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Modelling of Accidental Impacts of Hazardous Chemical Substances in the Czech Republic

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Abstract

The issue of major chemical accidents in the Czech Republic is first mentioned from a historical point of view. The following are the main hazardous impacts of chemical accidents. The next part is a comparison of the accidental impacts of major emergencies, such as toxic leakage, explosion and fire, even with examples of several typical chemical substances. Some factors of the main hazardous chemicals with a focus on toxic substances are discussed in detail. The modelling of accident impacts is presented in the next section on a detailed comparison of the accident impacts of nine main industrial chemical toxicants. The article also draws attention to the serious danger of the possible misuse of toxic substances in particular for hostile acts of chemical terrorism

KEY WORDS: *accidents, major accidents, major chemical accidents, hazardous chemicals and mixtures, accident impact modelling*

1. Introduction

From the point of view of history, it is interesting that the Czech Republic has a long and rich history both in the prevention of serious chemical accidents and in modeling their consequences. As early as 1981, the binding nationwide aid CO-51-5 [1] was issued, which included both prevention and the basics of modelling the impacts of the basic twelve hazardous industrial chemicals, but also contained guidelines and clear instructions for creating an internal emergency plan.

With progress in meeting the growing needs of humanity, industrial activity also brings a number of negative manifestations and impacts. One of them is the possibility of a major accident, which may be associated with the release of hazardous chemicals of toxic, flammable or explosive nature. In addition, hazardous chemicals and mixtures may have other significant hazardous properties, as discussed in more detail below.

A number of major chemical accidents have been known in history, which have had all sorts of negative effects on people's lives and health, the environment and property. It is indisputable that major chemical accidents will continue in the future. European and Czech legislation, together with a system of various state and branch technical standards, organizational and technical safety measures, seeks to prevent their occurrence, or to minimize their dangerous accidental impacts in the event of major chemical accidents.

Major chemical accidents and their impacts have been gradually published in the Czech professional literature [2-7], or Czech translations of important works, such as the valuable OECD professional publication [8].

2. Major Chemical Accidents and Their Impacts

Industrial sources of risk - especially hazardous chemicals and chemical mixtures - are very easily exploited by terrorists. The offender only needs to know how to cause, for example, the leakage of a dangerous substance into the vicinity of the source of the risk, or how to "effectively" damage it and thus initiate a major chemical accident. There are a large number of industrial sources of risk that are easily exploited in industrialized countries and, in addition, they are often located close to human settlements, or directly in towns, villages and settlements.

Extraordinary events (accidents and incidents, major accidents) in the chemical industry and traffic accidents

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associated with the leakage, explosion or fire of hazardous chemicals have their own specifics. It is therefore important to study the records of these cases in order to anticipate their occurrence and to establish, adopt and implement a number of preventive measures. We most often encounter fires, followed by explosions and outbursts of toxic gases, vapors or aerosols. An overview of the types, probabilities and impacts of these adverse events is given in Table 1.

Table 1.

Scheme of chemical accidents in terms of probability of occurrence and impacts

Type of chemical accident	Probability of an accident	Deadly danger to persons	Economic potential of losses
fire	high	small	medium
explosion	medium	medium	high
release of toxic gases	small	high	small

If we rank these accidents according to the number of fatalities, then the order is exactly the opposite, because the toxicity of gaseous effluents is the greatest fatal danger. This fact will be further documented in detail on specific examples.

Economic losses are correspondingly higher for accidents in which an explosion occurs. The worst types of explosions are Unconfined Vapor Cloud Explosion (UVCE). A large cloud of volatile and flammable vapors is released from the plant and dispersed across the plant or outside. Subsequent initiation will cause an explosion.

Chemical facilities, equipment, plants, technologies and warehouses are relatively safe because many are very well secured. On the other hand, it is necessary to take into account that there is a high and dangerous accumulated energy and toxic potential, which can, with a certain combination of different factors, cause an accident with catastrophic consequences.

Many hazardous chemicals have various accidental impacts, which are mainly caused by the toxicity, explosiveness and flammability of hazardous chemicals and mixtures. Accidental effects have a significant impact not only on humans, but also on livestock and other animals, or they can cause serious destruction or damage to property or the environment. In addition, the impacts can also be political, social, economic, international, etc. Finally, emergency impacts can also have an adverse effect on the functionality of a company's critical infrastructure.

