Flame Heights of Di-tert-butyl Peroxide Pool Fires – Experimental Study and Modeling

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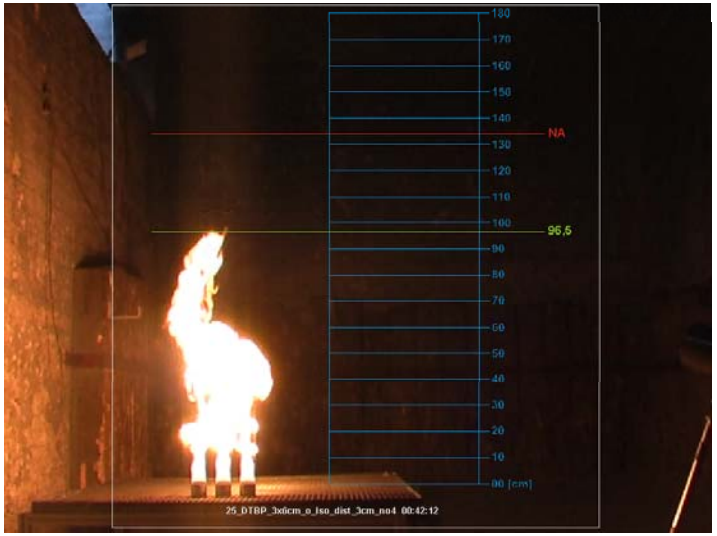
Flame heights

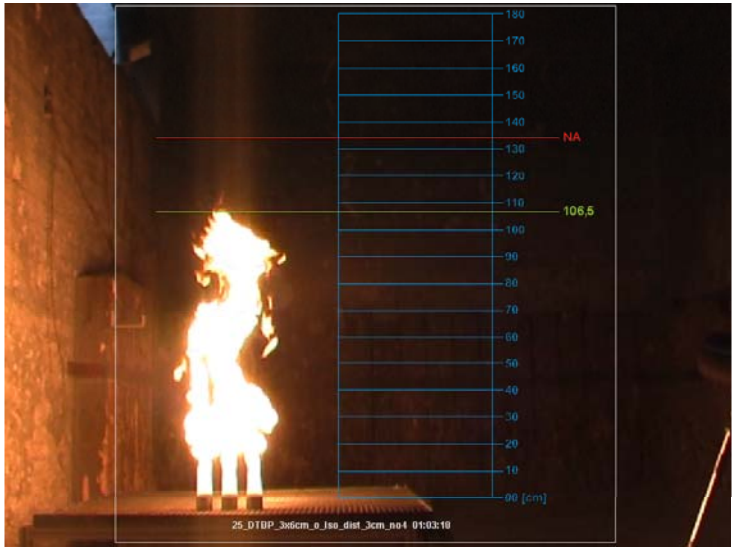
Digital images (25 frames per second) are obtained from the VHS videos.

The length of one pixel is determined.

The RGB colour (R 255, G 242, B 199) is used as a criterium for the instantaneouse flame height.

A MATLAB-code is used to search line-by-line for the first pixel of the above mentioned colour.





