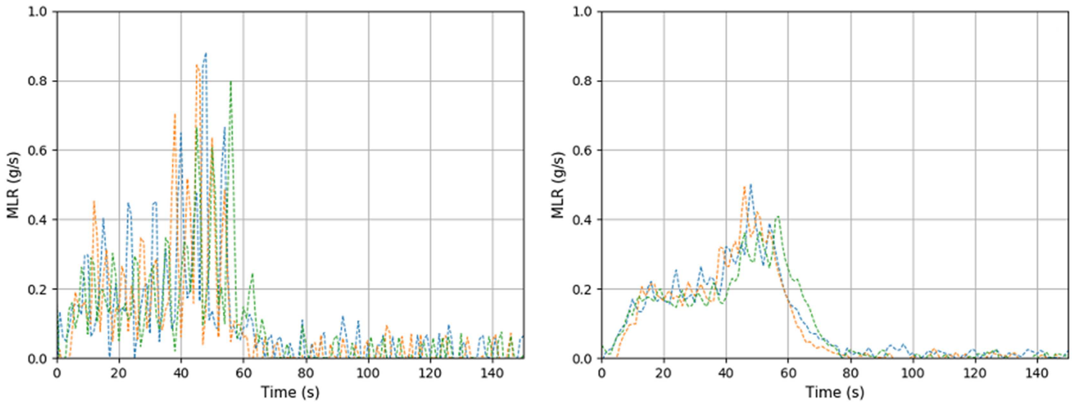

Fig. 1. Processing of mass loss rate data using a low frequency filter (irradiance level equal to 70kW/m^2, one dashed curve per repeated test). (a) Raw data; (b) Filtered results.

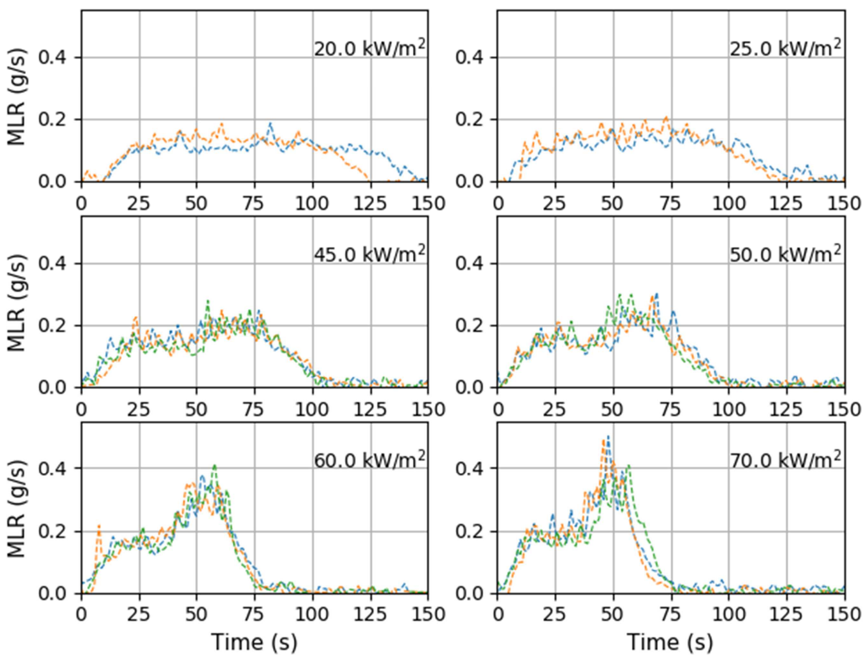

Fig. 2. Mass loss rate for polyurethane foam during cone calorimeter tests at irradiance levels ranging from 20 to 70 kW/m^2 (one dashed curve per repeat).

The results for irradiance levels from 20 to 70 kW/m^2 are shown in Fig. 2. Two stages of MLR can be distinguished for high values of irradiance level (greater than 45 kW/m^2). The first stage corresponds to a steady phase quickly reached after ignition, followed by a second stage where the

MLR grows toward a maximum value. These observations are in accordance with previous results [6] and a proposed decomposition scheme for polyurethane foam [13]. For lower irradiance levels, the MLR curves are quasi-stationary. Figure 2 also shows a good repeatability for the tests.