However, hazardous chemicals and mixtures can have a number of other hazardous properties; may be explosive, oxidising, extremely flammable, highly flammable, highly toxic, toxic, explosive, harmful, corrosive, irritating, sensitizing, carcinogenic, mutagenic, toxic for reproduction, dangerous for the environment. Some hazardous chemicals and mixtures can also react violently with water or release toxic gas on contact with water.

Below is a simple and clear table (Table 2) on the possible accident impacts of major chemical accidents. It is quite clear from this that in terms of endangering people, it is toxic (toxic) dangerous chemicals and mixtures that are the most dangerous. As a model, the basic data are given in the following illustrative table for three widespread and hazardous chemicals - toxic: chlorine; explosive: propane-butane; flammable substance: motor gasoline.

Table 2.

Basic comparison of the impacts of some major accident impacts

Hazard-ous chem-ical	Accident	Description of a possible emergency	The main accident impact	Amount of substance [t]	Impact of the emergency impact in terms of the risk of personal injury [m]
liquefied chlorine	escape	one-time leakage of equipment contents, or immediate leakage of contents	poison	10 50 100	4 330 7 070 9 280
liquefied propane - butane	explosion	one-time leakage of boiling liquid with rapid evaporation into the cloud	pressure wave, debris fragments spread (explosiveness)	10 50 100	570 1 000 1 280
motor gasoline	**fire**	endangerment of the tank by a flat fire	**thermal radiation (combustibility)**	**10** 50 100	**80** 190 270

While the effect of thermal radiation from fires or pressure waves (or debris fragments) after the explosion is spatially limited to a range of tens to hundreds of meters, in the event of a toxic leak can be expected both fatal and injuring impacts on people, fauna and flora in the order hundreds of meters or even several kilometers. It depends on many factors, the main ones being the type, amount and physical form of the leaked hazardous toxic substance, the mode of escape and the local weather situation. Dangerous chemical industrial toxic substances are considered to be the most dangerous because their toxicity can cause considerable mortality or even serious health damage, especially to people or animals, or the environment.

The molecular weight of a selected hazardous chemical industrial toxicant can also be of great importance. Air has a molecular weight of 29 and toxic gases can be divided into heavy and light.

Heavy gases, listed below, which are heavier as the surrounding air behaves by "flowing" into cellars, depressions, canals and sticking to the surface. From this point of view, these toxic gases are very dangerous. In addition, they can be easily and "advantageously" misused as a means of chemical terrorism. The following substances are the main representatives of heavy toxic gases (their molecular weight is given in parentheses) and the physical state under normal conditions. The following substances are listed in descending order of molecular weight:

- *phosgene COCl2 (98.9) - gas,*
- *carbon disulphide CS2 (76) - volatile liquid,*
- *chlorine Cl2 (71) - gas,*
- *sulfur dioxide SO2 (64) - gas,*
- *methyl isocyanate CH3 NCO (57) - volatile liquid,*
- *hydrogen chloride HCl (36) - gas,*
- *hydrogen phosphide (phosphine) PH3 (34) - gas,*
- *hydrogen sulfide (sulfane) H2S (34) - gas.*

Even in this brief overview, it is clear that phosgene is a poisonous gas, the most dangerous (or best misused for the "needs" of chemical terrorism).

By summarizing the group of dangerous chemical industrial toxic substances, it can be stated that the main danger is the very highly toxic gas phosgene. The conclusion is supported by the following facts:

- *Toxicity of the substance: phosgene is considered to be a gas of very high toxicity.*
- *Molecular weight of the substance: phosgene is one of the heaviest toxic gases due to its molecular weight (98.9).*
- *Achieved results of emergency impact modelling: phosgene is one of the longest of selected hazardous chemical industrial toxic substances.*
- *Historical experience: during the First World War, phosgene caused about 80-85% of the fatal medical losses of the total number of people affected by chemical weapons (this amounted to 73 to 78 thousand in absolute numbers).*

The main representatives of light toxic gases are carbon monoxide CO (30), hydrogen cyanide HCN (27) and ammonia NH3 (17).

The accidental impacts and impacts of light gas leaks are much smaller in terms of their molecular weight and behavior in the ground layer of the atmosphere than in the case of heavy toxic gases. Under no circumstances can these substances be underestimated or even "discarded". In some specific conditions, the dangers of these substances can be very high, eg in enclosed spaces (such as large supermarkets and other spaces).

