# Risk area estimation and consequence based analysis using 3D terrain modeling

## Case study:
## -an accidental phosgene release scenario near Râmnicu-Vâlcea, Romania-

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## Abstract

Risk area estimations are an important tool for the authorities responsible with intervention in case of a major chemical accident, aiding in their Emergency Response Plans by providing accurate and detailed information on the site, weather conditions, hazardous chemicals involved, and their dispersion patterns. By using SEVEX View, a complex three dimensional dispersion model can be developed, and its effects analyzed and compared in detail.

Phosgene is one of these toxic substances, and has severe effects on human health and the environment. Our project describes a “worst-case scenario” type release of phosgene and analyses its consequences by looking at the number of persons affected.

A more relevant overview of the effects of such an accident will be possible by correlating the dispersion patterns with demographical data collected from the Râmnicu-Vâlcea area.

**Keywords:** risk areas, phosgene, SEVEX View, consequence based analysis

## Introduction

Phosgene ($Cl_2CO$) gained its notoriety in World War I as a chemical weapon, it’s currently used as a chemical reagent and is a basic component in organic synthesis.

Industrially, phosgene is produced by passing chlorine gas and purified carbon monoxide through a bed of porous activated carbon, which serves as a catalyst. The equation is described as follows:

$$CO + Cl_2 \rightarrow COCl_2 \ \Delta H_{rxn} = -107.6 kJ/mol$$

Phosgene is corrosive to exposed tissues; inhalation of vapors may result in pulmonary edema and chemical pneumonia. Nonflammable, but on contact with moisture reacts violently and decomposes to toxic compounds, including chlorine.(Wikipedia, 2009)

Phosgene is 4 times denser than air, therefore it tends to remain close to the ground and to collect in low areas.

Although due to its high toxicity, storage is very strictly controlled, usually in confined areas with ventilation towards a neutralization system. In spite of these safety measures accidents do occur, for example a phosgene-containing pipe rupture on September 8, 1994, in Yeochon, Korea, resulted in multiple injuries and 3 deaths.(CRRNE, Lung-Damaging Agents, Phosgene, 2009)

Usually, are considered to be strategic objectives in case of war or terrorist attacks the facilities which store and process highly dangerous substances.

## Implementing Seveso III in Romania

Romania, as a recent member of the European Union has specific goals to achieve in order to meet the EU standards. A major goal is represented by the environmental and industrial sector's ability to achieve specific standards.

A major guideline is represented by the Seveso Directive. The Directive's scope was both broadened and simplified. It is applicable to any establishment where dangerous substances are present or likely to be produced as a result of an accident, in quantities equal to or in excess of the quantities listed in the Annex. The list of named substances in the Annex was reduced from 180 to 50, but is accompanied by a list of categories of substances, which in practice broadens the scope.

Directive 2003/105/EC (Seveso III) extended the scope and applicability of the Seveso II Directive to cover the processing and storage of minerals containing dangerous substances. For establishments which subsequently fall within the scope of Directive 96/82/EC, it has been shown necessary in Sveso III to introduce minimum periods for notifications and the establishment of major accident prevention policies, safety reports and emergency plans. (SCAD Plus, Major Accidents involving Dangerous Substances, 2009)

This approach also facilitates the public's access to information, and gives the public a more important role in the decision-making process. The operator and the authorities must actively raise awareness regarding potential hazards concerning the site and surroundings through campaigns and similar dissemination methods. Romania has a total of 281 Seveso facilities.(Ozunu and Anghel, 2007)

Therefore reliable data must be obtained in order to evaluate the risk factor with high accuracy. The method presented is through a simulation of a phosgene release and dispersion.

Our site meets the qualifying phosgene quantities required in art.6, art.7 (0.3 tons) and art.9 (0.75 tons) of the Seveso Directive, therefore is considered to be a Seveso objective. (SCAD Plus, Major Accidents involving Dangerous Substances, 2009)

## Consequence based risk analysis

Generally, risk assessment methods begin with the identification
of hazards and vulnerabilities, frequency and consequence analysis of each of these vulnerabilities and hazards. Consequence based risk analysis has an approach that starts with the identification of the major consequences by analyzing the potential accident scenarios and the effects of the accidents upon the environment, human factor and structures. The process then searches for combinations of hazard and vulnerability that could result in the most serious consequences.(TNO „Purple Book, 1999)

The advantage of the consequence based risk analysis is that it will show how qualitative threat, vulnerability and consequence information can be combined to derive a qualitative value for risk and offer an easy-to-understand graphical way to present risk assessment results. (American Institute of Chemical Engineers, 1989)

## Simulation

The model used in the simulation of the chemical accident with phosgene release and dispersion is the SEVEX (SEVeso EXpert) complex 3D terrain dispersion model.