DATA ANALYSIS

Modelling functions

Figure 3 shows a schematic representation of MLR results observed for irradiance levels higher than 45 kW/m^2. As mentioned before, PU burning in cone calorimeter can be divided in two stages (see solid red and hatched blue fills): a quasi-steady phase (see MLR_{first}) followed by a rapid increase to a maximum MLR ($MLR_{\max}$). The first stage accounts for approximately one third of the mass loss, so its end time is referred to as $t_{1/3}$.

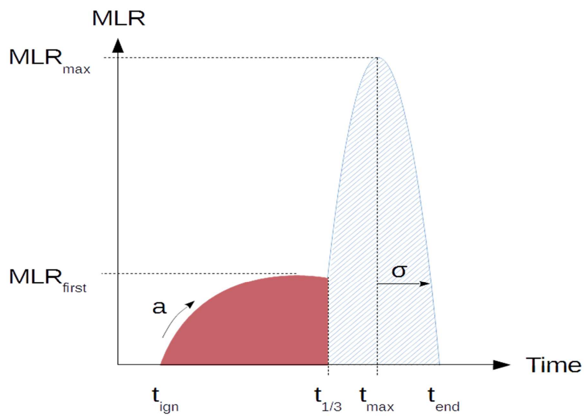

Fig. 3. Schematic view of the mass loss rate results observed for irradiance levels higher than 45 kW/m^2. The parts referred to as first and second stages are represented in red (solid) and blue (hashed) respectively.

In order to describe these two stages, simple mathematical functions were chosen. The first part (see solid red part in Fig. 3) could be approximated by an exponential or a hyperbolic tangent function. Both options were evaluated and the later showed a better agreement with the experimental data. This part of the mass loss rate was thus modelled using

$$MLR(t) = MLR_{first} \tanh(a\,t), \tag{2}$$

where MLR_{first} is the asymptote of the hyperbolic tangent function (i.e. the MLR for the steady phase) and a (s^{-1}) describes the growth of the curve to its asymptote (the higher the value of a, the faster the growth toward MLR_{first}).

The second part of experimental MLR curves (see hatched blue part in Fig. 3) fits well with a Gaussian function given by

$$MLR(t) = MLR_{\max} \exp\left(-\frac{(t-t_{\max})^2}{2\sigma^2}\right), \tag{3}$$

where $MLR_{\max}$ is the maximum MLR value, $t_{\max}$ is the time when it is reached (mean of the Gaussian function), and σ the standard deviation (the width of the curve). The higher the irradiance level, the smaller $t_{\max}$ and σ.

CORRELATIONS WITH HEAT FLUX

In order to build a model predicting MLR based on incident heat flux from the cone heater, correlations between irradiance level and the parameters listed in the previous section (see also Fig. 3) were investigated. The authors note that here irradiance level refers to the radiative heat flux delivered by the cone calorimeter according to the ISO standard [11]: other important factors (e.g. heat flux from the flame) should be accounted for in the future to give more accurate results.

For each parameter, values were extracted from average test results for three irradiance levels (25, 45 and 60 kW/m^2), and correlated to the heat flux. The other test results (i.e. 20, 50 and 70 kW/m^2) will be used to assess the predictive capability of the model.

Times of ignition and flameout, t_{ign} and t_{end} respectively, are based on the observations of the test operator (i.e. when the specimen ignited and when it extinguished). They were correlated to the incident heat flux as shown in Table 1 (where all equations are summarized).

Table 1. Examples of empirical correlations (based on 25, 45 and 60 kW/m^2 test results)

Parameter (unit)	Parameter values based on	Correlation (heat flux ϕ in kW/m^2)	
t_{ign} (s)	User input during the test (from first to last visible flames)	$1/t_{ign} = 0.0159\phi - 0.252$	(4)
t_{end} (s)		$t_{end} = -1.89\phi + 188$	(5)
$t_{1/3}$ (s)	Minimization of Eq. (12)	$t_{1/3} = -0.362\phi + 63.0$	(6)
MLR_{first} (g/s)	Fit of MLR using Eq. (2) (for $t_{ign} < t < t_{1/3}$)	$MLR_{first} = 0.000814\phi + 0.114$	(7)
a (s^{-1})		$a = 2.81\phi + 49.4$	(8)
$MLR_{\max}$ (g/s)	Fit of MLR using Eq. (3) (for $t_{1/3} < t < t_{end}$)	$MLR_{\max} = 0.0812\exp(0.0228\phi)$	(9)
$t_{\max}$ (s)		$t_{\max} = -0.586\phi + 90.1$	(10)
σ (s)		$\sigma = -0.425\phi + 38.3$	(11)

The time to burn one third of the mass, $t_{1/3}$, corresponds to time t_i which minimizes the following function:

$$\left|\frac{1}{3}\int_0^{t_{end}} MLR(t)dt - \int_0^{t_i} MLR(t)dt\right|. \tag{12}$$

This procedure is illustrated with data from 60 kW/m^2 tests in Fig. 4 (top graph).

