Large pool fires in the process industry. A simple model for safety distances estimation

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ABSTRACT In recent years, the global production growth and the complexity of processes operation have increased safety concern, especially during the design project, considering potential accidental events. Pool fire is one of the most frequent accidental events. Some procedures for safety distances (SDs) estimation from it were reported. However, there is a lack of adequate simple models to directly estimate SDs covering a wide range of substances and pool diameters, considering a continuous interval of receptor vulnerabilities. In this paper, simple models to estimate SDs are proposed, suitable to be incorporated into complex models (e.g., safety management systems, layout optimization). A surrogate model is achieved by adopting a reference one. Methodologically, the main variables that play a key role modelling a pool fire were selected and their influence on the SD was analyzed to propose simple mathematical expressions. NLP optimization problems were solved to optimize the model parameters. Models with R-squared values of more than 0.99 were obtained when compared to the reference model. A conservative, accurate and easy-to-use model was achieved with the aim of developing safer plants or for their safe operation by improving the optimal process design, or implementing safe management systems, considering risks.

KEYWORDS Fire; Safety distance; Thermal Radiation; NLP; GAMS

1. Introduction

It is known that safety issues have been considered as a crucial aspect covering all stages of process design projects. In fact, Inherently Safer Design Philosophy (ISD) or the Risk-Based Design approach (RBD) have been progressively incorporated in early steps of the process design task during the last decades.

Several methodologies were reported to implement or facilitate design strategies under these new paradigms (intensification or minimization, substitution, attenuation or moderation, limitation of effects, simplicity, avoiding knock-on effects, among others). For more detail see Athar et al. (2019) and Gao et al. (2020). However, there is still a lack of adequate models linking critical design variables and the estimation of safety distances (SDs), capable of being easily incorporated into more complex (typical) models for chemical process design. In fact, certain modelling aspects represent strong drawbacks for the design of inherently safer processes at a conceptual stage of the project, or for optimizing complex process layouts considering risk thresholds. Rigorous models of different complexity are available to evaluate the consequences of accidental events, such as fires, explosions, and toxic dispersion. They are appropriate and must be used at final stages of design for vulnerability and/or risk analysis. They are not applicable when complex design optimization models must be implemented (at firsts steps of the design), as the input parameters are often undefined.

So, adequate methodologies for SD estimation are critical for conceptual design, considering risk at early stages.

In general, loss-of-containment (LOC) events are the origin of accidents such as fires, explosions and/or eventual toxic dispersions. Pool fires are known to be one of the most frequent accidental events. In fact, most of the catastrophic accidents have started with a pool fire that triggered other fires and/or explosions (Vipin et al., 2018). The domino effect and pool fires are strongly related and have been extensively analysed (Yang et al., 2020). SDs are a key point to avoid the propagation of the domino effect and it is usually difficult to estimate them at the beginning of the design project. Therefore, it is important from the economic perspective and from the safe operation point of view, to develop suitable simplified models to estimate SDs directly and easily in case of a pool fire.

From the management point of view, 580 (2016) and 581 (2016) standards provides conceptual and quantitative procedures to define inspection programs using risk-based methods for hydrocarbon and chemical processes. The first is focused on definitions and conceptualizations, covering a complete description of the requirements for establishing inspection intervals following a Risk Based Inspection (RBI) methodology. The second describes methodologies for quantitative risk analysis (QRA) for each unit of a process. Risk is defined as a composition of the frequencies and consequences of all potential accidental events. The consequence analysis following API RBI guided assessment is performed to establish a ranking of equipment items based on risk (for establishing priorities for inspection programs). In API RBI, the consequences of LOCs are expressed as the affected impact area or in financial terms by fixing impact thresholds. The affected area is determined by two methods differing by their complexity: the level one consequence analysis is performed

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using simplified methods to estimate affected zones for a limited number of hazardous fluids, and the level two involves a rigorous consequence analysis to solve the deficiencies of the first one. These deficiencies are largely referenced in 581 (2016). Note that the availability of reliable models for the estimation of SDs for different accidental events is of paramount importance in the context of RBI since the simple models used in the level one method could be replaced by quite accurate simplified methods to estimate adequate SDs, reducing the actual deficiencies.

RBD methodologies also impose to perform complex QRA evaluations from the early stages of the project design. A set of safety indexes have been introduced attempting to facilitate the design of safer processes (DOW F&EI, Mond, among others). Safety indexes are considered useful tools for preliminary process synthesis and design. Most indexes attempt to associate a measure of relative hazards with a radius of exposure. However, there is a lack of simple models relating critical variables linking management, design and QRA. Reduced models for SD estimation could be directly applied to make an adequate estimation of unit hazard rankings considering the influence on the impact distances in a similar way as expressed in APIs, but in this case from the design perspective (Sultana and Haugen, 2022). Here, simplified models are developed to estimate SDs given a pool fire, useful for both tasks (RBD and RBI).

Alileche et al. (2015) presented an extensive review of existing regulations that establish thresholds for domino effects and SDs for the process industry. Since regulations change from country to country, establishing SDs for a few impact thresholds is a good approach to facilitate a safety design, but it also has limitations. A further step for the estimation procedure of such SDs calls for simple models allowing to obtain them for each given radiation intensity threshold based in a few critical and accessible design variables at first steps of the conceptual design. In other words, these models should cover different scenarios, varying continuously from the radiation thresholds associated with the impact on people to those associated with the escalation possibilities of domino effects. Therefore, a suitable range of incident radiation intensities should be selected as an input for the simple/reduced models to be used.

Some reported works for process layout optimization use empirical tables to define separation distances among units (CCPS, 2018; Jung, 2010). This procedure segregates both effects, the one related with the adoption of relevant design variables (at conceptual/early design stages) and the consequences of the decisions made during the design/optimization of the layout (after the process flowsheet and dimensions of units were decided).

Other authors reported different approaches to overcome these limitations, achieving specific "*ad hoc simple functions*" to estimate SDs. For example, de Lira-Flores et al. (2018) obtained simple functions correlating SDs achieved through parametric simulations using ALOHA, making the impact level explicit by a correlated function of the distance to optimize a layout. Similarly, Jung (2010) achieved "*ad hoc*" functions to incorporate them into a layout optimization model using PHAST. These simple relationships are achieved "offline" making several parametric simulations and are associated with a specific scenario; just for a certain substance and for some fixed values of specific design variables; for example, tank volumes or dike areas (Mishra et al., 2013).

It is important to note that the above procedures are generally expensive from a computational point of view, requiring many "offline" simulations and correlations based on appropriate mathematical expressions for each event and involved substance, considering in most cases a fixed set of values of the relevant design variables for a given design problem. Curiously, there is a lack of simple models ensuring simultaneously the attributes we emphasize here: a simple analytical expression of general validity, applicable to a wide range of substances and operative conditions, easy to use for the direct estimation of SDs or for the incorporation into more complex models (risk-based design or layout optimization).