In SEVEX are included three modules:

The *SEVEX-Meso* is a complex 3D terrain and meteorological model which solves the Navier-Stokes equations, considering the terrain roughness (the topography of the terrain), the land use of the terrain (five categories: water, forest, urban, grass-land and the mixture of the previous four) and the solar radiation and heat transfer between the ground and the atmosphere.

The *SEVEX-Toxic* module is a Lagrangian 3D dispersion model that simulates the passive transport and dispersion of toxic and flammable material.

The *SEVEX-Source* module simulates different types of releases, effects and consequences of accidents. (ATM PRO, 2009)

These three modules combined in SEVEX View software compute the worst-case realistic conditions of an accident. SEVEX View is the only software that considers both the SEVESO directives of the European Commission, and U.S. EPA guidelines. The software was built to simulate major industrial accidents, so the model is designed for impact zones from 1 to 18 km.(Ozunu et al, 2007)

## Case study

The site is located at a height of 150 m above sea level, at 10 km from the city of Ramnicu-Valcea on the right bank of the Olt River on a alluvial terrace 7 meters above Govora Lake. The facility is 2 km long and 1,5 wide, covering 2.143.852,3 $m^2$, with buildings covering 645.573,8 $m^2$.

The site is surrounded by hills with a maximum altitude of 450 m, and the mean absolute altitude is 150 m.

With the building of the dams on the Olt valley, the surface covered by water increased, resulting in an increase of the relative humidity in the site's area, with a mean of 76%. The total anual precipitation in the area is 710,5 mm.

The wind circulation, both direction and speed, are influenced by the area's landscape. The Olt Valley has an obvious funneling effect, the highest wind frequencies occuring from the north(10,2%) and south(13%). The atmospheric calm situation has the highest occurace rate(37,4%). The mean wind speed varies between 0.8 and 2 m/s. On the predominant wind direction we find Lake Govora and Stolniceni and Stupărei villages. The dominant atmospheric stability conditions are class D (neutral), E (slightly stable) and F (stable).

## Technical specifications:

The storage vessel has the following technical characteristics: length, L = 6 m, diameter d = 2.6 m, maximum capacity of storage equal to 37.64 tons of phosgene at $20^{o}$C storage temperature, 85% filling level and at 3 bar service pressure. The storage tank is located underground, in an enclosed concrete room with ventilation leading to neutralization system.

We have two possible release scenarios:

The first release scenario takes into consideration catastrophic rupture of the storage vessel, followed by the release of the entire quantity of liquefied phosgene.

The second scenario consists in a 10 minute continuous release of phosgene with a transient release of 0.9 tons of phosgene from a ruptured pipe.

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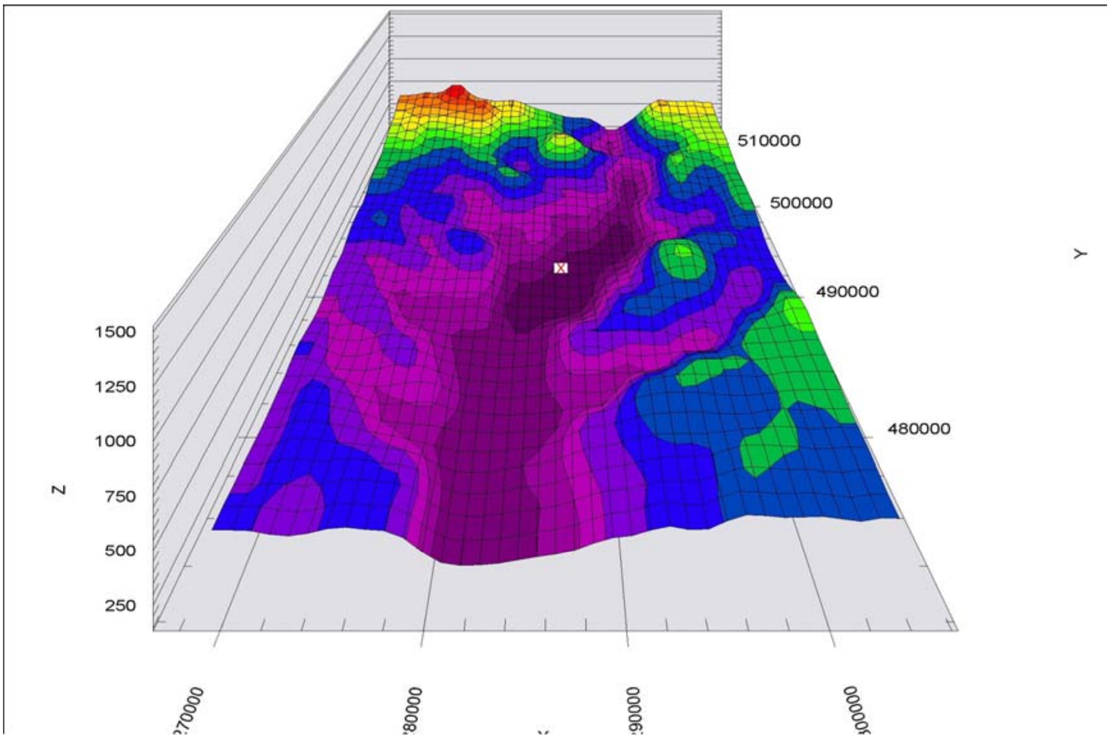