Flame heights

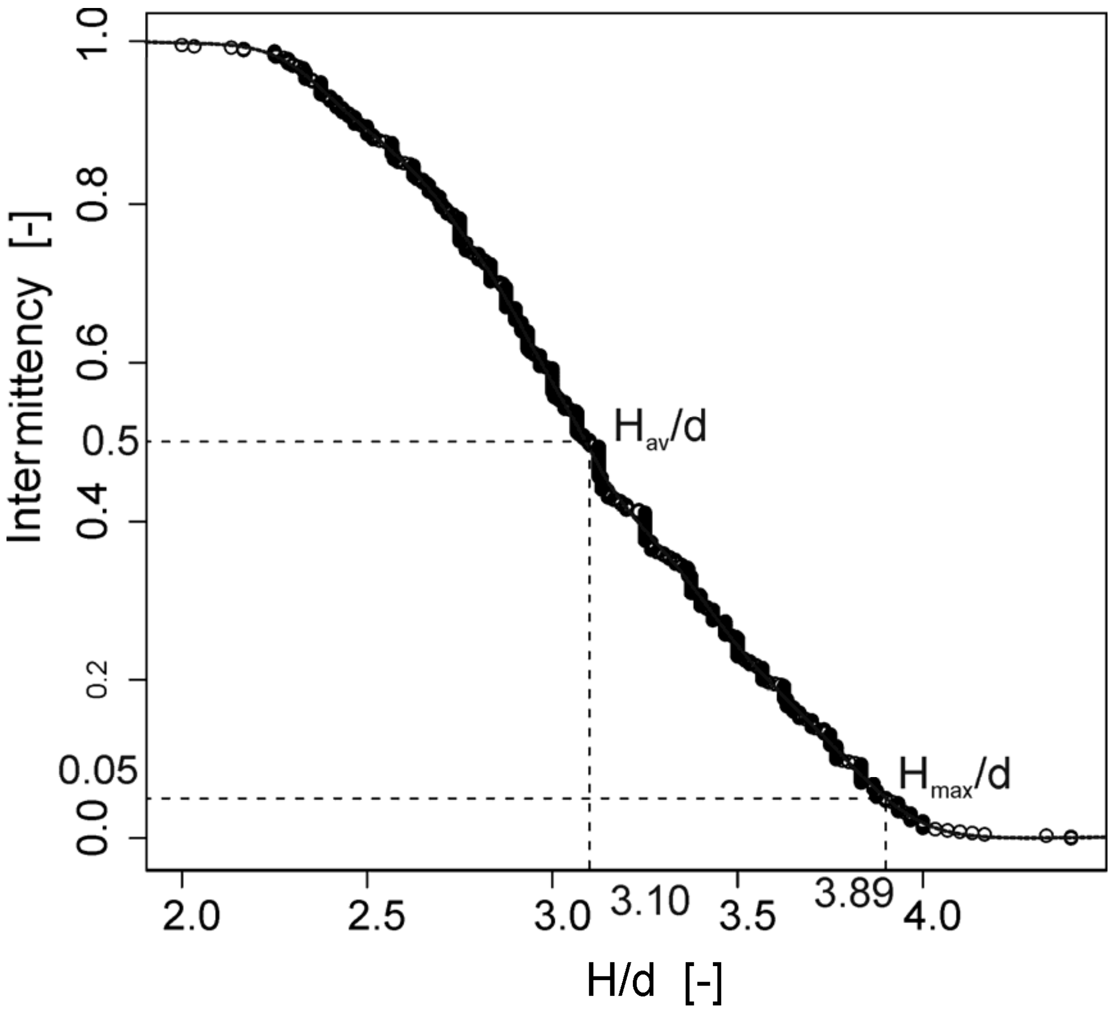
The intermittency criterium is used to obtain avaraged and maximum flame heights.

The intermittency describes the instantenouse flame heights as distributions.

I(H/d) = 0.5 criterium for the averaged flame height.

I(H/d) = 0.05 criterium for the maximum flame height.

No comparison of instantaneouse heights, but a comparison of the position of a distribution.



Intermittency of a DTBP pool fire d = 3.4 m

Flame heights

$$\overline{H}/d = a\,Fr_f^{\,b}\,\overline{u}_w^{*c} \qquad H_{max}/d = a\,Fr_f^{\,b}\,\overline{u}_w^{*c}$$