Although some works reported simple analytical models to estimate radiation levels, avoiding an explicit calculation of all the phenomena involved; they lack some of the critical requirements listed above. In fact, representative models of this group are the classic and widely known point source model (with a small application range of pool diameters) or the correlation developed by Shokri and Beyler (1989) that incorporate many simplifying assumptions and the estimated SDs are excessively overestimated, a fact that is unacceptable when searching optimal solutions.

To overcome this problem, many strategies have been reported to simplify the estimation of SDs from pool fires that are at the same time reliable and general, mainly oriented to the design of chemical processes. Cozzani et al. (2006) proposed fixed conservative SDs (regardless of the involved substance and pool fire diameter) to prevent domino effect. This approach has limitations to achieve optimal designs because the achieved generality simultaneously implies in many cases excessive overestimations. Later, Cozzani et al. (2009) improved their estimations by introducing a functionality of the pool diameter. In a report published by RIVM (2003) called 'Instrument Domino-Effecten (IDE)', a similar methodology is proposed for SD estimations for pool fire events. Both cited works proposed a dependency of the SDs for a set of fixed radiation thresholds. More precisely, in the second one, SDs were estimated for two fixed radiation thresholds, based on the TNO model (Van Den Bosch and Weterings, 2005). In both cases significant overestimations are the price to pay to cover a wide set of substances. Furthermore, the SD is not expressed as a continuous function of incident radiation thresholds.

Summarizing, simplified models should easily link critical design variables and relevant safety indicators allowing the consideration of the critical trade-offs among them. In this context, this work does not focus on searching new rigorous pool fire models. Instead, here we introduce two simple models fulfilling all the requirements mentioned above. The objective is to capture in a simple equation the relationships among the critical variables to estimate SDs minimizing the overestimation with respect to the ones provided by a suitable reference model (*RefM*), whatever the substance involved in the pool fire, for a wide range of pool dimensions and fixed incident radiation levels. The methodology to achieve the simplified models is presented in Section 2, followed by an analysis of model performance in Section 3. Additionally, some application examples are shown in Section 4. Finally, conclusions are included in Section 5.

2. Methodology

The existing pool fire models are aimed at calculating the radiation intensity for a given distance from the fire. Therefore, an iterative procedure must be used when pursuing the inverse calculation (the distance associated with a given radiation intensity), which we want to avoid here. In fact, the simple models (*Safety Distance Reduced Models -SDRMs-*) are inversely oriented with respect to the *RefM*. Although they are surrogate models, the structure of the input-output variables is different from that corresponding to the *RefM*.

To select a *RefM* considering the objectives of this work, two types of models appear as candidates: *differential models* and *solid flame models*. *Differential models* are the most accurate but at the same time the most complex from a mathematical perspective, requiring the resolution of differential equations (conservation of mass, momentum, and energy). They are implemented through numerical simulation tools (CFD). In addition to the complexity associated with their resolution, they require many input data. *Solid flame models* are semiempirical models covering different complexity levels. In general, they mainly consider a single homogeneous flame surface that emits with constant emissive power over the entire fire surface (McGrattan et al., 2000; Mudan, 1984; Shokri and Beyler, 1989; Van Den Bosch and Weterings, 2005). There are also more accurate ones assuming two or more flame areas with different characteristics (Muñoz, 2005).

Solid flame models are the most suitable for developing a reduced model as they are commonly used in QRA. The most rigorous methods (CFD-type) require a large computational effort and considerable amount of empirical information, not available along the initial stages of the process design. Furthermore, it is important to note that to achieve a proper fit with respect to the *RefM*, several simulations must be performed to achieve a dense grid of reference points.

The methodology used to obtain the *SDRMs* is summarized in Fig. 1. It involves the following steps: select an adequate reference model that can accurately estimate the radiation for a wide range of input variables, select an adequate set of input variables for the *SDRM* for the estimation of SDs, adopt simple functions to build *SDRMs* capturing the influence of the selected set of input variables on the SDs and solve NLP models to estimate the model parameters. Finally, check the accuracy of the obtained model. If the overestimation of SDs is not admissible, an iterative procedure proposing other functionalities must be performed.

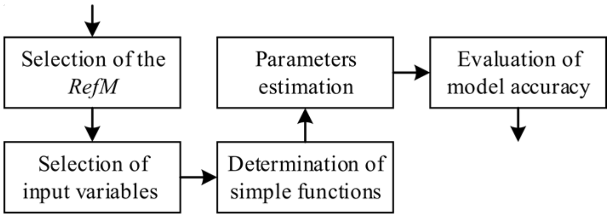

Figure 1: Methodology to obtain *SDRMs*.

2.1 Reference model selection (*RefM*)

An analysis of the main reported solid flame models is developed, and the most appropriate *RefM* is selected considering accuracy, generality, application range, general acceptance, among other attributes above mentioned. For the adoption of the appropriate *RefM*, the radiation fields estimated by different models were analysed considering that the objective of this paper is to obtain SDs from large pool fires (see appendix).

It is known that the main problem associated with most of the existing models is the need to extrapolate them for diameters outside their valid application range. The model of McGrattan et al. (2000) was selected as *RefM* because it proved to be the most appropriate for estimating SDs for a wide range of fire dimensions. The main disadvantage is that it does not consider wind effects. However, as indicated by McGrattan et al. (2000), the estimation difference is compensated by the inherent safety factor established in the formulation of the *RefM*. It is important to mention that the radiation estimated by the *RefM* could be quite conservative for short distances from the edge of the flame in the absence of wind. However, since the main objective here is to achieve SDs, conservative values must be assured for each used rigorous model, for all fire dimensions, all potentially involved substances, radiation levels and wind speeds. Considering these requirements, the trade-off among overestimations and generality along the full valid application space is inherently quite acceptable for the selected *RefM*. In addition, it should be considered that we also impose overestimations for the surrogate *SDRMs* with respect to the *RefM*, assuring a known maximum overestimation bound, along the valid *SDRMs* input space.

Next, the relationships between the involved variables will be analysed to determine the minimum set of input ones, considering the trade-off between the number of variables and the model performance.

2.2 Input variables (IVs) selection for the *SDRMs*

The principal involved variables for the estimation of SDs can be classified according to the following sets:

- Variables that characterize substances: *parameters included in physicochemical correlations.*
- Stochastics variables: those not exactly known before the accidental event. For example, the environmental parameters (wind speed and direction, am-

bient temperature, humidity, among others). This type of variables requires a statistical analysis to adopt a representative value. In the case of a pool fire, if the equipment dike is considered, a substantial portion of this probabilistic chain is avoided. Regarding atmospheric variables, wind direction, speed, and humidity, influence radiation fields.