Fig. 1
37x37 km 3D representation of the area

**Results and discussions**

Simulations of the accident were performed considering the meteorological "worst case scenarios" for the two types of release, for daytime (complete cloud cover, a 70% relative humidity, stability class D, a ground temperature of 19$^{o}$C was calculated, air temperature of 20$^{o}$C) and for nighttime (no cloud cover, a 90% relative humidity, stability class F, a calculated ground temperature of 10.13$^{o}$C, air temperature of 10$^{o}$C). Two worst case scenarios were chosen, each with a specific set of meteorological data, because the vulnerability of the population potentially affected varies from day to night.

In all simulation cases a map with 37 km x 37 km area was used. The simulation considers the complex topography and the land use of the terrain, calculating the wind direction and velocity for every 1 km x 1 km square.

The wind speeds for 36 directions were computed, in every 10$^{o}$, from 0$^{o}$ to 350$^{o}$. For this reason, the overall area of danger is estimated based on a discrete set of result, so called plume fingers.

Three different concentration levels were selected, 17 ppm for $LC_{50}$ (lethal concentration 50 % kill) dangerous concentration indoor (evacuation of population is necessary), 5 ppm for IDLH (immediately dangerous for life and health) and 0.2 ppm causing temporary affections (avoiding exposure is advised).

The graphical representations show the concentration levels indicated above, which could occur during 60 minutes in low wind condition calculated using a 2 m/s synoptic wind. The maps don't represent exposure time and toxic dose. These concentration levels (17 ppm, 5 ppm, 0.2 ppm) were chosen in order to separate different emergency actions (evacuation, self-confinement, avoiding exposure), that need to be implemented for each type of health effect.(NIOSH, 2009)

The meteorological simulation results regarding the wind directions are confirmed by the local measured data (see Fig 2-9).

