Modelling the occupational exposure of workers to certain hazardous chemicals

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Abstract. Hazardous substances are considered to be liquids, gases or solids which are of risk for the health and safety of workers and they may be found in almost all workplaces, including in SME's. Hazardous substances include chemical agents, but also biological ones, such as bacteria, viruses, mould etc. Most chemicals used in the industry present risk for the workers, depending on their physico-chemical properties. Directive 2012/18/EU is the legal act which regulates the chemical substances field within the Member States, regulation dealing with the control of hazards involving dangerous substances which may lead to major accidents. In Romania, Law 59 dated April 2016 on controlling the hazard of major accidents caused by hazardous substances evaluates “hazardous chemicals”, describing the risk for people and regulating concentrations of such substances. By using the commercially available Phast consequence modelling package, within this study were modelled leaks of several chemical substances used in the industry, in order to estimate their hazardous influence extent. The current article is a significant work on modelling of discharge and atmospheric dispersion of hazardous substances using state-of-the-art consequence modelling software. Emergency Response Planning Guidelines (ERPG) are used as reference exposure levels within the present study. Output data of computational modelling are significantly influenced by input parameters. In this regard, the effects of the latter for ensuring robustness of the simulation and for identifying improvements have proven to be necessary.

1 Introduction

In the industrial field, there are used many chemicals which present various risks depending on and whose physical-chemical properties may change drastically with

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concentration [1, 2, 3]. Such chemicals can be used in industrial processes as solutions with water.

In Romania, Law 59 dated April 2016 on controlling the hazard of major accidents caused by hazardous substances evaluates “hazardous chemicals”, describing the risk for people and regulating concentrations of such substances [4, 5]. In order to be prepared for possible accidents, it is a common practice nowadays to develop computational analyses regarding the potential damage extent in case of accidents [6-10].

Chemical substances used in the manufacturing sector must be controlled at national level as there are risks associated with chemical substances in the raw materials themselves [11-15]. The differences in regulated concentration of chemical substances between countries suggest a serious issue. Countries with low chemical regulatory concentrations may be over-regulated. On the other hand, countries with high levels of chemical regulations can not manage low concentration chemicals, so chemical accidents can occur at low concentrations.

This study used PHAST 8.22. modelling program to measure values according to the toxic concentration Emergency Response Planning Guideline (ERPG-1, ERPG-2 and ERPG-3), in case of unexpected leaks of a tank located within an industrial facility and which contains such chemicals [15, 16, 17].

2 Chemical substances involved

Within the study are selected chemical substances that are used in many industries, that have almost identical physical and chemical properties and which are being used in various industrial processes: hydrogen chloride, hydrogen fluoride, and hydrogen peroxide, for which the basic chemical and physical properties are presented in Table 1.

Table 1. Physical/chemical properties of analysed substances

Property	Hydrogen chloride	Hydrogen fluoride	Hydrogen peroxide
Chemical Abstracts Service (CAS) number	7647-01-0	7644-39-3	7722-84-1
Formula	HCl	HF	H ₂ O ₂
Molecular weight	36.4606	20.0063	34.0147
Melting point (deg C)	-114.18	-83.36	-0.425
Normal boiling point (deg C)	-85	19.52	150.2
Vapour density (g/L)	1.268 (25 deg c)	0.92 (0 deg C)	1.17 (25 deg C)
Vapour pressure (mmHg)	31,652 (20 deg C)	917 (25 deg C)	1.97 (25 deg C)
Odour	Foul smelling	Strong, irritating	No odour or weak odour
Colour	Colourless liquid/gas	Colourless liquid/gas	Colourless liquid
Purpose	Production, vinyl chloride polymer	Manufacturing disinfectants, refrigerants, cleaners etc.	Disinfectant, bleach, detergent, oxidizing agent

2.1 Concentration

Concentration level recommendations and guidelines are used for determining whether individuals in an emergency response scenario will be impacted by their proximity to certain hazardous chemicals. Emergency Response Planning Guidelines – ERPG are the best known and most commonly measures used worldwide [18].

For the substances to which they are applicable, these criteria use a three-category system to rate exposure values; individual ratings are unique to each chemical dose, but the three categories are identical.

A compound may have up to three ERPG levels, each leading to a different level of health effects. The three ERPG tiers are defined as follows: a level 1 value indicates temporary damage, a level 2 value indicates failure or serious health effects, and a level 3 value indicates life-threatening effects.

- ERPG-1 specifies the total airborne level at which almost all individuals could be exposed for up to one hour without experiencing more than mild, intermittent adverse health effects or without perceiving a clearly defined adverse odor.
- ERPG-2 specifies the total airborne levels to which individuals may be exposed for up to one hour without permanent or other serious health effects or symptoms.
- ERPG-3 is the peak airborne concentration at which almost all people could be exposed for up to 1 hour without life-threatening health effects [18].