$$Fr_f \equiv \frac{\dot{m}_f''}{\rho_a\sqrt{gd}}$$

Fuel Froude number

$$\overline{u}_w^{*} = \frac{\overline{u}_w}{\overline{u}_c}$$

dimensionales wind speed

ρ_a [kg/m³] air density

g [m/s²] gravitational acceleration

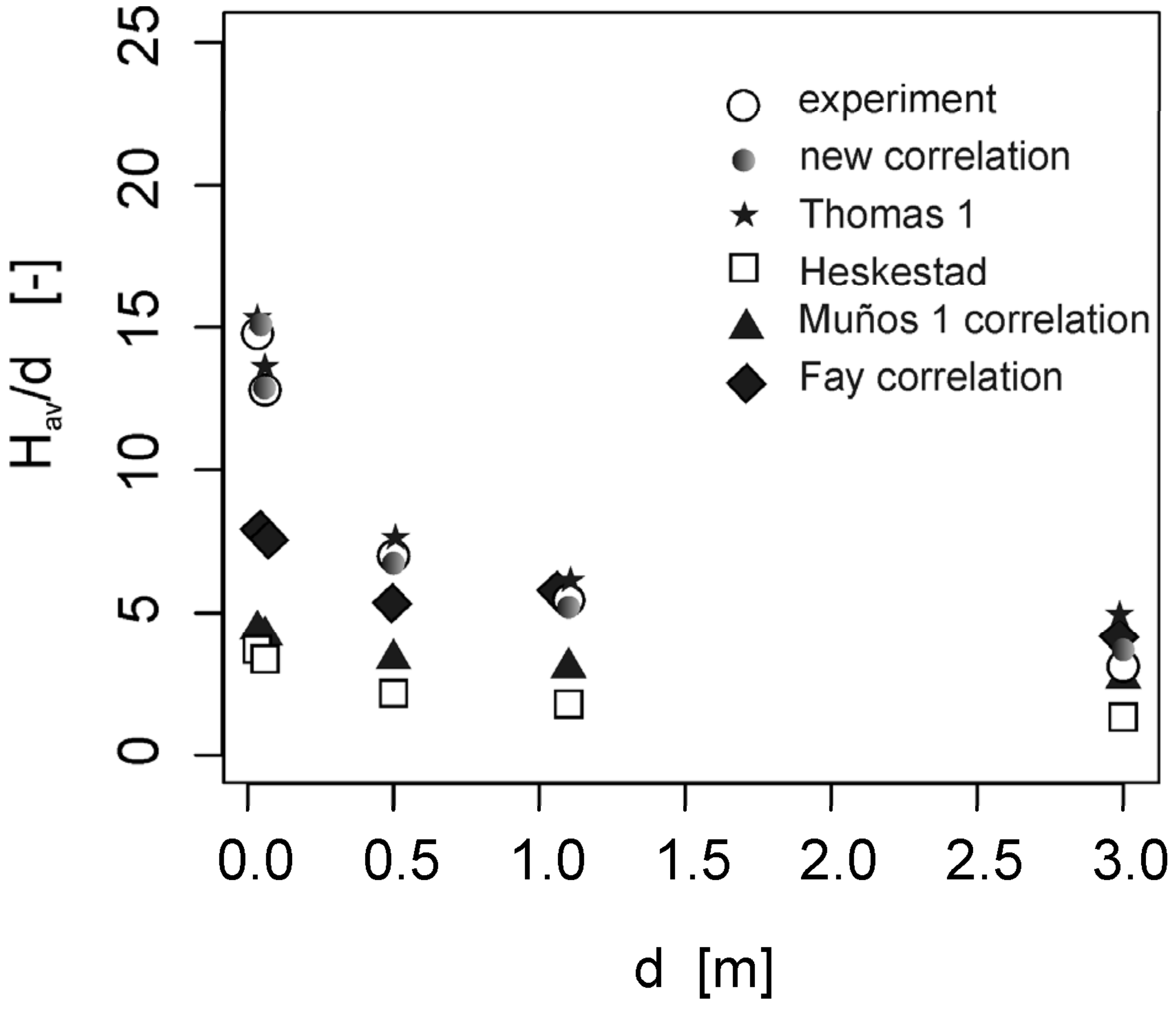
d [m] pool diameter

u_w [m/s] wind speed

u_c [m/s] characteristic wind speed

correlation	a	b	c	
Thomas	55	0.07	-0.21	as measured by wood crib fires; $(H/d)_{max}$
Moorhouse	6.2	0.254	-0.044	as measured by cylindrical LNG fires; $(H/d)_{max}$
Muños	7.74	0.375	-0.096	as measured by gasoline and diesel fires; $\overline{H}/d$