- Variables that characterize the receptor: those that identify the maximum impact level tolerated by different targets, *the maximum tolerated radiation level*.
- Extensive or design variables: those that allow to quantify the event magnitude, associated with the mass involved, dimensions of the fire, among others. The main variable to determine the size of a pool fire is the burning area which under certain conditions can be represented by the *equivalent diameter of the fire*.

At a first analysis, and considering the existing simplified models above cited, three key variables arising from the physical nature of the accidental event are the maximum incident radiation tolerated by the receptor (I), the diameter of the pool fire (D), and a characterization of the substance. Note that they are key design variables, known at first steps of the process design. *RefM* uses *Heat Release Rate* (*HRR*) to identify the substance, so we consider it as a potential input variable (IV). As a result, functions $L(D,\ I,\ HRR)$ to estimate SD (that we denote as L) of at least the mentioned variables will be analyzed to achieve the *SDRM*.

It is important to consider that (*HRR*) can be obtained from tables or can be estimated by the product of the heat of combustion (ΔH_c [kJ/kg]) and the maximum mass burning rate (m_∞ [kg/s·m^2]). The last one can be determined from the heat of combustion and the heat of vaporization that combined, result in Eq. 1.

$$HRR = \Delta H_c m_\infty = 10^{-3}\left(\frac{\text{kg}}{\text{m}^2\text{s}}\right)\frac{\Delta H_c^2}{\lambda + \int_{T_o}^{T_b} c_p dT} \tag{1}$$

In the case where T_b (boiling point [K]) is close to the atmospheric value, a usual conservative simplification is to neglect the sensible heat.

Considering stochastic variables, relative humidity (*RH*) can be evaluated as an *IV* (*RefM* does not consider wind effects because of its inherent overestimation).

To decide if new variables should be incorporated, in addition to the above-mentioned three (D, I, *HRR*), a local sensitivity analysis is performed to select the input variables for the *SDRM* assessing their relative impact on the model output. In fact, Relative Marginal Value RMV_q (Eq. 2) is used to measure the sensitivity of the SDs with respect to a relative infinitesimal variation of each one of the potential input variables q, considering the remaining ones as constant values (Kraft et al., 2023).

$$RMV_q = \frac{\partial f\left(IV_1, IV_2, \ldots, IV_Q\right)/f\left(IV_1, IV_2, \ldots, IV_Q\right)}{\partial IV_q/IV_q} \tag{2}$$

Representing Q the total set of IVs with $q = 1, 2, \ldots, Q$.

We cover a dense grid of the potential set of IVs along a real application range from an industrial perspective. This range includes practically all flammable substances (*HRR* from 340 to 5700 kW/m^2), radiation intensities associated to all potential receptors (1.5 to 40 kW/m^2), pool diameters from 3 to 200 m, and *RH* from 0 to 100 %.

In addition to the three potential mentioned IVs (I, *HRR* and D) we include for evaluation, the relative humidity (*RH*) as an additional IV. Note that the effect of all physicochemical parameters is captured by *HRR*.

Procedurally, we estimate RMV_q by implementing the *RefM* in GAMS to obtain L as an output variable, and so we estimate the partial derivates of L with respect to all considered IVs along the considered range of values.

Finally, we obtain a four-dimensional hypermatrix for each q, that we define as $RMV_q^{D,HRR,I,RH}$. We estimate the mean ($R\bar{M}V$) and standard deviation (σ_{RMV}) considering all calculated values of the hypermatrix $RMV_q^{D,HRR,I,RH}$ (Table 1). The dimension of the hypermatrix is ($198 \times 10 \times 10 \times 10$) considering a homogeneous partition of the analysed range of the IVs. The range of the IVs will be deeply analysed in the next section.

A segmentation is imposed on diameter due to the nature of the *RefM* for the estimation of the flame length.

From the values of Table 1 ($R\bar{M}V$ and σ_{RMV}), clearly the contribution of *RH* to the output is negligible. In addition, Refenes and Zapranis (1999) suggested a threshold value (up to 0.15 as a maximum) for $R\bar{M}V$ to discard an input variable. We can conclude that D, I and *HRR* are here the key input variables, and the influence of relative humidity (*RH*) can be ignored. So, *RH* is assumed considering the worst-case scenario ($RH = 0$, transmissivity$= 1$). On the other hand, if any variable of the input set (D, I, *HRR*) is omitted, the reduced model will be excessively conservative in case we impose an overestimation as a restriction like here is the case. This fact will be verified in case study 3, concluding that methods to estimate SDs avoiding one or more of them overestimate excessively SDs. Therefore, we adopt *SDRMs* of the form $L(D, I, HRR)$.

2.3 Selection of simple functions to fit the *SDRMs*

After defined the set of IVs, a valid input space for the *SDRM* must be defined more precisely.

To determine SDs for domino effects prevention, it is necessary to characterize the source of the fire (*HRR* and

Table 1: Relative marginal values of the potential IVs.

interval	IV	$R\bar{M}V$	σ_{RMV}	CV
D <20 m	D	0,8049	0,1543	19 %
	HRR	0,3349	0,1922	57 %
	I	-1,0187	0,3505	-34 %
	RH	-0,0635	0,0078	-12 %
$D \geq 20$ m	D	0,3167	0,1433	45 %
	HRR	0,6833	0,1433	21 %
	I	-0,8478	0,2783	-33 %
	RH	-0,0651	0,0061	-9 %

D), then set the maximum response time of the emergency group (t_r) and estimate the radiation threshold (I) according to the receptor characteristics (Landucci et al., 2009; Ricci et al., 2021). Therefore, the estimation of SDs to prevent domino effects is greatly facilitated if adequate and simplified models are at hand.

The fire diameter interval has been a key criterion for the selection of the *RefM*. According to Steinhaus et al. (2007), the term "large pool fires" colloquially refers to sources of great extent, represented by fires associated with liquid storage tanks with diameters from 10 to 100 m. In this paper, fire diameters from 3 to 200 m are considered for the *SDRMs* as the strict application interval. In other words, the range of values for which optimal parameters will be determined.

Regarding the HRR interval, the adopted lower bound is 340 kW/m^2, which corresponds to methanol ($D \leq 3$ m) (SFPE and NFPA, 2002), while the upper extreme corresponds to pentane and is 5,700 kW/m^2 (McGrattan et al., 2000). Hence, almost all substances involved in process industries are covered. It is necessary to highlight that the *RefM* is not applicable to LNG pool fires (Raj, 2007). Therefore, the same is valid for the *SDRMs*. Finally, for the radiation level range, the adopted lower value is 1.5 kW/m^2 corresponding to a conservative value for the damage to people. The upper value arises from the threshold used for the escalation of domino effect for pressurized units (40 kW/m^2), as considered by Cozzani et al. (2006, 2007). To prevent domino effect, the SD should be high enough to ensure that the time to failure (TTF) is higher than the duration of the fire or the time required to mitigate it by the emergency response group. For atmospheric vessels, TTF is assumed higher than 10 min for $I < 15$ kW/m^2 and for pressurized vessels, TTF is assumed higher than 30 min for $I < 40$ kW/m^2 (Cozzani et al., 2006, 2007).