3. Modelling ff Emergency Impacts of Hazardous Chemical Substances

It is also possible to emphasize that professional publications dealing with hazardous chemicals, prevention and modelling of emergency consequences were also published later. The publication of the General Directorate of the Fire and Rescue Service [9] was particularly useful, as was the expert publication on the toxicological aspects of chemical accidents [10].

In addition to the above, Table 2 clearly shows the need to model (forecast) the various accidental impacts of chemical accidents (or terrorist attacks using dangerous chemicals). The need for modelling of emergency impacts arises from the Act on the Prevention of Major Accidents, because modelling of emergency impacts is required, which will reach "beyond the company" or in the area of the so-called emergency planning zone. From this point of view, the emergency planning zone is the area around the operators where the emergency impacts of major accidents are expected. Emergency impact modelling must be thoroughly performed by the operator himself or a professional entity that is able to perform a high-quality and qualified analysis and risk assessment of hazardous chemicals and chemical mixtures.

Another obligation arising from the same law is the modelling of emergency impacts by administrative authorities. The regional authority has a legal obligation on the basis of prescribed documents from individual operators. The completely irreplaceable role of regional authorities is that they must carefully and thoroughly consider the possibilities of domino effects, on which possible accidental impacts have a fundamental impact.

At present, it is possible to advantageously use modern modelling computer programmes, such as the Czech product ROZEX-Alarm or TerEx, or you can use a freely downloadable SW tool from the USA called ALOHA (Areal Locations of Hazardous Atmospheres). Alternatively, the professional international methodology REPRA can be used.

Due to the practical need to model accident impacts, it is possible to recommend the Czech software tool ROZEX-Alarm/TerEx, which relatively easily models the impacts of major chemical accidents. It includes both hazardous chemical industrial toxic substances and accidents associated with the release of flammable and explosive industrial substances. The mentioned SW tool is easy to use with a pleasant user environment and in addition the provided results can be electronically archived, or they can be printed in the form of an output report.

There are a number of other foreign high quality computer modelling programmes such as: EFFECTS (Netherlands), DAMAGE (Netherlands), PHAST (United Kingdom), SAVE (Netherlands), DOW INDEX MODEL FOR TOXIC (USA), CHARM (USA), DEGADIS (USA), HEGADAS (United Kingdom), DENZ / CRUNCH (United Kingdom), HASTE (USA), SLAB (USA), TRACE (USA), DRIFT (United Kingdom), NBC WARNING (Denmark), NBC ANALYSIS (Denmark), H-PACK (USA). Another programme for possible use is a Danish SW tool called ARGOS [11]. Foreign modelling tools are usually highly sophisticated, but on the other hand very expensive.

In general, programmes for assessing emergency impacts in chemical accidents differ in their accuracy, which is given by the accuracy of dispersion algorithms and their connection to other modules that take into account local weather conditions, the impact of terrain and terrain or demographic characteristics in a given space. The use of these models for practice was made possible mainly by the development of personal computers and their possible connection with other data sources.

The next table (Table 3) shows the values of the results of modelling the accidental impacts of selected toxic substances in order to make clear how different data the individual substances show.

Evaluated as a one-time leakage of device content or an immediate leakage of content. Fluid temperature in device 20 C. Total amount of leaked substance: see table 3. Wind speed in the ground layer of the atmosphere 1 m / s. Atmospheric stability type: inversion. Surface type in the direction of material propagation: industrial area. Personal exposure to toxic substances: see table 3.

Table 3.

Comparison of the accidental impacts of some major toxic substances for a "unit quantity" of 10 tonnes for each substance

Hazardous chemical industrial toxic substanbces	**Chemical formula**	**Classification of hazardous chemical industrial toxic substances**	**Danger of persons with toxic contcentration [m]**
Phosgene	$COCl_2$	Gas with particularly high toxicity	5 800
Hydrogen phosphine (phosphine)	PH_3	Gas with particularly high toxicity	6 250
Methyl isocyanate	CH_3NCO	Liquid / gas with particularly high toxicity	7 170
Chlorine	Cl_2	Highly toxic gas	4 330
Hydrogen chloride	HCl	Highly toxic gas	4 060
Hydrogen sulfide (sulfane)	H_2S	Highly toxic gas	1 750
Hydrogen cyanide	HCN	Highly toxic liquid / gas	6 890
Ammonia	NH_3	Medium toxic gas	1 920
Sulfur dioxide	SO_2	Medium toxic gas	3 400

The classification of hazardous chemical toxic substances is given in this table according to the methodology of the International Atomic Energy Agency in Vienna, TECDOC-727 (1996) [12]. The presented literary source represents a highly prestigious professional document, prepared by an international team of UN experts.

