Three dimensional CFD simulation of LPG tank exposed to partially engulfing pool fires

Supplementary Material

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Figure S1: Comparison between experimental and CFD lading temperatures along array II (See Figure 2 in the main text) at different instants of time for cases C and D.



Figure S2: Comparison between experimental and CFD lading temperatures along array IV (See Figure 2 in the main text) at different instants of time for cases C and D.



Figure S3: Comparison between experimental and CFD lading temperatures along array V (See Figure 2 in the main text) at different instants of time for cases C and D.



Figure S4: Comparison between experimental and CFD lading temperatures along array I (See Figure 2 in the main text).



Figure S5: Comparison between experimental and CFD lading temperatures along array II (See Figure 2 in the main text).



Figure S6: Comparison between experimental and CFD lading temperatures along array IV (See Figure 2 in the main text).



Figure S7: Comparison between experimental and CFD lading temperatures along array V (See Figure 2 in the main text).



Figure S8: Maximum $(\Delta T_{i,max})$ and average $(\overline{\Delta T}_i)$ difference between the calculated and measured temperature for the *i*-*th* thermocouple calculated for each array considering simulation case C.

With respect to Figure S8 is should be remarked that array I also has a thermocouple in the vapour space, which is not present in arrays II, IV and V.

Estimation of the correction due to radiation error with regard to thermocouple 0

From an energy balance around the thermocouple bead, under a series of simplifying assumption discussed (discussed in Brady et al., 2015), the vapor temperature ($T_{v,T0}$) can be calculated from the thermocouple reading (T_{T0}) according to Eq. S1:

$$T_{\nu,T0} = T_{T0} + \frac{\sigma \, d_{T0} \, \varepsilon_{T0}}{Nu \, k_{\nu}} \left(T_{T0}^{4} - F_{w \to T0} \, T_{w}^{4} \right)$$
(Eq. S1)
$$Nu = (0.24 + 0.56 Re^{0.45})$$
(Eq. S2)

where σ is the Stefan-Boltzmann constant, d_{T0} and ε_{T0} are the diameter and the emissivity of the thermocouple respectively, k_v is the thermal conductivity of the vapor surrounding the thermocouple, $F_{w \to T0}$ is the view factor between the thermocouple and the vapor wetted wall, T_w is the average wall temperature and Nu is Nusselt number, calculated using Eq. S2 (Brady et al., 2015). Based on Eq. S1 and considering the assumptions reported in Table S1, the red dotted line in **Errore. L'origine riferimento non è stata trovata.** a was obtained. As emphasized by Brady and co workers (2015), the estimation of the radiation correction is very sensitive to both the emissivity of the thermocouple bead (which may vary considerably according to the condition of the thermocouple bead surface) and the Nusselt number (which depends on the correlation used for its estimation). The same is true for the value of view factor ($F_{w \to T0}$), which is affected by a strong uncertainty.

Parameter / variable	Value / Estimation method
T_{T0}	From thermocouple T0 reading
T _w	Average temperature (varying with time) from vapor wetted wall thermocouples (i.e. from thermocouples W0, W1, W2, W3, W4, W5, W6 and W12)
d_{T0}	3 mm (as sated in the experimental report)
ε_{T0}	0.18 – Typical value for k-type thermocouples (Brady et al., 2015)
k_v	\approx 0.24 (average thermal conductivity of pure propane in the range 20 ÷ 120 °C)
Re	\approx 126 – calculated from CFD simulation results of case C (at 300 s), at the point corresponding to the position of thermocouple 0, considering the thermocouple diameter as characteristic length
Nu	\approx 5 (from Eq. S2)
$F_{w \to T0}$	= 0.5 - it was assumed that half of the surface of thermocouple bead sees the vapor wetted wall and the other half sees the liquid surface, exchanging with it a negligible amount of thermal radiation

Table S1: values of variable and parameters considered for the calculation $T_{v,T0}$

Details on the simulation carried out with RADMOD

The RADMOD model is based on the partition of the tank into different zones (or nodes), each one described by a simple set of parameters. Such parameters represent physical quantities (e.g. temperature, pressure, thermal conductivity, etc.) averaged over each node. For each node, conservation equations for energy and mass are solved. In this way, the transient evolution of temperature and pressure in the tank calculated. Further details on the model setup can be found in the literature (Cozzani et al., 2006; Gubinelli, 2005).

The original version of the RADMOD was developed to simulate full engulfment conditions. In the present work, the RADMOD code was slightly modified in order to simulate the partial engulfment conditions of the test described in Section 2. In particular, the engulfed area was reduced to the 25 % of the total surface of the tank. A heat flux of 94 kW/m² was set as boundary condition within the engulfed region. This corresponds to the heat emissive power of the flame. Table S2 summarizes the input parameters considered to run the simulation in RADMOD.

Parameter	Value
Initial temperature	14 °C
Initial pressure	7.1 bar
Initial liquid filling level	80 %
Tank inner diameter	0.953 m
Tank length	3.05 m
Wall thickness	0.0071 m
Engulfed surface area	25 % of the total tank surface area
Heat flux to the engulfed surface	95.4 kW/m ²
Heat flux outside the engulfed area	0 kW/m^2

Table S2: input parameters considered to run the simulation in RADMOD