MLR for the first stage (MLR_{first}) was computed by fitting the chosen function (see Eq. (2)) on experimental data from t_{ign} to $t_{1/3}$, as illustrated in Fig. 4 (bottom left). This also provided parameter a. Equation (7) (MLR_{first} as a function of the irradiance level) is shown in Fig. 5 (left).

The second stage was also fitted using the function described earlier (see Eq. (3)), to provide values for $MLR_{\max}$, $t_{\max}$ and σ. This is illustrated in Fig. 4 (bottom right graph), and the correlation in

Eq. (9) is shown in Fig. 5 (right plot). Note that the standard deviation σ will be used to adjust the function in the next section (and can thus be modified).

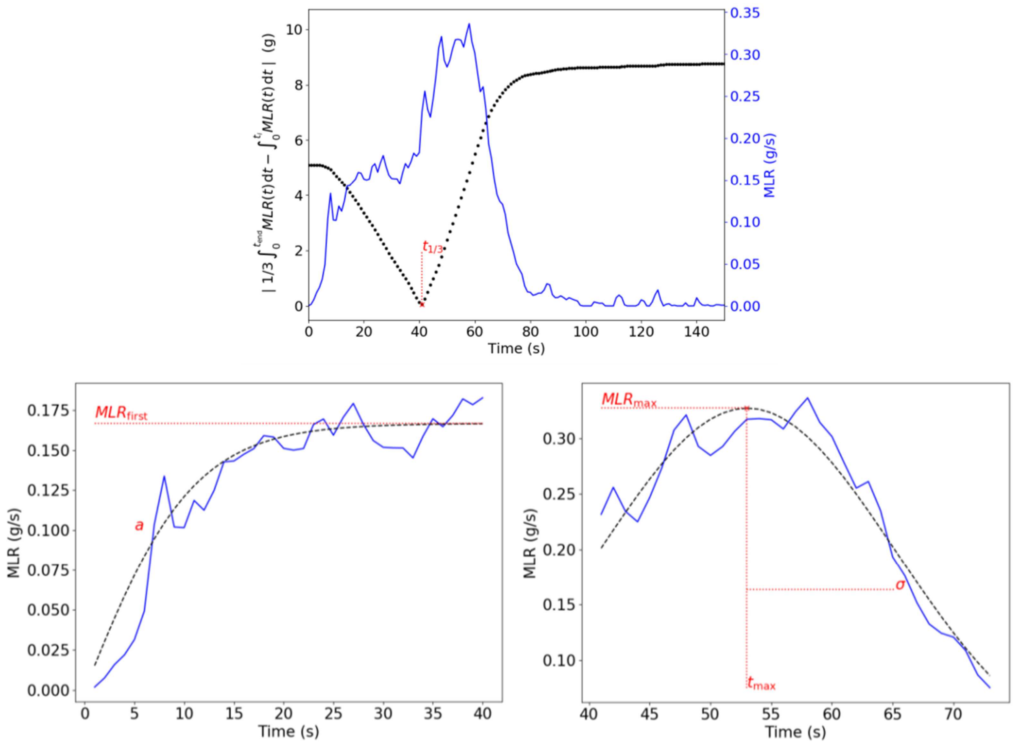

Fig. 4. Examples of how parameters were determined from average data for the 60 kW/m^2 tests. Top: $t_{1/3}$; bottom left: MLR_{first} and a ; bottom right: MLR_{max} , t_{max} and σ .