Flame heights

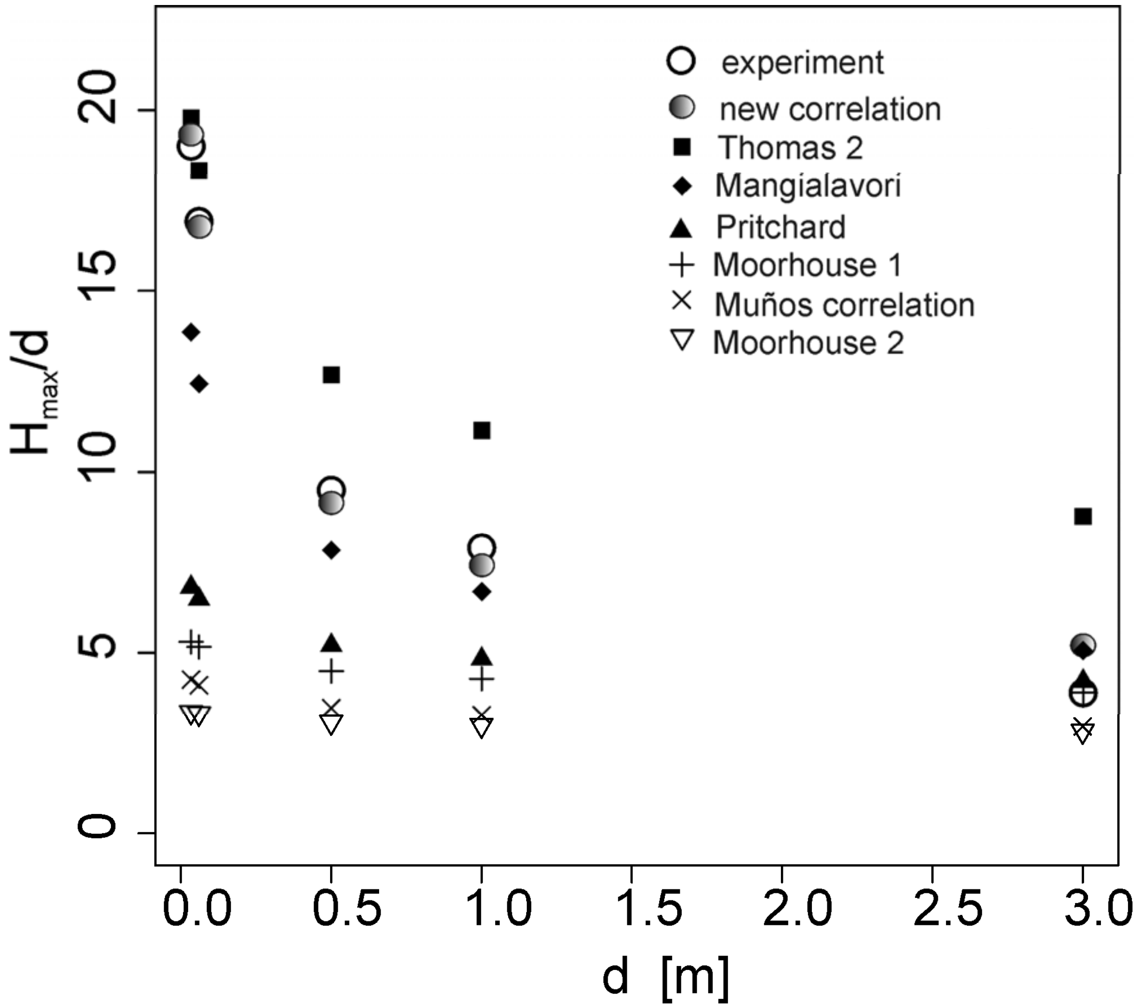


Neglecting factor c caused by windless conditions

Correlation for the averaged flame heights $\overline{H}$ against the fuel froude numbers Fr_f for DTBP pool fires:

$$\boxed{\overline{H} / d = 46.05\, Fr_f^{0.80}}$$

Flame heights



Correlation for the averaged flame heights H_{max} against the fuel froude numbers Fr_f for DTBP pool fires:

$$\boxed{H_{max} / d = 56.96\, Fr_f^{0.76}}$$

Mass burning rates according to Hottel (1959):