Once the valid space for the input variables is determined, the *RefM* is solved parametrically for a set of defined scenarios assuring a dense grid covering the full range of input variables detailed in Table 2. Therefore, a set of SDs corresponding to the set of parameterized input variables (substance characteristics, fire diameters and incident radiation levels) is obtained. A hyper-matrix is generated according to the discretized evaluations points. More precisely, the intervals used for parametric simulations are defined by dividing the selected HRR range into 10 partitions as well as the range of thermal radiation intensity, while the diameter interval is partitioned per meter, resulting 198 evaluation points. The set of discrete values are denoted with the suffix i for diameters (D_i), j for the radiation intensity (I_j) and k for the Heat Release Rate (HRR_k). So, after solving the *RefM* for all these points (19,800 input sets of variables and simulations), it is possible to graphically analyze the variation of SD (L) as a function of each input parameter to propose simple and suitable functionalities for the *SDRMs*.

Table 2: Parameter range discretization.

Parameter	Lower bound	Upper bound	Number of partitions
D (m)	3	200	198
HRR (kW/m^2)	340	5700	10
I (kW/m^2)	1.5	40	10

As was mentioned, it is important to achieve simple mathematical expressions for the *SDRMs* considering their future incorporation into more complex optimization problems (for example for layout optimization). In addition, it is particularly important to minimize overestimations since the quality of the optimal solutions strongly depend on these estimations. Clearly, the global model complexity and non-linearities will depend on the type of adopted *SDRM* mathematical expressions. Specifically, the more complex the function, the better the *SDRMs* fit but, at the same time, a more complex mathematical expression should be incorporated to complex (hard combinatory) optimization design models. At an extreme, the simplified model proposed by Shokri and Beyler (1989) –which presents a linear relationship between the distance and the pool diameter– is very easy to use, but at the same time SDs are substantially overestimated. To explore adequate relationships among the set of values achieved from the parametric simulations, some important relationships among them are presented here, after making a qualitative and quantitative analysis.

First, a qualitative analysis of the relationships between SDs and each IV is made. In Fig. 2, the logarithm of the distance is shown as a function of the logarithm of the fire diameter for different substances (HRR) and fixed radiation levels (I). The effect of the disjunction for the calculation of the flame length can be observed at $D = 20$ m. Based on this, reduced models represented through a segmented function ($D = 20$ m) are proposed here to avoid the incorporation of more complex terms or a correlation with excessive overestimations.

From Fig. 2, an almost linear trend is observed for low levels of radiation intensity; consequently in Eq. 3 a potential relationship between the diameter and L is proposed for both defined intervals.

$$L \simeq D^{k_4} f_2 (HRR, I) \tag{3}$$

The region of high radiation intensity levels depicted in Fig. 2b is the hardest to be suited by a potential relation. In this region, the calculated distances by the *RefM* are small, so errors will not be relevant in absolute terms. However, it is necessary to note that this fact could affect the statistical indicators that are based on a relative nature if they are used as the objective function for parameters estimation. Logically, if k_4 were expressed as a function of HRR and I, the final correlation will better fit the *RefM*, but making the mathematical expression more complex. Considering that varying HRR or I the slopes change little, k_4 was assumed independent of these terms.

For both partitions of the *SDRM* correlation, which are defined here as medium ($D = 3 - 20$ m) and large dimensions ($D \leq 20$ m), f_2 should be considered as a function of HRR and I. The relationship between logarithm of

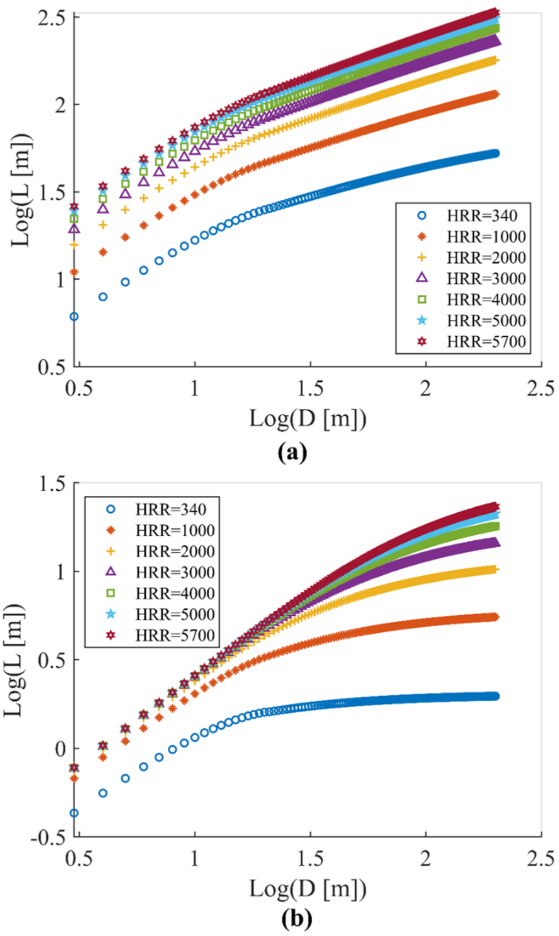

Figure 2: Influence of fire diameter on the safety distance. (a) $I = 1.5$ kW/m^2 (b) $I = 40$ kW/m^2

distance and the logarithm of *HRR* is quite similar to the function of distance and diameter. For large pool fire diameters, the slope is approximately independent of the radiation level while for small diameters this is only true for low radiation intensities. However, since the SD is small for low fire diameters and high radiation intensities this assumption does not significantly affect the SD approximation in absolute terms. In this form, the model is simplified by introducing Eq. 4. The function f_2 (from Eq. 3) is now disaggregated into two functions, one involving the *HRR* effect and the other to account for the effect of I. In other words, it is assumed that in the simplified model, k_3 is independent of I.

$$L \simeq f_3(I)\, HRR^{k_3} D^{k_4} \tag{4}$$

The characteristics of $f_3(I)$ are like the ones observed for the functions previously analyzed. There is a linear trend between the logarithm of the SD and the logarithm of the radiation intensity for different diameters and *HRRs* for low levels of radiation intensities. As intensity increases, linearity is progressively lost. For these radiation levels, the corresponding SD is relatively low, so errors in absolute terms should not be relatively important.

