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From laboratory simulation to scale-up and design of spray barriers mitigating toxic gaseous releases

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ABSTRACT

Simulation of a process by means of physical models at a reduced scale is an essential tool in many application, allowing to perform a large number of experimental runs, so as to obtain a quantitative representation of the involved phenomena, at relatively low cost. Some difficulties can arise when the mathematical model derived from the simulation is applied to a real scale problem, in that the scaling of some empirical coefficients with the system size is not obvious at all. As fluid barrier scaling is a difficult task, still not deeply investigated in the scientific literature, the focus of this study is to translate knowledge from research on this topic into practice for industrial application. Following an extensive and accurate experimental work in wind tunnel, the main parameters determining the effectiveness of containment, absorption and dilution of chlorine releases were determined and a mathematical model is developed. In order to frame proper scale-up strategies, the most important result of this study rests on the explicit formulae giving, as a function of the aforesaid parameters, the single pass efficiency, the global absorption efficiency, and the toxic gas concentration downwind the barrier. In the far field, the gas concentration is practically determined only by the rate of atmospheric dispersion of the mass flow-rate of gas escaping the abatement. The absorption efficiencies are related to the drop size and to the mass transfer coefficients in the gas and liquid phases. The mean drop diameter plays an essential role in the absorption efficiency, since it simultaneously acts on air entrainment, interfacial surface and mass transfer coefficient in the gas phase. The evaluation of the mitigation effect for an industrial installation requires the scaling of the entrainment coefficient experimentally determined from wind tunnel testing. All the scaling criteria needed for adapting the proposed model to the design of a spray curtain suitable for the protection from a chlorine release, are amply discussed presenting some carefully designed simulations. Owing to its rather general structure, the model can be applied to different gaseous releases and/or absorbing solutions, provided that proper values of the parameters related with the chemical and physical absorption of the involved substances be theoretically or experimentally obtained in advance.

Keywords: Chlorine; Mitigation; Modelling; Nozzles; Scale-up; Toxic release

1. Introduction

Notwithstanding significant improvement in safety design, layout and management procedures, accidental releases of flammable or toxic gases still represent a serious concern in the process and petrochemical industries. A detailed survey about industrial accidents involving hazardous materials, which caused or could have caused severe damage and danger, revealed that 6004 accidents were due to gaseous releases, over the time span from the end of the 1970–2007. Among them, we identified 670 chlorine release accidents, with fatalities in 67 events and injuries in 439 events. Main activities involved in chlorine releases were processing (32.8%) transport by rail, road and pipe (16.3%) and storage (8.5%), while the main locations were chemical and process factories (51.5%) followed by storage parks (6.3%). These findings are in good agreement with a statistical analysis of historical data taken from the MHIDAS database ("Major Hazard Incident Data Service") performed by Planas-Cuchi et al. (1997). The analysis of 6099 accidents occurred up to the end of 1993 showed that the highest percentage (52.15%) corresponded to release, followed by fire (41.52%). Spray curtains are considered among the most

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Nomenclature

a_c	air flow rate induced by the curtain ($kg\,s^{-1}$)
a_{dil}	total diluting air flow ($kg\,s^{-1}$)
a_e	air flow rate entrained by the curtain ($kg\,s^{-1}$)
A	function of the spray angle
d	equivalent spray diameter (m)
D_F	mitigating factor
g	acceleration of gravity ($m\,s^{-2}$)
h	curtain height (m)
$k_g p$	mass transfer coefficient in the gas-phase ($kmol\,m^{-2}\,s^{-1}$)
l_n	nozzle pitch (m)
L	curtain length (m)
m_{abs}	mass flow rate of the absorbed substance ($kg\,s^{-1}$)
m_d	residual mass flow rate ($kg\,s^{-1}$)
m_r	mass flow rate of the release ($kg\,s^{-1}$)
M_a	mean molar mass of air ($kg\,kmol^{-1}$)
s	liquid flow rate ($kg\,s^{-1}$)
v_j	liquid velocity at the end of the jet phase ($m\,s^{-1}$)
v_0	liquid velocity at nozzle exit ($m\,s^{-1}$)
v_∞	free fall velocity ($m\,s^{-1}$)
x_t	distance from the release source (m)
X_g	intrinsic single-pass absorption efficiency of chlorine