4. Sub-Limit Sources or Risk in the Czech Republic

Until 2017, it was not at all clear how to approach dangerous objects that are not included in category A or B according to the Act on the Prevention of Major Accidents. Individual regions or cities approached this completely differently, which was influenced by a number of factors. The effort to unify the approach to the registration of sub-limit sources of risk was only the issuance of the Instruction of the General Director of the Fire and Rescue Service of the Czech Republic No. 35/2017 (instruction). [*full name: Instruction of the General Director of the Fire and Rescue Service of the Czech Republic No. 35/2017 of 14 September 2017, which sets out the minimum requirements for assessing the risk of a major accident and processing documentation for a specified hazard zone of a building with below-limit amount of hazardous substance*]

The professional instruction itself is quite detailed and contains, including appendices (samples), a total of 17 pages of professional text. As expected, this guideline covers the following hazardous chemicals and their limit weight:

- Anhydrous ammonia in quantities of more than 1 tonne,
- Chlorine in quantities of more than 400 kg,
- Liquefied LPG, CNG in quantities greater than 1 ton.

It is not the purpose of this article to evaluate this guideline in full, because despite its undeniable quality, necessity and systemic advantage, we could argue that, for example, for ammonia and chlorine the set limit values could be even lower. modeling of various small accidental releases of both chlorine and ammonia. The masses of both toxic gases were deliberately chosen as relatively low for emergency modeling. The specific weights are given in a certain scale for both toxic substances in the tables.

The first problem that perhaps all regional fire brigades solves is the identification of sub-limit sources of risk. Operators do not have a reporting obligation to the Department of Civil Protection and Crisis Management, but cooperation with the Prevention Department and also with the Department of the Environment of the Regional Office, which is responsible for major accident prevention and to which operators have a reporting obligation. Even so, it is very difficult to detect individual objects, and especially to continuously monitor the amount of used, handled and stored hazardous chemicals and mixtures.

The model emergency card, which is an annex to the issued professional instruction, is prepared for the winter stadium for ammonia leakage. Some parts of the emergency card are the same for all establishments that handle the same hazardous chemical (hazardous properties of the substance, warning symbols, H-phrases and P-phrases, part of the activities of the components of the integrated rescue system). As there are only four of the hazardous chemicals specified in the instruction (ammonia, chlorine, LPG and CNG), a sample card could be prepared for all of the hazardous chemicals listed.

In short, it can be stated that the issued Instruction was a very useful helper, which clearly leads to higher safety of persons, but also intervening rescuers, in the entire spectrum of the Integrated Rescue System in the Czech Republic. This expert guide could thus be very inspiring for other countries that do not have the issue addressed.

The TerEx software tool was chosen for modeling emergency impacts, which is an abbreviation of the words Terrorist Expert, specifically application version 3.0.0.0. of T-Soft Praha. The input parameters for modeling software with the TerEx tool are as follows: toxic gas - chlorine (UN 1017) as liquefied gas, emergency event: PUFF = single leakage of boiling liquid with rapid evaporation into the cloud, temperature 200 C, amount / weight of leaked hazardous substance see table, wind speed in the ground layer 1 m / s (and also alternatively also for wind speeds 3 and 5 m / s), sky coverage clouds 50%, type of atmospheric stability INVERSION (very stable conditions), type of surface in the direction of cloud propagation - industrial flat. The modeling results are summarized in Table 4.

Table 4.