## Catastrophic release of phosgene

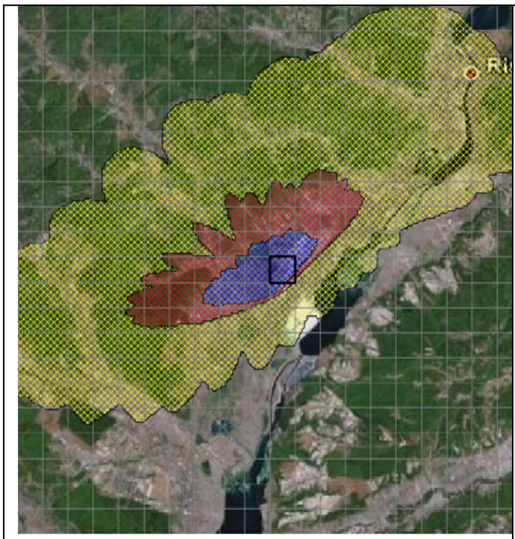


Fig. 2

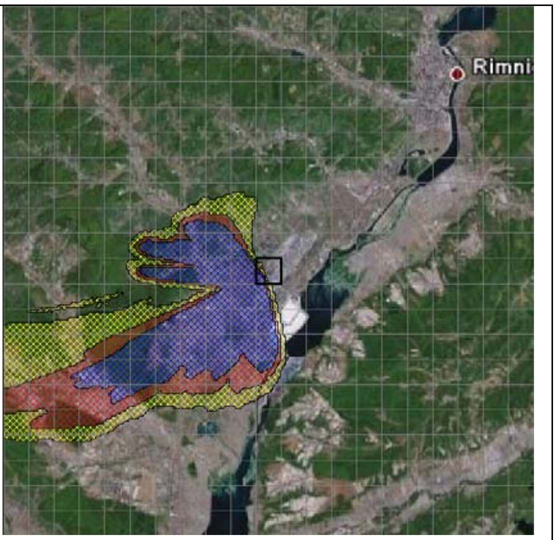


Fig. 3

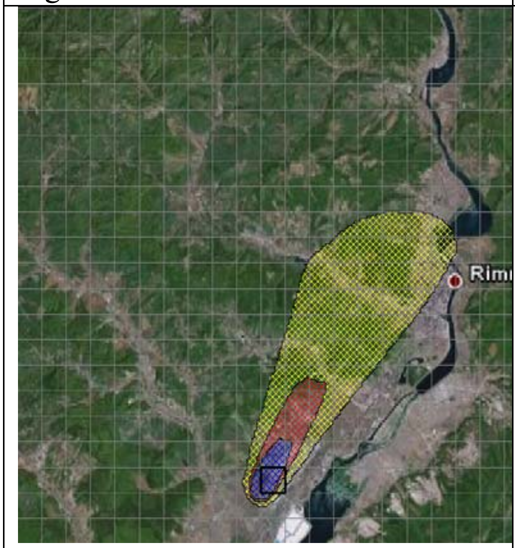


Fig. 4

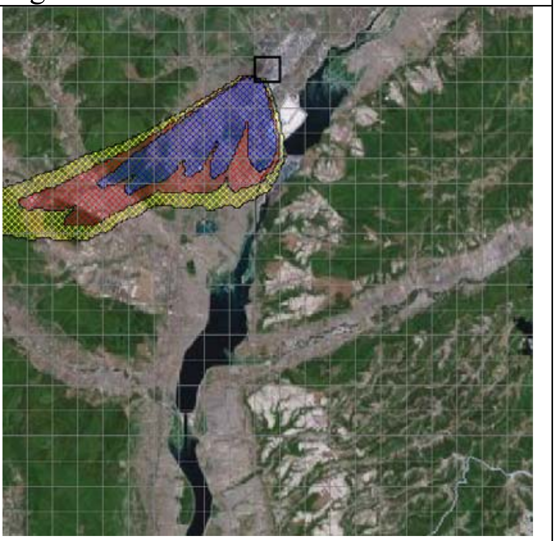


Fig. 5

**Fig. 2 - Low wind daytime dispersion**
**Fig. 3 - Low wind nighttime dispersion**
**Fig. 4 - 2 m/s synoptic wind from S, daytime**
**Fig. 5 - 2 m/s synoptic wind from N, nighttime**

| Risk | | Orders | Criteria |
|---|---|---|---|
| None | | No change in behaviour | C < 0.2 ppm |
| Temporary diseases<br>Superficial injuries | 🟨 | Avoiding exposure advised | 0.2 < C < 5.0 ppm |
| Permanent injuries out door | 🟥 | Self-confinement exclusion | 5.0 < C < 17.0 ppm |
| Danger indoor | 🟦 | Evacuation | 17.0 < C ppm |