Greek letters

δ	drop mean diameter (m)
η_{abs}	absorption efficiency
η_{dil}	dilution efficiency
η_{disp}	efficiency due to atmospheric dispersion
η_0	efficiency during initial dilution of the release
λ	length scale factor
ρ_a	air density ($kg\,m^{-3}$)
ρ_s	mean density of the liquid (curtain) ($kg\,m^{-3}$)
ϕ	spray angle
ψ	parameter defined by Eq. (22)
ω_d	concentration of released substance downwind the curtain (ppm)
ω_t	concentration of released substance at x_t (ppm)

Superscript

$'$	parameters per unit curtain length

Subscripts

f	real scale
t	wind tunnel

common devices suitable to mitigate the risk connected to these accidental events. The mixing and dispersion of dense gas clouds are often much slower than those of buoyant clouds and, consequently, it is desirable to increase their natural dispersion by enhancing the dilution rate. In this respect, spray curtains can represent an effective method to control the spreading of a cloud and mitigate the environmental/toxic effects. The release concentration is reduced by means of two mechanisms: diluting action due to air entrainment by the sprays, particularly effective in case of stable atmospheric conditions and low ventilation; containment action, which, extending the "transient phase", reduces the maximum gas concentration, especially when dealing with a release of short duration. When dealing with flammable gases of low solubility and reactivity, as saturated hydrocarbons, the primary purpose of the barrier is a fast dilution of the released substances, so that the possible contact of the cloud with ignition sources occurs by far below the low flammability limit (LFL). In this respect, inert vapour or gas curtains, located as near as possible the release, can often represent the best technical solution (Rulkens et al., 1983). An extended review on the application of water sprays by Jones and Thomas (1993) gives an insight into the potential mitigation mechanism and effectiveness against propagating explosions. Watts used water sprays to reduce the concentration of ethylene–air mixtures to below LFL, proving their effectiveness in this instance, due to the air entrainment effect connected to water spray motion (Watts, 1976).

The effectiveness of the chemico-physical mitigation of a barrier depends on the characteristics of the liquid solution and, particularly, on the reagent concentration. The effectiveness of water spraying systems in removing water-soluble gases was studied theoretically using the model HGSPRAY developed by Fthenakis (1989) and implemented by Fthenakis and Blewitt (1993, 1995). Their application was recently extended also to the application of indoor releases of water-soluble gases (Fthenakis, 2001). Only few researchers, (Griolet et al., 1995) developed a model to optimise the reactive curtain design for toxic gas dispersion. Dealing with reacting curtains, the authors performed a detailed study at laboratory scale, on the transient behaviour of a chlorine release (Fabiano et al., 2003; Palazzi et al., 2007a). Subsequently, the authors developed a mathematical model of a two-phase jet to evaluate the entrained air rate into a spray barrier, taking into account as well the chemical reaction due to chlorine absorption in alkaline solutions (Palazzi et al., 2007b).

As fluid barrier scaling is a difficult task, not deeply investigated in the scientific literature up to now, the focus of this study is to translate knowledge from research on this topic, obtained from a simulation study in wind tunnel, into practice for industrial application.

Following an extensive and accurate experimental work in wind tunnel, the main parameters determining the effectiveness of containment, absorption and dilution of gaseous toxic releases were assessed. In order to frame proper scale-up strategies for practical applications, the most important result of this study rests on the explicit formulae giving, as a function of the aforesaid parameters, the single pass efficiency, X_g, the global absorption efficiency, η_{abs} and the toxic gas concentration downwind the barrier, ω_d. In fact, the protective action of a curtain can be essentially related to the mitigation factor, D_F, i.e. the ratio between the chlorine concentration without the curtain and that resulting from the sprays activation. At far field dispersion from the barrier, the gas concentration is practically determined only by the rate of atmospheric dispersion of the mass flow-rate of gas escaping the abatement. Then, according to the model, D_F directly depends on X_g, or else on η_{abs}. The absorption efficiencies, on the other hand, are related to the drop size and to the mass transfer coefficients in the gas and liquid phases. According to literature, the mean drop diameter can be scaled with the square root of the system size. This parameter plays an essential role in the absorption efficiency, since it simultaneously acts on air entrainment, interfacial surface and mass transfer coefficient in the gas phase. Immediately downwind the barrier, the gas concentration, and then D_F, also depends on the dilution due to mixing of the partially decontaminated air leaving the curtain with the air entrained externally to it. The evaluation of D_F for an industrial installation then requires also the scaling