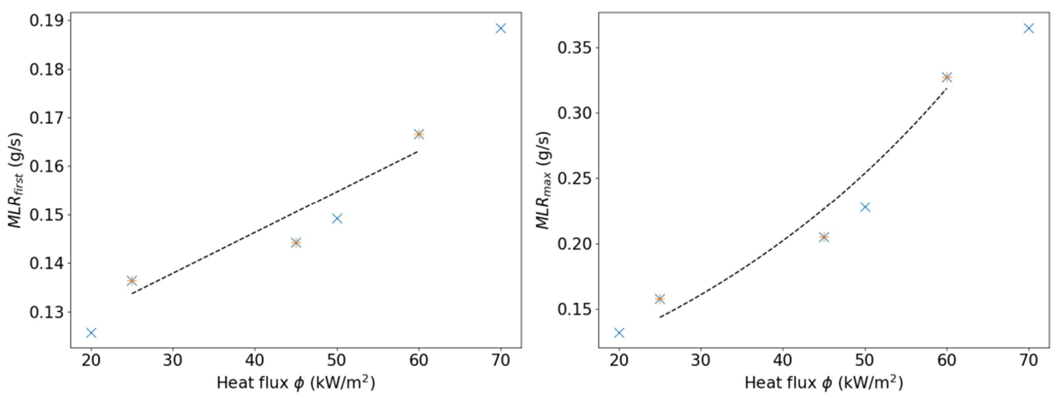

Fig. 5. Values of mass loss rate for the first stage (MLR_{first}) and maximum MLR (MLR_{max}).

Dashed line for correlations (see Eq. (7) and (9), respectively), symbols for experimental data (points with a + sign were used to compute the correlations).

MASS LOSS RATE PREDICTION

The previous section showed that key quantities describing the foam burning behaviour correlate well with the incident heat flux (see Table 1). Two modelling functions were also chosen to describe the stages of the foam combustion (see Eq. (2) and (3)). To summarize, the model follows

$$MLR(t,\phi) = \begin{cases} MLR_{first}(\phi)\tanh\left(a(\phi)\, t\right), & t < t_{1/3} \\ MLR_{\max}(\phi)\exp\left(-\dfrac{(t-t_{\max})^2}{2\sigma^2}\right), & t \geq t_{1/3} \end{cases} . \quad (13)$$

The junction at $t_{1/3}$ is made by satisfying

$$MLR_{first}(\phi)\tanh\left(a(\phi)t\right) < MLR_{\max}(\phi)\exp\left(-\frac{(t-t_{\max})^2}{2\sigma^2}\right). \quad (14)$$

If needed, σ is increased until this condition is verified. The resulting standard deviation is shown in Fig. 6, along with the original correlation (see Eq. (11) in Table 1).

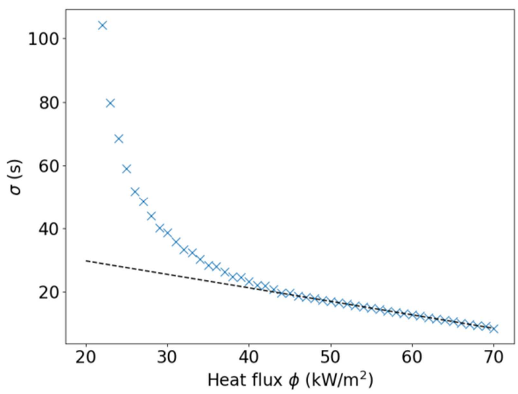

Fig. 6. Standard deviation for the Gaussian function, see Eq. (3). Dashed line: initial correlation, Eq. (11); symbols: corrected values to satisfy Eq. (12).

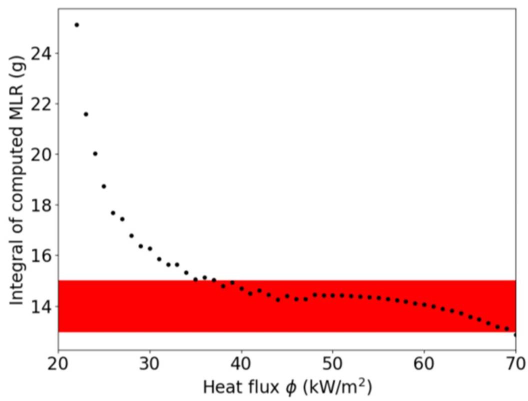

Fig. 7. Burned masses according to the model (black dots). The red rectangle shows the mass of the tested samples (14±1 g).