The potential relationships inferred by the previous qualitative analysis can be examined, as a first step, by a sensibility analysis over the entire space of IVs avoiding

Table 3: Relative marginal values of the IV.

interval	IV	$R\bar{M}V$	σ_{RMV}	CV
D <20 m	D	0,7473	0,1382	18 %
	HRR	0,4446	0,1053	24 %
	I	-0,7466	0,1391	-19 %
$D \geq 20$ m	D	0,3467	0,0935	27 %
	HRR	0,6533	0,0915	14 %
	I	-0,7295	0,0915	-13 %

highest radiations as the qualitative analysis indicated. An extensive analysis of the applications of sensibility analysis is presented for example in Iooss and Lemaître (2015). In case of a potential relation among SDs and all the input variables (as Eq. 4 considering a potential function for f_3), RMV_q should result constant values, and equal to the exponent of each IV$_q$ along the analysed space. Considering it, we create a three-dimensional hypermatrix for each IV$_q$ ($RMV_q^{D,HRR,I}$). We calculate mean, standard deviation, and coefficient of variation (CV) for each IV$_q$ (Table 3). We calculate $R\bar{M}V_q$ by considering a range of I from 1.5 to 15 kW/m^2 and the full interval of HRR and D.

From Table 3 we can suspect that a potential relationship could fit relatively well the *RefM* because RMV_q values are approximately constant for the entire space of the input variables; considering the low values obtained for standard deviations and CVs. As a general guide if CVs are lower than 30 %, our assumption about RMV_q constant can be adequate.

So, according to the set of characteristics imposed to *SDRMs* and considering Eq. 4, we propose Eq. 5 to define the *SDRM1*.

$$L = \left\{ \begin{array}{ll} a_1 I^{a_2} HRR^{a_3} D^{a_4} & D < 20 \text{ m} \\ b_1 I^{b_2} HRR^{b_3} D^{b_4} & D \geq 20 \text{ m} \end{array} \right\} \tag{5}$$

In addition, we introduce a more complex model to improve the fit as shown in Eq. 6 (*SDRM2*) by adding new parameters, increasing the degree of freedom.

$$L = \left\{ \begin{array}{ll} a_1 \left(I^{a_2} + a_3\right)^{a_4} \left(HRR^{a_5} + a_6\right) D^{a_7} & D < 20 \text{ m} \\ b_1 \left(I^{b_2} + b_3\right)^{b_4} \left(HRR^{b_5} + b_6\right) D^{b_7} & D \geq 20 \text{ m} \end{array} \right\} \tag{6}$$

The models are dimensional, I and HRR must be expressed in kW/m^2, L and D in m.

In the next section we will obtain the model parameters by solving NLP optimization problems using adequate statistical indicators as objective functions (OFs). According to our previous analysis, it can be expected that the estimated parameters values (the exponents) should be similar to the $R\bar{M}V_q$ indicated in Table 3.

2.4 Parameter estimation

After defined the IVs and the functionalities of the *SDRMs*, according to Fig. 1, here we proceed to estimate the model parameters. They are obtained by solving Nonlinear optimization problems. The optimization model can be symbolically expressed as follows (Eqs. 7 to 10). The OFs are different statistical quantitative indicators representing the correlation quality of each reduced model. Some of them are chosen for the evaluation of the absolute error and/or for the relative one. Here is presented the coefficient of determination (r^2) as *OF* (Eq. 7) involving absolute terms. However, other statistical indicators considering the absolute and relative error were tested as the Relative Root Mean Square Error (*RRMSE*) and the Root Mean Squared Relative Error (*RMSRE*) (Despotovic et al., 2016).

$$\text{Max.} \qquad r^2 = \frac{\sum\sum\sum\left(l_{ijk}^{RefM} - l_{ijk}^{SDRM}\right)^2}{\sum\sum\sum\left(l_{ijk}^{RefM} - l_{m}^{RefM}\right)^2} \tag{7}$$

s.t.

$$l_{ijk}^{SDRM} = SDRM\left(D_i, I_j, HRR_k, \underline{x}\right) \tag{8}$$

$$l_{ijk}^{SDRM} \geq l_{ijk}^{RefM} \tag{9}$$

$$l_{ijk}^{SDRM} \leq l_{ijk}^{RefM} + \Delta l_{max} \tag{10}$$

$\underline{x} \in ¡^{n_p}$

where $\underline{x}$ is a vector containing the parameters of the model and n_p is the number of parameters involved in each *SDRM*. l_{ijk}^{SDRM} indicates the estimated distances by applying alternatively each of the *SDRMs* (Eq. 5 or 6), while l_{ijk}^{RefM} represents the corresponding ones estimated by the *RefM*, l_m is the mean distance calculated by the *RefM* and n represents the total number of evaluated points (19,800). The set of values l_{ijk}^{RefM}, as was mentioned, were previously calculated by parametric simulations covering all the points defined by the discretization of the adopted input variable intervals. These values are incorporated to the optimization problem as parameters.

The set of inequality constraints (Eq. 9) are imposed to assure that estimated distances by *SDRMs* always overestimate the ones calculated by *RefM* which is desirable for the estimation of SDs. Moreover, the constraints imposed by Eq. 10 bound the maximum overestimation produced by *SDRMs*. To minimize the maximum overestimation measure (Δl_{max}), the optimization problem is parametrically solved using decreasing values of Δl_{max} until the problem results infeasible.

The optimal parameters were achieved by solving the optimization problems in GAMS using the CONOPT solver. The models include 19,800 variables, which corresponds to the *SDRMs* estimations in each evaluated point. The equality restrictions are 19,800, while the inequalities are 39,600. Finally, the optimization variables are the 8 parameters for *SDRM1* and the 14 parameters for *SDRM2*. In each case, half of them are defined for each of the partition (4 and 7 for each interval of each respective model). The results will be presented and discussed in the following section.

3. Model performance analysis

In Table 4 are shown the values of the statistical quantitative indicators obtained by using r^2 as *OF* for both *SDRMs*. The statistical indicators and the achieved parameters present little variations modifying the objective

Table 4: Statistical quantitative indicators of *SDRMs*.

Model	r^2	*RMSRE*	*RRMSE*
*SDRM*1	0.97740	0.66151	19.14 %
*SDRM*2	0.99659	0.28483	7.43 %

functions because Eq. 10 strongly constrain the feasible region. The definitions of *RRMSE* and *RMSRE* are included in Eqs. 11 and 12.

$$RMSRE = \sqrt{\frac{1}{n}\sum_{i\in D}\sum_{j\in I}\sum_{k\in HRR}\left(\frac{l_{ijk}^{RefM} - l_{ijk}^{SDRM}}{l_{ijk}^{RefM}}\right)^2} \tag{11}$$

$$RRMSE = \frac{\sqrt{\frac{1}{n}\sum_{i\in D}\sum_{j\in I}\sum_{k\in HRR}\left(l_{ijk}^{RefM} - l_{ijk}^{SDRM}\right)^2}}{\frac{1}{n}\sum_{i\in D}\sum_{j\in I}\sum_{k\in HRR} l_{ijk}^{RefM}}100 \tag{12}$$

R-squared (r^2) is interpreted as the proportion of the total variation of the values estimated by the *RefM* with respect to its arithmetic mean l_m^{RefM}, explained by the *SDRMs*. Therefore, values close to unity are desired.

