

## Generalized Mathematical Model of Reacting Spray Curtains Mitigating Hazardous Releases

Bruno Fabiano<sup>1\*</sup>, Andrea P. Reverberi<sup>2</sup>, Fabio Currò<sup>1</sup>, Emilio Palazzi<sup>1</sup>

*1 DICCA – Department of Civil, Chemical and Environmental Engineering, Polytechnic School, Genoa University, via Opera Pia 15, 16145 Genoa (Italy); 2 DCCI – Dept of Chemistry and Industrial Chemistry, Genoa University via Dodecaneso 31, 16146 Genoa (Italy).*

*\*Corresponding author: brown@unige.it*

### Highlights

- Absorption of a toxic gaseous component into reacting or non-reacting spray.
- Mathematical model for the performance of a reacting curtain.
- Experimental characterization of chlorine physical and chemical absorption by a barrier.
- Estimation of design parameters for spray curtain industrial application.

### 1. Introduction

Notwithstanding extensive regulations set in place for improving process operations, process safety and environmental protection offer limitless opportunities from fundamental research to applied research for sustainable chemical production. Despite the development of novel technologies and processes for the efficient and safer production of chemicals and the move towards inherently safe materials, accidental releases of dangerous toxic/ flammable gases still represent a serious concern in the process industries. Even if spray curtains have been applied since the 80', further methodological development is required to make the results directly applicable to the current industry needs in many emerging applications. In this regard, recent studies were carried to assess the effectiveness of water curtains in LNG vapor cloud dispersion and clarify the main controlling phenomena involved during vapor and water curtain interaction [1]. A further noteworthy example with reacting curtains relates to recent experimental studies focused on ammonia release mitigation by small-sized water curtain, in which the additives involved were surfactants and three organic acids, i.e. citric acid, malic acid and acetic acid [2]. In this paper, we present the results obtained during a long-term program, aiming at developing a fundamental model and set-up comprehensive design guidelines for reacting spray curtains, addressing environmental protection by mitigating hazardous gaseous releases.

### 2. Methods

A rather general model is developed for the absorption of a toxic gaseous component into reacting or non-reacting solutions. The particular case of chlorine abatement is then considered, both as an example of application of the absorption model and to the end of subsequent validation of the model itself.

Based on a large number of experiments on chlorine releases in a laboratory-scale wind tunnel, we developed a unified mathematical model suitable to be adopted as a real-scale design tool of a barrier accounting for both still air and windy conditions. The mathematical representation of the system, based on a careful analysis of the main aspects and of the reciprocal correlations of the single subsystem, required the development and the assembling of some specific sub-models, i.e.:

- a fluid-dynamic model, describing the rate of air entrainment and the flow-field either in still air, or windy conditions;
- an absorption model, for evaluating the spray absorption efficiency, assuming instantaneous and non reversible reaction [3];
- a mixing-dispersion model, predicting the overall efficiency of the barrier in release mitigation.

The physical model represented in Fig. 1 allowed considering both the cases of still air and windy conditions, a fraction of the chlorine escaping downwind the curtain is recycled to the curtain itself, while the remaining one is dispersed into the external environment. The whole system can be considered as a recycle absorber

characterized by an intrinsic absorption efficiency of the curtain,  $X_c$ , and an overall absorption efficiency of the safety device in chlorine abatement,  $\eta$ .

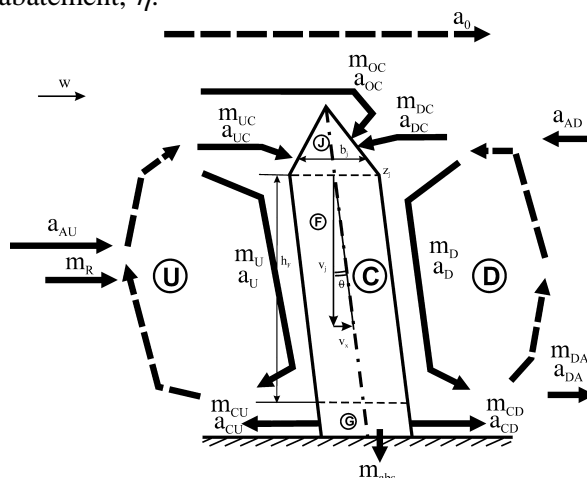


Figure 1. Physical model of the reacting spray curtains.

The overall experimental design includes:

- preliminary runs, carried out to select a curtain of adequate capability of containment and air entrainment;
- fluid-dynamic runs, aimed the characterization of the air entrainment as a function of the curtain characteristics and of the operative conditions;
- absorption runs, for determining the efficiency of the safety device in abatement and dilution of the gaseous release.

### 3. Results and discussion

A fairly good agreement was verified between model results and wind tunnel experimental data obtained simulating a chlorine release mitigated by a liquid spray curtain. The goodness of fit between experimental and calculated values for physical absorption in water corresponded to an overall correlation coefficient equal to 0.83, while the correlation coefficient considering absorption with conversion in alkaline solution corresponded to 0.79. The major contribution of this work is a unified analytical description of the curtain behavior both a unified analytical description of the curtain behavior under both still and windy conditions and the attainment of constraints for optimal design. The proposed model comprehensively describes the complex system of transport and reaction, providing a direct input to the design of chemical spray curtain for chlorine abatement. Additionally, the framework can be extended to releases of other hazardous gaseous releases, provided that proper modifications on the absorption and reaction kinetics be taken into account.

### 4. Conclusions

We developed a unified mathematical model suitable to be adopted as a real-scale design tool of a barrier accounting for both still air and windy conditions. The model was validated by a large number of experiments on chlorine releases in a laboratory-scale wind tunnel. The developed methodology can be applied to complex situations allowing the attainment of a more generalized approach for the design of a curtain, once given the release parameters, the site layout and the vulnerable target specifications.

### References

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### Keywords

Environmental protection; hazardous release; reacting film; spray absorption efficiency.