As can be seen, the correction to satisfy Eq. (12) yields very large σ values for low heat fluxes, which in turn produce unrealistic results. This was expected because the two-stage behaviour (on which the model presented here is based) was not observed at 20 or 25 kW/m^2. However, it is believed that a simple threshold would allow determining the lowest irradiance level beyond which the model is not valid anymore (e.g. here around 40 kW/m^2). This limit is in agreement with the predicted burned mass, shown in Fig. 7, as it is consistent with the sample mass (see red rectangle, 14±1 g) for heat fluxes higher than 40 kW/m^2.

Comparisons with experiments at 20, 50 and 70 kW/m^2 (i.e. that were not used to compute the correlations) are shown in Fig. 8. As expected, prediction at 20 kW/m^2 is poor (combustion decay is not captured). Results at higher heat fluxes (50 and 70 kW/m^2 in Fig. 8, but also 45 and 60 kW/m^2) are far more consistent with cone calorimeter data. This confirms that this simple approach can produce valid MLR predictions at intermediate irradiance levels (i.e. approximately 40 to 70 kW/m^2).

CONCLUSIONS

Numerous tests were performed in cone calorimeter, at irradiance levels ranging from 20 to 70 kW/m^2. The results, and more specifically mass loss rates, were used to determine modelling functions that could describe MLR evolution in time. Two stages were identified for irradiance level greater than 45 kW/m^2 (in accordance with the literature [6,13]). A hyperbolic tangent function (Eq. (2)) and a Gaussian function (Eq. (3)) were chosen to model the first and second part respectively. The parameters for each function were then correlated to the heat flux (see Table 1), using part of the experimental data (25, 45 and 60 kW/m^2). The resulting equations (Eq. (13)) were used to predict MLR from 20 to 70 kW/m^2. As expected, the agreement is poor for low heat fluxes (approximately below 40 kW/m^2) because foam did not display the two-stage behaviour (see data for 20 and 25 kW/m^2 in Fig. 2). For higher irradiance levels, predicted MLR are close to experimental values, even for tests not used when establishing the correlations (i.e. 50 and 70 kW/m^2, see Fig. 8).

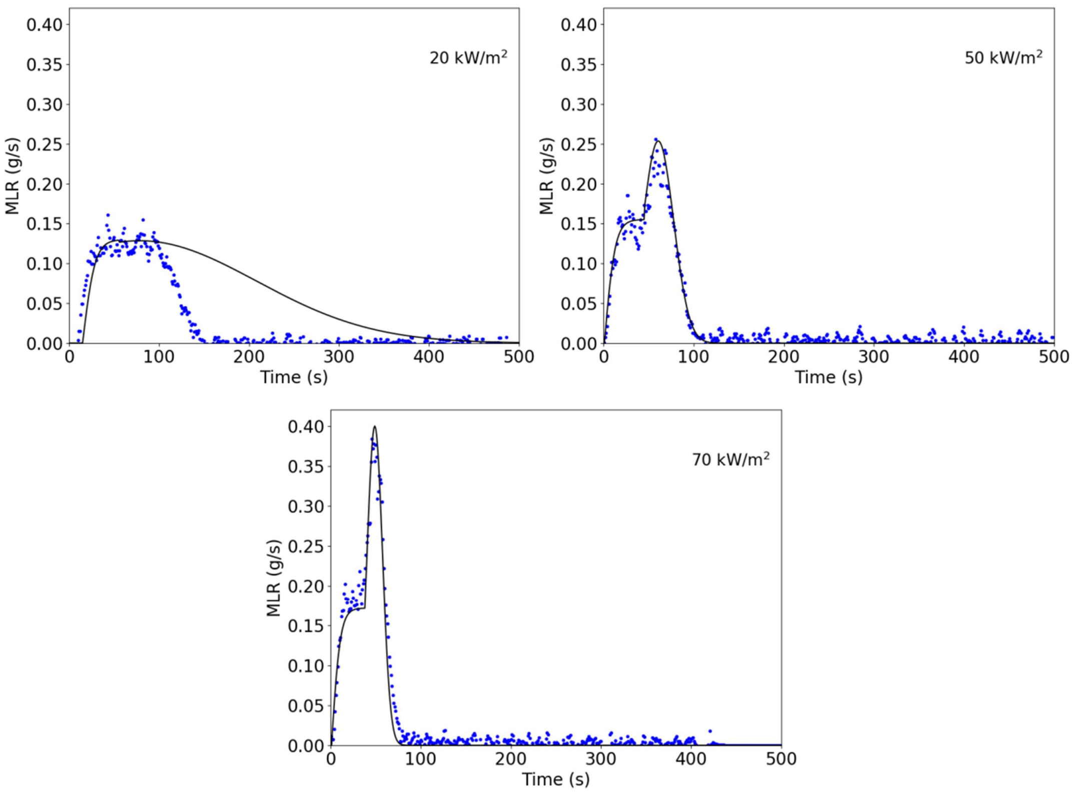

Fig. 8. MLR predictions (solid black lines) compared to experimental data (blue points). Top left: 20 kW/m^2; top right: 50 kW/m^2; bottom: 70 kW/m^2.