Table 5 shows the optimal parameters for both *SDRMs*. It is important to remark that the exponents obtained for the *SDRM1* are similar, as was expected, to the ones above obtained through the RMV analysis for all the input variables and for both partitions of the model (Table 3). The differences arise from the constrained imposed to avoid underestimations. This verifies the reasonability of the assumptions made to propose the simplified models. In fact, the chosen variables, and functionalities can adequately capture (in a similar form to the *RefM*, as it is our objective) the relationships among the set of IVs and the SD.

In Fig. 3 are indicated the *SDRM2* estimation errors for three significant radiation levels, for different *HRRs*

Table 5: Parameters of SDRM.

Par.	Value $D < 20$ m	Par.	Value $D \geq 20$ m
	SDRM1		
a_1	0.3602	b_1	0.2981
a_2	-0.6376	b_2	-0.6361
a_3	0.4660	b_3	0.6022
a_4	0.6961	b_4	0.3978
	SDRM2		
a_1	0.4744	b_1	0.3179
a_2	-0.6478	b_2	-0.7913
a_3	-0.0689	b_3	-0.0395
a_4	0.7989	b_4	0.6889
a_5	0.4380	b_5	0.5798
a_6	-2.5246	b_6	-0.3698
a_7	0.6998	b_7	0.4175

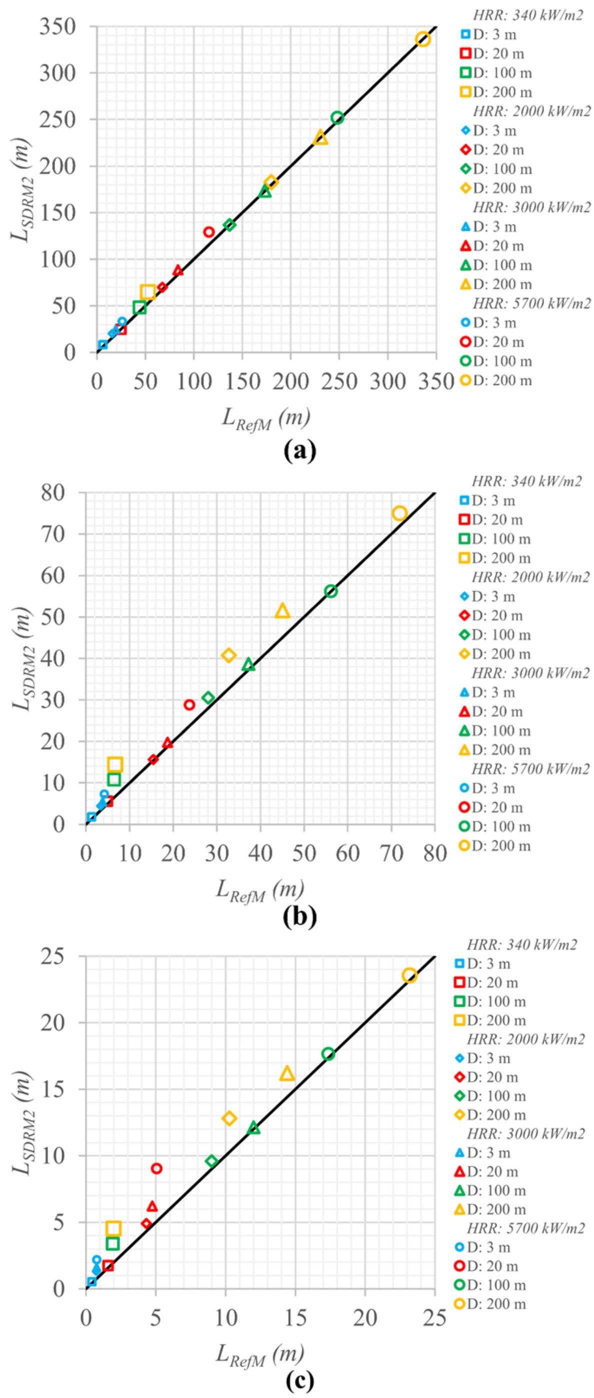

Figure 3: Performance of the *SDRM2* vs *RefM*. (a) $I = 1.5$ kW/m^2 (b) $I = 15$ kW/m^2 (c) $I = 40$ kW/m^2.

values and for the set of diameters: 3 m, 20 m, 100 m, and 200 m. An adequate fit can be observed in Fig. 3.

The maximum overestimation of *SDRM2* with respect to the *RefM* is 13 m. This upper bound was achieved by solving parametrically a set of optimization problems, using decreasing values of Δl_{max} as indicated by Eq. e10. The problem becomes infeasible for values lower than 13 m. Subsequently, 13 m is the maximum overestimation that can be obtained (using *SDRM2*) over the SD estimated by the *RefM*. Overestimations are significantly reduced for other values of the valid input space, for example, for smaller values of *HRR* the maximum overestimation is 5 m (for $HRR = 3000$ kW/m^2 and $I = 1.5$ kW/m^2).

The principal contributions to the relative error indicator (*RMSRE*) are the high relative errors associated with small pool fire diameters (with high radiations thresholds and *HRR* values). However, this fact occurs for overestimations lower than 4 m, which are a negligible difference for practical applications (layout design, contingency plan). This can be observed in Fig. 3(c).

Regarding *SDRM1*, as expected, the maximum overestimation is greater than the corresponding one of *SDRM2* (23 m) for $I = 1.5$ kW/m^2 and $HRR = 5{,}700$ kW/m^2. Similarly, for lower values of *HRR*, the maximum overestimation is significantly reduced (10 m for $HRR = 3{,}000$ kW/m^2 and $I = 1.5$ kW/m^2).

According to the *RRMSE*, an adequate fit for the simplified *SDRMs* was obtained when compared with the *RefM*. In fact, the calculated value is 7.43 %, which represent an excellent performance for *SDRM2*. For *SDRM1* the calculated value for *RRMSE* is 19.14 %, representing still a good performance (Despotovic et al., 2016).

Based on this analysis, we can conclude that *SDRMs* can adequately fit the *RefM*. In the next section, we will demonstrate the effectiveness of *SDRMs* in different study cases.

4. Application examples of the reduced models

In the first study case the *SDRMs* estimations are compared with the TNO model considering different substances and scenarios characterized by the absence or presence of wind. In the second case, both *SDRMs* are compared with other published methods to estimate SDs. In the third study case, the *SDRM2* estimations are compared with experimental pool fires.