Results of modeling chlorine leakage

Leaked weight in kg	THREATS TO PERSONS WITH TOXIC SUBSTANCE, EVACUATION OF PERSONS TO A DISTANCE IN METERS Wind speed 1 m / s	THREATS TO PERSONS WITH TOXIC SUBSTANCE, EVACUATION OF PERSONS TO A DISTANCE IN METERS Wind speed 3 m / s	THREATS TO PERSONS WITH TOXIC SUBSTANCE, EVACUATION OF PERSONS TO A DISTANCE IN METERS Wind speed 5 m / s
50	758	580	474
100	974	744	609
150	1 128	861	706
200	1 252	955	783
250	1 358	1 034	850
300	1 075	1 105	908
350	1 382	1 167	960
400	1 601	1 225	1 007
450	1 776	1 278	1 051
500	1 745	1 327	1 092
550	1 806	1 373	1 130
600	1 864	1 419	1 167

The same TerEx software tool was chosen for modeling emergency impacts of ammonia. The input parameters for modeling software with the TerEx tool are as follows: toxic gas - ammonia (UN 1005) as liquefied gas, emergency event: PUFF = single leakage of boiling liquid with rapid evaporation into the cloud, temperature 200 C. Sky coverage clouds 50%, type of atmospheric stability INVERSION (very stable conditions), type of surface in the direction of cloud propagation - industrial flat. The modeling results are summarized in Table 5.

Table 5.

Results of modeling ammonia leakage

Leaked weight in kg	THREATS TO PERSONS WITH TOXIC SUBSTANCE, EVACUATION OF PERSONS TO A DISTANCE IN METERS Wind speed 1 m / s	THREATS TO PERSONS WITH TOXIC SUBSTANCE, EVACUATION OF PERSONS TO A DISTANCE IN METERS Wind speed 3 m / s	THREATS TO PERSONS WITH TOXIC SUBSTANCE, EVACUATION OF PERSONS TO A DISTANCE IN METERS Wind speed 5 m / s
100	467	358	295
200	600	460	375
300	695	532	435
400	772	590	482
500	837	639	523
1 000	1 075	821	673
2 000	1 382	1 053	865
3 000	1 601	1 218	1 002
4 000	1 776	1 351	1 112
5 000	1 926	1 464	1 205

Note for modeling results: The evaluated substance does not have exothermic manifestations such as UVCE and Flash Fire in the event of an accident.

The threat of persons with a toxic substance (range of toxic concentration) in the concept of this SW program means the necessary evacuation of persons. It is sufficiently clear from the modeling results in this table what is the fundamental effect of the air flow in the ground layer of the atmosphere, in other words that the speed of the ground wind fundamentally affects the formation and propagation of the cloud of polluted air. Among other things, it is commonly calculated that the wind speed and direction in the ground layer of the atmosphere are highly unstable and the measured values at the measuring point are usually only usable for a maximum of 2 hours. Only wind speeds in the range from 1 to a maximum of 10 m/s are taken into account for modeling emergency leaks. Ideally, it is more appropriate to use freshly measured values of the state of air flow in the ground layer of the atmosphere to evaluate accidental releases of chemicals.

The complete result of the calculation is significantly wider in the software program TerEx, in individual categories, as standard outputs from the program: Danger of persons with toxic substances, Evacuation of persons to a distance, Recommended survey of toxic concentration to a distance from the place of escape.

5. Conclusion

The very existence of large masses of hazardous chemicals creates a precondition for possible chemical accidents or even chemical attacks by terrorists. At the same time, huge weights of hazardous chemicals and mixtures are stored, handled and transported in many places in the Czech Republic. This data is relatively easily accessible and therefore unfortunately also misuse.

There are a large number of exploitable sources of risk in industrialized countries and they are often located close to human settlements. In addition, there are many large-scale sources of risk in the form of mobile sources (road and rail tanks), which can be directly targeted at a selected site of chemical attack.

It is also interesting that the first law on the prevention of major accidents was not issued in the Czech Republic until 1999, but since then there have been other significant changes in the law. Therefore, new laws were gradually issued, the latest valid version is Act No. 224/2015 Coll. [13]

Although there are a number of different software tools for calculating the accidental impacts of major chemical accidents, their use is not specified in the legislation. At the same time, it is quite clear that the need for modelling of emergency impacts is not only given by the requirements of the "Act on the Prevention of Major Accidents" and its implementing regulations, but the use of modelling results is much wider.

The results of modelling the accidental impacts of major chemical accidents must then be used quickly and efficiently for the preparation and subsequent implementation of various preventive, protective, rescue and liquidation measures. And the various measures just mentioned above will have a fundamental impact on the protection of the lives and health of people at risk, affected and injured. In other words, the results of modelling can indirectly save many lives, or quickly and effectively protect their endangered health.

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