$$\dot{m}_f'' = \frac{\dot{Q}_{ba,tot}}{A_P(\Delta h_v + c_{p,v} T_{f,bp} - c_{p,f} T_{f,a})}$$

n-pentane, d = 25 m

$$\dot{m}_f'' \approx 0.06\,kg/(m^2 s)$$

$\dot{m}_f''$	[kg/(m² s)]	mass burning rate
$\dot{Q}_{ba,tot}$	[kW]	radiative heat rate to the fuel surface
A_P	[m²]	pool surface area
Δh_v	[kJ/kg]	enthalpy of vaporization
$c_{p,v}$	[kJ/(kg K)]	heat capacity of fuel vapor
$c_{p,f}$	[kJ/(kg K)]	heat capcity of the liquid fuel
$T_{f,bp}$	[K]	boiling temperature
$T_{f,a}$	[K]	ambient temperature

Model for the mass burning rate of HC pool fires according to Burgess und Hertzberg (1962):

$$\boxed{\dot{m}''_f = \beta \frac{-\Delta h_c}{\Delta h_v} \approx 10^{-3}\,\mathrm{kg/(m^2\,s)}\frac{-\Delta h_c}{\Delta h_v}}$$

$-\Delta h_c$ [kJ/kg] enthalpy of combustion

$$\boxed{\beta = f_{rad}\frac{\varepsilon_{F,f}}{\varepsilon_F}\varphi_{F,f}\,S_u\,c_f = 5.8\cdot 10^{-4}\,\mathrm{kg/(m^2\,s)}}$$

$f_{rad} = 0.5$: Fraction of heat radiated

$\varphi_{F,f} = 0.4$: View factor between flame and pool

$\frac{\varepsilon_{F,f}}{\varepsilon_F} = 0.5$: Emissivity ratio

$S_u = 0.06\,\mathrm{m/s}$: Limit burning velocity for natural convection

$c_f = \rho_v \cdot \mathrm{UEL} = 3.1\,\mathrm{kg/m^3}\cdot 0.031 = 0.096\,\mathrm{kg/m^3}$: Maximum fuel concentration for flame propagation

Di-tert-butyl peroxide, (DTBP), d = 3.4 m

$\dot{m}_f'' \approx 0.30\,\mathrm{kg/(m^2\,s)}$

Tert-butyl peroxybenzoate (TBPB), d = 3.4 m

$\dot{m}_f'' \approx 0.37\,\mathrm{kg/(m^2\,s)}$

Tert-butyl peroxy-2-ethyl hexanoate (TBPEH), d = 3.4 m

$\dot{m}_f'' \approx 0.53\,\mathrm{kg/(m^2\,s)}$

Microcalorimetric measurements for DTBP and TBPB show a 1st order kinetic:

$$T_{onset} \approx 365\,K \quad ,$$

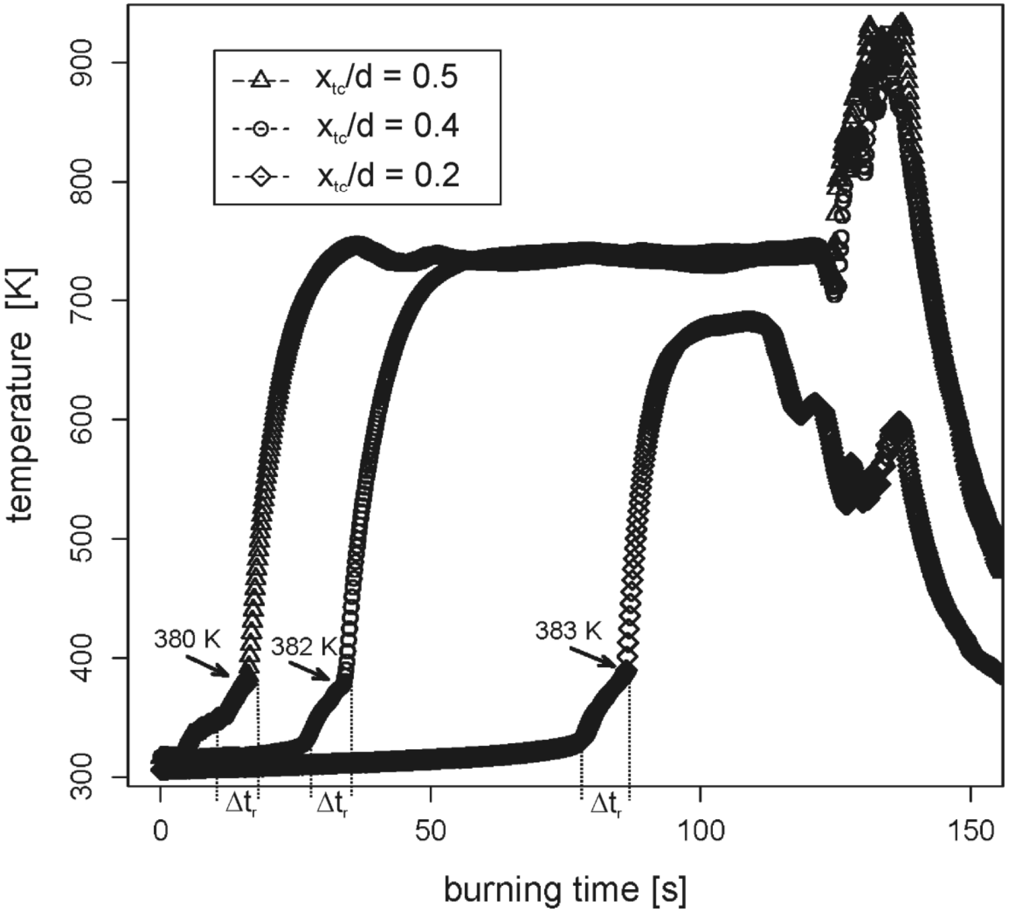
$$T_{SADT} \approx 358\,K \quad , \quad T_{SADT} \approx 338\,K$$

DTBP
(aliphatic)

TBPB
(aromatic)

Reason: Aromatic compounds show a lower heat capacity and can be heated up easier.

Liquid phase decomposition during the burning (residence time $\tau \approx 5 - 10$ s) has to be taken into account.



Thermocouple measurements at different heights of the liquid (left side of the arrows) und gas phase (right side of the arrows) of a DTBP pool fire (d = 0.06 m)

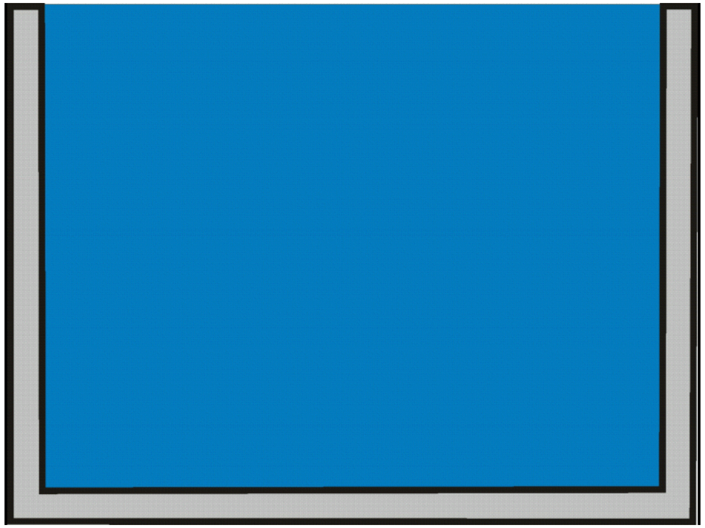
An additional heat rate due to liquid phase decomposition $\dot{Q}_d$ has to be taken into the energy balance:

$$\dot{m}_f'' = \frac{\dot{Q}_d + \dot{Q}_{ba,tot}}{A_P(\Delta h_v + c_{p,v} T_{f,bp} - c_{p,f} T_{f,a})}$$

$$\dot{Q}_d = U \, \dot{m}_f'' \, A_P \, (-\Delta h_d)$$

$-\Delta h_d$	[kJ/kg]	heat of decomposition
U	[–]	conversion

$\dot{Q}_d$ can be modeled as an ideal, isotherme, continuously stired tank reactor (CSTR):



$$Da = \tau \; k(T)$$

Da	[–]	first order Damköhler number
τ	[s]	residence time
k	[s^{-1}]	reaction rate constant