4.1 Study case I

The SD estimated using both *SDRMs* are compared here with those estimated by means of the TNO model for different substances, and considering diverse scenarios characterized by the absence or presence of wind. In Fig. 4 are shown the thermal radiation fields, for kerosene pool fires of 20 m diameter and for different wind velocities (TNO model: 20 m/s, 10 m/s, 5 m/s and 0 m/s) estimated by the three models. The values of m'' (mass burning rate) and ΔH_c were extracted from SFPE and NFPA (2002). Radiation fractions used in the TNO model were extracted from experimental data (Burgess and Herzberg, 1974; Koseki, 1989; Muñoz, 2005). Analogous results (not shown here) were obtained with different substances (benzene, gasoline, crude oil, among other), verifying that *SDRMs* always overestimate the results obtained with TNO model.

As can be seen in Fig. 4, even in the presence of reasonably high wind speeds, for the substances evaluated, both *SDRMs* ensure conservative SDs in all cases. *SDRM1* estimations, as expected, are greater than *SDRM2*. This fact should be considered to estimate SDs to process equipment (high radiation thresholds) in zones with extremely high wind speeds. The flame tilt for high wind speeds causes an increase in the view factors near the edge

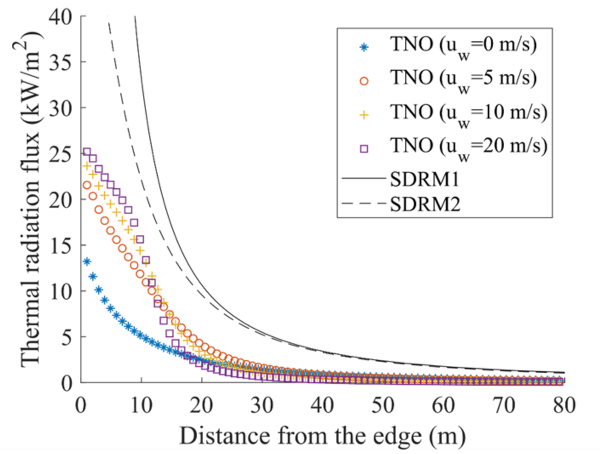

Figure 4: Comparison of *SDRM* with the model of TNO.

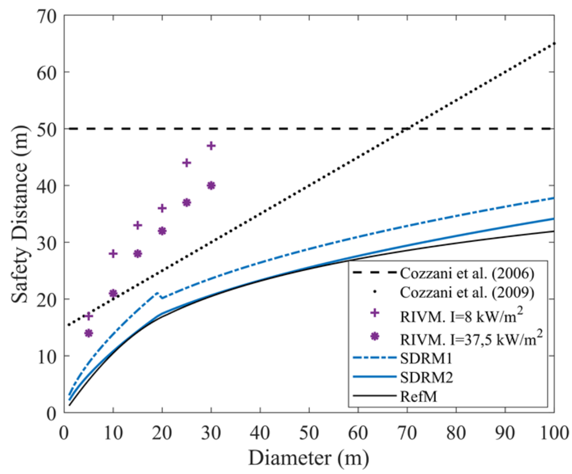

Figure 5: Comparison between *SDRMs* and other methods to estimate safety distances.

of the flame. Thus, when radiation thresholds are high, for substances with high flame heights (high *HRR*) and high radiation fractions, for high winds speed conditions, *SDRM1* could be more adequate.

Observe that *SDRMs* directly allow the estimation of SDs, while the TNO model is oriented to the calculation of the thermal radiation flux. The direction of the input/output variables and the characteristics of the *SDRMs* allow them to be applied in early design stages to establish a ranking of equipment items based on the affected zone from potential pool fires. Logically, this ranking can also be used in the context of RBI following the APIs procedures.

4.2 Study case II

Here, the SD estimations provided by both *SDRMs* are compared with existing and commonly used approaches for the estimation of SDs.

Cozzani et al. (2006) suggested a separation distance of 50 m to prevent domino effect triggered by pool fires for atmospheric units and 20 m for pressurized ones.

Figure 5 shows the estimations of SDs applying different approaches for a gasoline pool fire, considering a radiation threshold for atmospheric equipment (15 kW/m^2).

One is the mentioned constant values proposed by Cozzani et al. (2006), other is the improved model of Cozzani et al. (2009), and the other the procedure proposed by RIVM (2003), defining certain SDs for fixed radiation levels (8 and 37.5 kW/m^2) aimed at preventing domino effects. Both cited methods take the TNO model as reference.

As can be seen in Fig. 5, the SD suggested by Cozzani et al. (2006) as a constant value (50 m) largely overestimate all other values for pool fires diameters lower than 70 m. It can also be seen that using the linear relationship proposed by Cozzani et al. (2009), the estimated SDs are improved (for this substance) but are still relatively higher. Specially, for large pool fires ($D \geq 70$ m), SDs are progressively and significantly overestimated.

It is important to note that SDs estimated by using RIVM (2003) are related to fixed radiation thresholds (8 and 37.5 kW/m^2). Even those calculated for the highest radiation intensity are relatively greater than the SDs obtained by the other methods compared here, except for the value 50 m.

Clearly, all the mentioned methods provide better estimations for cases with larger *HRRs*, while for those with lower *HRRs* they are more conservatives. In case of the *SDRM* developed in this work, even the SDs estimated by the most conservative model (*SDRM1*) are significantly lower than the ones suggested by Cozzani et al. (2009) and the RIVM methodology, especially for large pool diameters. SDs estimations using both *SDRMs* assure overestimations over the adopted *RefM*.

Through this analysis, it can be concluded that the relative overestimations of the SDs are strongly dependent on the considered input variables. Methods considering only one or two input variables (*I* and/or *D*) without considering the characteristics of the involved substance are necessarily more conservative.

4.3 Study case III

Reduced models were successfully tested (guaranteeing conservative results) against experimental results of ethanol, gasoline and diesel pool fires with diameters up to 22 m (Burgess and Herzberg, 1974; Koseki, 1989; Muñoz, 2005; Sjöström et al., 2015). In Fig. 6, *SDRM2* estimations are compared with experimental data for gasoline pool fires extracted from Sjöström et al. (2015). The experimental data refers to the radiation observed for different pool areas and for different wind conditions. The SDs estimated by *SDRM2* are adequate since the radiation levels are overestimated and in terms of the added distance, does not result exaggerated.

Clearly *SDRM2* shows significant variations in added radiation intensity at low SDs. However, in terms of added SDs, the variation is not so extreme. The main reason for these deviations lies in the fact that the experimental data was obtained for pool fires with a wind speed of 2 m/s. The reduced models ensure conservative results, even in the presence of high wind speeds. The overestimation in SDs is not a drawback compared to previous methods used to date to estimate SDs (Fig. 5).