The methodology presented here should allow predicting the MLR at cone calorimeter scale for various heat fluxes, based only on a few measurements. The parameters in Table 1 still have to be correlated to the net heat flux experienced by the sample, and not only the incident heat flux from the cone heater (e.g. by accounting for heat flux from the flame [4, 14] or for sample regression during the tests [15]). Application to full-scale foam combustion will require additional models, for thickness scaling for example [4].

When finalized, the proposed modelling approach is meant to be coupled to a heat transfer model predicting the incident heat flux at the fuel surface (based, for example, on flame size/geometry, fuel type, etc.), in order to predict MLR, and consequently flame spread. The same methodology could also be applied to other fuels, by choosing appropriate functions depending on the observed fire behaviour.

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REFERENCES

[1] F.V. Lundström, P. van Hees, É. Guillaume, A review on prediction models for full-scale fire behaviour of building products, Fire Mater. 41 (2017) 225–44.

[2] L. Bustamante Valencia, Experimental and numerical investigation of the thermal decomposition of materials at three scales: application to polyether polyurethane foam used in upholstered furniture phdthesis, PhD thesis, École nationale supérieure de mécanique et d'aérotechnique, Poitiers, France, 2009.

[3] M. Ravey, E.M. Pearce, Flexible polyurethane foam. I. Thermal decomposition of a polyether-based, water-blown commercial type of flexible polyurethane foam, J. Appl. Polym. Sci. 63 (1997) 47–74.

[4] B. Sundström, CBUF, Fire Safety of Upholstered Furniture - the final report of the CBUF research programme, 1995.

[5] J.U. Ezinwa, L.D. Robson, M.R. Obach, D.A. Torvi, E.J. Weckman, Evaluating Models for Predicting Full-Scale Fire Behaviour of Polyurethane Foam Using Cone Calorimeter Data, Fire Technol. 50 (2014) 693–719.

[6] L.D. Robson, Scalability of Cone Calorimeter Test Results for the Prediction of Full Scale Fire Behavior of Polyurethane Foam, University of Saskatchewan, Saskatoon, Canada, 2014.

[7] U. Wickström, U. Göransson, Full-scale/Bench-Scale correlations of wall and ceiling linings, Fire Mater. 16 (1992) 15–22.

[8] B. Messerschmidt, P. van Hees, U. Wickström, Prediction of SBI (Single Burning Item) test results by means of cone calorimeter test results, Interflam'99 (Edinburgh, UK: Interscience Communications Ltd), pp 11–22, 1999.

[9] T. Hakkarainen, M. A. Kokkala, Application of a one-dimensional thermal flame spread model on predicting the rate of heat release in the SBI test, Fire Mater. 25 (2001) 61–70.

[10] A.S. Hansen, Prediction of heat release in the single burning item test, Fire Mater. 26 (2002) 87–97

[11] ISO 5660-1 2002 Reaction-to-fire tests – Heat release, smoke production and mass loss rate - Part 1: Heat release rate (cone calorimeter method).

[12] V. Babrauskas, W.H. Twilley, W.J. Parker, The effects of specimen edge conditions on heat release rate, Fire Mater. 17 (1993) 51–63.

[13] W.M. Pitts, Role of two stage pyrolysis in fire growth on flexible polyurethane foam slabs, Fire Mater. 38 (2014) 323–38.

[14] F. Hermouet, Développement d'une approche innovante de modélisation de la cinétique de décomposition thermique des matériaux solides en espaces confinés sous-ventilés. Application aux incendies en tunnel, École nationale supérieure de mécanique et d'aérotechnique, Chasseneuil-du-Poitou, France, 2015.

[15] W. M. Pitts, Applied Heat Flux Distribution and Time Response Effects on Cone Calorimeter Characterization of a Commercial Flexible Polyurethane Foam, Fire Technol. 50 (2014) 635–72.