3 Accident modelling

Based on each material in the modelling, the hazardous distances downwind for two leaks differing in diameter are determined, ERPG-1, 2 and 3 levels of toxic concentrations being set as endpoints, taking into account that all substances were released under the same operating conditions. Saturation vapour pressure varies for each concentration, given both leakage exist under the same conditions; concentration and saturation vapour pressure can therefore be adjusted in a simulation system. Phast software uses for modelling the Gaussian atmospheric diffusion which is used widely for assessing the environmental impact in case of accidental releases of hazardous substances. In the paper, for modelling purposes, there has been assumed a constant leak rate and also that no chemical reaction occurs during the leak. This characteristic is consistent with the theory of modelling assuming that due to the vapour pressure, the chemical forms a pool and continually evaporates and diffuses. The release direction has been assumed to be horizontal.

3.1 Input parameters

3.1.1 Weather

- Ambient temperature: 20° C
- Atmospheric humidity: 70 %
- Wind speed: 1.5 m/
- Pasquil stability class: D - Neutral conditions
- Solar Radiation: 0.5 kW/m²

3.1.2 Endpoint concentration

The present study calculated the hazardous distances downwind for each chemical substance by setting the ERPG-1, 2 and 3 endpoint concentrations as the concentrations of interest, as presented in Table 2:

Table 2. Endpoint concentrations

ERPG Levels	Hydrogen chloride	Hydrogen fluoride	Hydrogen peroxide
ERPG-1	3 ppm	2 ppm	10 ppm
ERPG-2	20 ppm	20 ppm	50 ppm
ERPG-3	150 ppm	50 ppm	100 ppm

3.1.3 Scenario

The three chemicals in liquid form involved where assumed to leak from a tank, through a 10 mm and a 100 mm leak, at atmospheric temperature and pressure. The leaking tank has been assumed to contain 3000 kg of chemical substance.

For measuring the ERPG-2 level concentrations have been selected three distances of interest: 50 m, 100 m, and 250 m.

3.2 Results obtained

The distances downwind to the concentrations of interest calculated under the same conditions for each of the three chemical substances are presented in Table 3. For the three distances of interest, results of concentrations are presented in Table 4.

Table 3. Distance downwind to defined concentrations

Chemical substance	Scenario	Concentration of interest	Distance downwind to concentration of interest [m]
Hydrogen chloride	10 mm leak	20 ppm	475.042
	100 mm leak		4207.76
Hydrogen fluoride	10 mm leak	20 ppm	580.597
	100 mm leak		2440.58
Hydrogen peroxide	10 mm leak	50 ppm	30.6874
	100 mm leak		26.8138

Table 4. Concentrations at defined distances of interest downwind

Chemical substance	Scenario	Distance of Interest	Concentration at distance of interest [ppm]
HCL	10 mm leak	50 m	3023.89
HF			2902.45
H2O2			62.521
HCL	100 mm leak		166176
HF			15491.3
H2O2			65.9066
HCL	10 mm leak	100 m	665.973
HF			960.301
H2O2			18.3037
HCL	100 mm leak		43634.7
HF			170703
H2O2			30.4744
HCL	10 mm leak	250 m	155.183
HF			232.439
H2O2			0
HCL	100 mm leak		6414.03
HF			27373.5
H2O2			0

Table 5. Distance downwind to ERPG Levels

Chemical substance / Scenario	Distance downwind to ERPG-1 [m]	Distance downwind to ERPG-2 [m]	Distance downwind to ERPG-3 [m]
HCl 10 mm leak	1534	475.474	131.778
HCl 100 mm leak	10168.9	4281.58	1749.16
HF 10 mm leak	2189.25	581.483	338.717
HF 100 mm leak	8869.76	2463.66	1562
H ₂ O ₂ 10 mm leak	77.8441	30.7122	21.2185
H ₂ O ₂ 100 mm leak	105.419	26.8337	19.5642

Fig. 1. Toxic gas cloud – Side view

Fig. 2. Maxim Concentration vs Distance

Fig. 3. Dispersion Cloud maximum footprint for 10 ppm effect zone

Figures 1, 2 and 3 present the dispersed cloud and maximum concentrations of hydrogen chloride, hydrogen fluoride and hydrogen peroxide with the distance downwind from the possible leak.

4 Conclusions and final remarks

Modelling programs existing nowadays are widely used for taking precautions and preventive measures against chemical accidents which may have unwanted consequences upon the workers and surrounding environment. However, the results of the predicted models may be different from the ones which can be generated by such accidents, thus the limitation of the computational modelling. Anyway, if additional results from real-life experiments cannot be obtained for comparing the values obtained by modelling, such preventive works are trustful since the mathematical models which are implement within commercially available software are validated.

The paper presented the distances for representative ERPG-2 concentrations, distances obtained for representative scenarios of chemical accidents involved by widely used chemicals: hydrogen chloride, hydrogen fluoride and hydrogen peroxide. Graphs presented in the paper can be used for emergency plans residing in the fast evacuation of workers in case of accidental releases of one of the three substances analysed.

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