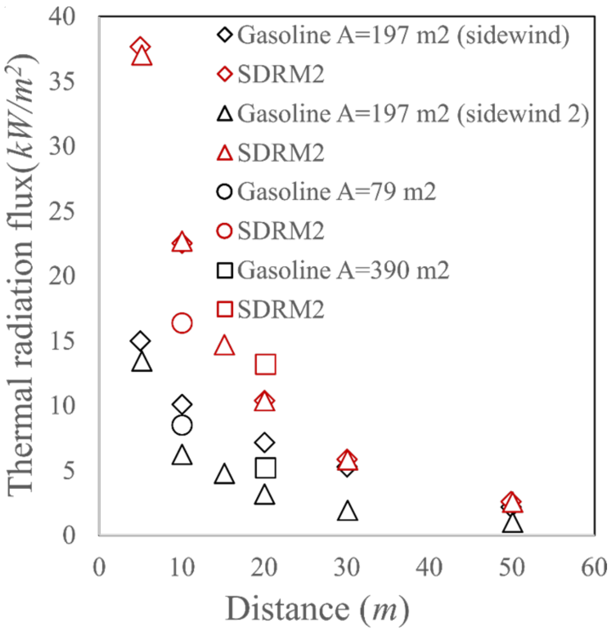

Figure 6: *SDRM2* vs. experimental data.

5. Conclusions

A detailed procedure for the development of *SDRMs* from pool fires was presented. As shown in the study cases, the *SDRMs* developed here are a further step in the estimation of SDs from accidental pool fires. In fact, both *SDRMs* make it easy based on the diameter of the pool fire and covering continuously a set of thermal radiation thresholds relevant for practical design decisions, such as, people death or domino effects.

The study cases show that *SDRMs* accurately estimate SDs even for the worst conditions compared to rigorous models and against experimental data. Although *SDRMs* show significant variations in added radiation intensity at low SDs (Fig. 6), the variation in terms of added SDs is not considerable for practical purposes. This is an advantage over other SD estimation methods, as both *SDRMs* avoid excessive overestimations. The selection of one of them depends on the model complexity and the tolerated overestimation. *SDRM1* is simpler than *SDRM2*, and inherently yields higher overestimations, assuring a more conservative SD. For cases in which it is desirable to reduce the overestimations at an achievable minimum, the *SDRM2* should be used.

The valid application space covers a wide spectrum including not only small processes but also large tanks and storage areas (ranging from relatively small pool fires of 3 m to extremely large pool fires of 200 m). This can be guaranteed by the used methodology; and contrasting the *SDRMs* results against the ones obtained by the selected *RefM* which is applicable to pool fires of large dimensions.

In the RBI context, the application of *SDRMs* is straightforward since the procedure presented in 581 (2016) requires estimating the affected area by setting an impact threshold. It can be calculated directly from the SD obtained with the *SDRMs* for a pool fire. In the process design context, *SDRMs* improve the way that SD matrixes are assumed. In fact, from the layout perspective, the achieved *SDRMs* provide a close link among the basic variables to estimate SDs and those used to design optimal layouts in real problems considering risk. Traditional Facility Layout Problem modelling uses the dimensions and the minimum separation distance among units (SDs) as input parameters. By including *SDRMs*, the layout, and the preliminary conceptual design of facilities can be optimized simultaneously. It is important to mention that in these problems, the *SDRMs* introduce a discontinuity when the pool diameter is a free variable. This requires a set of binary variables or a relaxation of the disjunctions. Future works will be oriented to reduce the gap to model simultaneously the trade-offs among different design steps (process and layout design).

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Appendix: Selection of the reference model

Radiation fields estimated by different models were evaluated as a function of the pool diameter and distance from the edge for different hydrocarbons. The difunded models of Mudan (1984) and Shokri and Beyler (1989) predict extremely low radiation fields near the flame for large diameter pool fires. The model of Shokri and Beyler predicts a maximum radiation intensity at a certain diameter. This fact is also verified with the model proposed by Mudan for high radiation intensities. This behavior arises due to extrapolations outside their valid application limits to calculate the flame length (h) and the surface emissive power (E). These models estimate extremely high flame length for large diameter pool fires and compensate the flame length overestimation by a restricted estimation of E, low enough to maintain the product hE (proportional to the radiant energy released per unit of pool perimeter). However, low emissive powers and high flame lengths cause that the radiation at ground level and near to the flame be relatively lower even though the product hE is maintained as a constant. This fact explains the presence of the observed maximum values.

In the implementation of TNO model, a conservative high radiation fraction was assumed, considering the experimental data obtained for radiant fraction factor (Fs) for low diameter pool fires. Moreover, the use of Thomas Equation for the flame length is conservative too (Thomas, 1963). The TNO model and those above mentioned are valid up to fire diameters of 20 m. The difference among the TNO model and those proposed by Mudan and Shokri & Beyler is that the first does not consider a decreasing emissive power with the diameter (if Fs remains constant). This fact explains the absence of the maximum in the radiation fields.

Even the conservative hypotheses, the model of TNO estimates radiation levels lower than those estimated by the model of McGrattan et al. (2000). This fact is observed particularly near of the edge of the flame, and it is caused by the estimation of a high flame length and a relatively low emissive power by the first. The model of McGrattan considers a constant flame length above 20 m diameter and a constant emissive power. Thus, it shows increasing radiation levels with the diameter, due to the view factor increment.

Given our objective, the model of McGrattan et al. (2000) was selected as the most appropriate one for estimating SDs for a wide range of fire dimensions. However, it does not consider wind influence. According to McGrattan et al. (2000), the view factor calculation given the flame tilt, will yield marginally different results when the receptor is at a distance of a few diameters from the pool. That is, the estimation difference (when considering the wind) is compensated by the inherent safety factor established for their model and calculation procedure. Even though, it is important to mention that the flame could largely approximate or even directly take contact with some equipment in case of high wind speeds. In such situation, specially the second case, care must be taken because the heat transfer will be much higher than the one calculated without this effect consideration. To complete the previous analysis, the overestimation degree of the selected *RefM* compared to other models was evaluated, including more rigorous models for pool fires –in this case for relatively low diameters (6 m)–. The overestimation of the model of McGrattan was verified comparing it with the model proposed by Muñoz (2005), applied to a gasoline pool fire considering multiple emissive zones. The *RefM* assumes a high value of the emissive power, so the calculated flame length is low and therefore the radiation fields at ground level at nearby distances are conservative. Comparison of the *RefM* with more rigorous models like the proposed by Muñoz (2005) for larger pool fires is not possible due to the absence of experimental data for the emissive power as a function of the vertical coordinate. For large pool fires, most of the flame is covered by smoke, so the use of a variable emissive power is not justified.

The estimated radiation field for large gasoline pool fires (50 and 100 m) by the *RefM* was successfully tested by comparing with the 2-zone model developed by Muñoz (2005). Models with zone partition estimate the highest radiation intensity near to the flame edge in comparison with the models of Mudan, Shokri & Beyler and TNO. Even though, the thermal radiation is always lower than the estimated by the *RefM*. The overestimation of the *RefM* is verified considering different substances, relevant for the calculation of SDs.