## 10 min transient release of phosgene

Fig. 6

Fig. 7

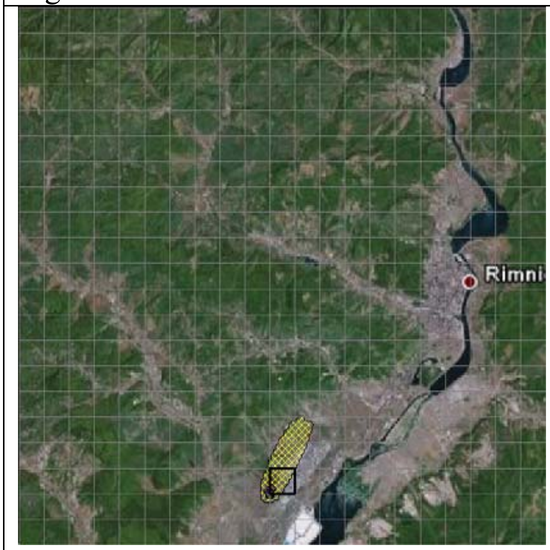


Fig. 8

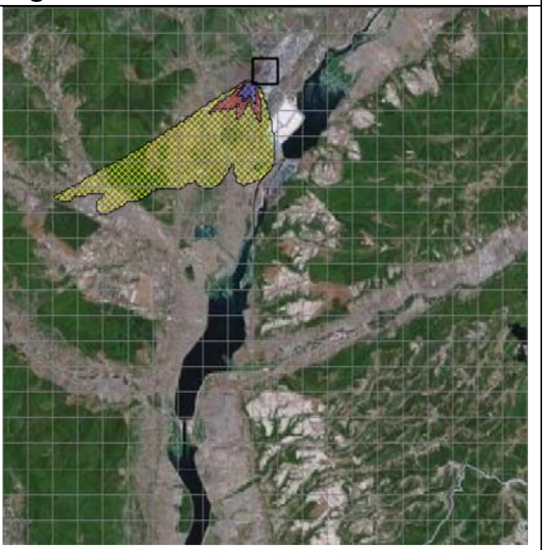
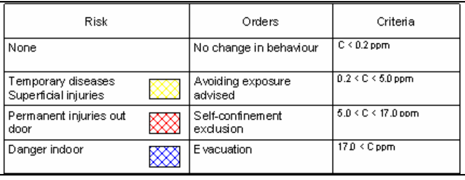


Fig. 9

**Fig. 6 - Low wind daytime dispersion**
**Fig. 7 - Low wind nighttime dispersion**
**Fig. 8 - 2 m/s synoptic wind from S, daytime**
**Fig. 9- 2 m/s synoptic wind from N, nighttime**



| Risk | | Orders | Criteria |
|---|---|---|---|
| None | | No change in behaviour | C < 0.2 ppm |
| Temporary diseases<br>Superficial injuries | 🟨 | Avoiding exposure advised | 0.2 < C < 5.0 ppm |
| Permanent injuries out door | 🟥 | Self-confinement exclusion | 5.0 < C < 17.0 ppm |
| Danger indoor | 🟦 | E vacuation | 17.0 < C ppm |

The daytime simulation for catastrophic release (Fig. 2) shows that the villages of Negreni and Buleta will be the most affected, being covered by the high concentration cloud with concentrations exceeding 17 ppm($LC_{50}$). The second danger zone corresponds to concentration levels between 5ppm (IDLH) and 17ppm ($LC_{50}$), covering Govora, Barsesti, Vulpesti, Scarisoara villages with a total population of 6297 inhabitants and also reaches Ocnele Mari city with a population of 3.578 inhabitants. The third concentration zone with concentrations under 5 ppm covers a large area reaching Ramnicu-Valcea with a population of 120.363 inhabitants. (Casa de Asigurari de Sanatate Valcea, Populatie, 2009)

In the nighttime simulation for catastrophic release (Fig.3) the high concentration cloud covers a much larger area and develops to the west and south-west affecting Negreni, Buleta, Mihaesti, Arsanca, Magura, Rugetu, Viisoara, Cosani with a total population exceeding 10 000 inhabitatns. The danger zone corresponding to the second concentration level covers Capu Dealului, Tatarani, Munteni, Manailesti, Firijaba. The zone with concentrations under 5 ppm is considerably smaller than in daytime conditions. Due to the fact that the high concentration area covers a much larger area, the nighttime scenario is considerably more dangerous. (Casa de Asigurari de Sanatate Valcea, Populatie, 2009)

Considering the 10 min transient release scenario, the only potentially dangerous situation for the surrounding population might occur during low wind conditions at nighttime(Fig. 7). The other three scenarios (Fig. 6, Fig. 8, Fig. 9), only poses danger to the workers inside the facility's boundaries.

Regarding the fact that the most common meteorological conditions present in the area, involve a 2m/s wind from the north at nighttime and from south at daytime, simulations representing these situations were also taken into consideration. The most dangerous situation is catastrophic release under these conditions (Fig. 5).

## Conclusions

The SEVEX concept is to represent the danger zones where these concentrations might occur during the dispersion period, therefore the exposure time is not so relevant, the focus should be on the dangerous concentration levels that might occur in a "worst case scenario" situation.

Using 3D topographic, land use and meteorological data together, the SEVEX software computes individual wind speeds in each 1x1 km square of the 37x37 km map, giving more accurate wind direction for the dispersion simulation. This way the potentially affected area is significantly reduced, and the accuracy of the model increases. In most cases of the 2D modeling without taking topography into consideration the affected areas of the plumes are overestimated. This doesn't reduce the consequences directly, the purpose is to increase the accuracy of the estimated area, and provide better quality data for the emergency response efforts, in order for them to better concentrate their resources.

The simulations show that the situation could become extremely dangerous to the nearby inhabitants, therefore an efficient external emergency plan must be developed and according o the Seveso III Directive, the population should be informed about the hazards involved, emergency individual and collective measures, warning and evacuation plans.

In order to achieve this, high quality data is required, following the principle: "good quality data leads to good decisions". With the use of high performance software like SEVEX, we can aid the Romanian stakeholders and decision makers with information they need in order to develop efficient plans and policies.

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