$k \approx 5 \cdot 10^{-3}$ s^{-1}

$$\boxed{U = \frac{Da}{1+Da} \approx 0.02 - 0.04}$$

Heat rates in peroxide pool fires

d = 3.4 m		DTBP	TBPB
$\dot{Q}_d$	[kW]	150	364
$\dot{Q}_{ba,rad}$	[kW]	379	366
$\dot{Q}_d / \dot{Q}_{ba,rad}$	[–]	0.4	0.99
$\dot{Q}_d / A_P$	[kW/m²]	21	51
$\dot{Q}_{ba,rad,P} / \dot{Q}_{ba,rad,HC}$	[–]	2	1.9

The observed higher mass burning rates of peroxide pool fires can be explained by the additional heat rate due to liquid phase decomposition $\dot{Q}_d$.

Model for the mass burning rates of peroxide pool fires based on the energy balance according to Burgess und Hertzberg:

$$\boxed{\dot{m}''_{f,th} = \frac{\beta(-\Delta h_c) + \left(1 + \frac{\beta}{S_u\, c_f}\right)\dot{Q}_d / A_P}{\Delta h_v + c_{p,v} T_{f,bp} - c_{p,f} T_{f,a}}}$$

$\dot{m}''_{f,exp} = 0.30\,\mathrm{kg}/(\mathrm{m}^2\mathrm{s})$	$\dot{m}''_{f,th} = 0.32\,\mathrm{kg}/(\mathrm{m}^2\mathrm{s})$	DTBP
$\dot{m}''_{f,exp} = 0.37\,\mathrm{kg}/(\mathrm{m}^2\mathrm{s})$	$\dot{m}''_{f,th} = 0.39\,\mathrm{kg}/(\mathrm{m}^2\mathrm{s})$	TBPB

Simplified model:

$$\boxed{\dot{m}''_{f,th} = \frac{1.1\alpha + \beta(-\Delta h_c)}{\gamma}}$$

As a first approximation for α a linear regression against the tabulated T_{onset} according to Wehrstedt und Malow (2005) can be used:

$$\alpha = \dot{Q}_d / A_P = -1.27\, T_{onset} + 501.07\, K$$

Calculating β using the particular decomposition products shows an average value for organic peroxides of:

$$\beta = 1.5 \cdot 10^{-3}\, kg/(m^2 s)$$

$$\gamma = \Delta h_v + c_{p,v} T_{f,bp} - c_{p,f} T_{f,a} = 220\, kJ/kg$$ aromatic compound

$$\gamma = \Delta h_v + c_{p,v} T_{f,bp} - c_{p,f} T_{f,a} = 250\, kJ/kg$$ aliphatic compound

Example for calculating the mass burning rate of TBPEH:

$$T_{onset} = 334\,K \quad , \quad -\Delta h_c = 34455\ kJ/kg$$

$$\alpha = \dot{Q}_d / A_P = -1.27 \cdot 334\,K + 501.07 = 77\,kW/m^2$$

$$\beta = 1.5 \cdot 10^{-3}\,kg/(m^2 s)$$

$$\gamma = \Delta h_v + c_{p,v} T_{f,bp} - c_{p,f} T_{f,a} = 250\,kJ/kg$$

$$\dot{m}''_{f,th} = \frac{1.1 \cdot 77\,kW/m^2 + 1.5 \cdot 10^{-3}\,kg/(m^2 s) \cdot 34455\,kJ/kg}{250\,kJ/kg} = 0.55\,kg/(m^2 s)$$

$$\dot{m}''_{f,exp} = 0.53\,kg/(m^2 s)$$

Conclusions

The averaged and maximum flame heights of DTBP pool fires can be described by a correlation based on the fuel Froude number.

A new model for the mass burning rates of peroxide pool fires including a liquid phase decomposition reaction has been developed.

Thank you very much for your attention.