PERIÓDICO TCHÊ QUÍMICA

Volume 17 - Número 35 - 2020 ISSN 2179-0302

Órgão de divulgação científica e informativa

www.periodico.tchequimica.com

PERIÓDICO TCHÊ QUÍMICA

ISSN - 1806-0374 (Impresso) - ISSN - 2179-0302 (Online)

Volume 17 **Número 35 – 2020** **ISSN 2179 - 0302**

Órgão de divulgação científica e informativa.

Dados Internacionais de Catalogação na Publicação (CIP)

Periódico Tchê Química: órgão de divulgação científica e informativa [recurso eletrônico] / Grupo Tchê Química – Vol. 1, n. 1 (Jan. 2004)- . – Porto Alegre: Grupo Tchê Química, 2005 - Semestral.
Sistema requerido: Adobe Acrobat Reader.
Modo de acesso: World Wide Web:
<http://www.tchequimica.com>

Descrição baseada em: Vol. 14, n. 28 (ago. 2017).
ISSN 1806-0374
ISSN 2179-0302
1. Química. I. Grupo Tchê Química.

CDD 540

Bibliotecário Responsável
Ednei de Freitas Silveira
CRB 10/1262

Welcome to the TCHÊ QUÍMICA JOURNAL

International multidisciplinary scientific journal

The Tchê Química Journal publishes original research papers, review articles, short communications (scientific publications), book reviews, forum articles, technical reports, articles on chemical education, interviews, announcements or letters. Articles suitable for publication in the Tchê Química Journal are those that cover the traditional fields of ***Chemistry, Physics, Mathematics, Biology, Pharmacy, Medicine, Engineering and Agriculture****. We are especially interested in those submissions that are highly relevant to theoretical and* ***applied contributions in the area of chemistry and related disciplines.***

PERIÓDICO TCHÊ QUÍMICA

Volume 17 Número 35 – 2020 ISSN 2179 - 0302

Órgão de divulgação científica e informativa.

Periódico Tchê Química

ISSN - 1806-0374 (Print)
ISSN - 2179-0302 (Online)

LCCN: 2010240735

Divulgação *on-line* em
http://www.periodico.tchequimica.com
http://www.journal.tchequimica.com
http://www.tchequimica.com

Esta revista é indexada e resumida pelo CAS, EBSCO,Latindex, Sumários, Index Copernicus, Scopus, OAIJ, CAB Abstracts, EuroPub e Reaxys.

Missão

O Periódico Tchê Química (PTQ) publica artigos de pesquisa originais, artigos de revisão, notas curtas (publicações científicas), revisões de livros, artigos de fórum, editoriais e entrevistas. Pesquisadores de todos os países são convidados a publicar nas páginas do PTQ.

A responsabilidade sobre os artigos é de exclusividade dos autores.

Correspondências

Rua Anita Garibaldi, 359/603.
Bairro Mon't Serrat. CEP: 90450-001
Porto Alegre – RS. Brasil.
Skype: tchequimica
www.periodico.tchequimica.com
tchequimica@tchequimica.com

Índice

PERIÓDICO TCHÊ QUÍMICA
ARTIGO ORIGINAL

AVALIAÇÃO OPERACIONAL DOS PARÂMETROS DE CONTAMINAÇÃO QUÍMICA

RAPID ASSESSMENT OF CHEMICAL CONTAMINATION PARAMETERS

ОПЕРАТИВНА ОЦІНКА ПАРАМЕТРІВ ХІМІЧНОГО ЗАРАЖЕННЯ

MELNYK, Oleksandr V.[1*]; SOVHIRA, Svitlana V.[2]; DUSHECHKINA, Nataliia Yu.[3]; AVRAMENKO, Oleg B.[4]; DUBOVA, Nataliia V.[5];

[1,4] Pavlo Tychyna Uman State Pedagogical University; Department of Technical and Technological Disciplines, Labor Protection and Life Safety; 2 Sadova Str.; zip code 20300; Uman – Ukraine

[2,3] Pavlo Tychyna Uman State Pedagogical University; Department of Chemistry, Ecology and Methods of Their Training; 2 Sadova Str.; zip code 20300; Uman – Ukraine

[5] Pavlo Tychyna Uman State Pedagogical University; Department of Professional Education and Technology for Profiles; 2 Sadova Str.; zip code 20300; Uman – Ukraine

** Correspondence author*
e-mail: aleksandr9949@ukr.net

Received 15 April 2020; received in revised form 01 June 2020; accepted 03 June 2020

RESUMO

O artigo descreve o risco químico que pode afetar adversamente o meio ambiente e as pessoas em caso de acidentes em instalações de alto risco, levar à poluição tecnogênica, grandes danos e mortes entre as pessoas. Foi realizada uma análise dos métodos existentes para avaliar os efeitos da contaminação química. As propriedades tóxicas de substâncias tóxicas (ST) foram reveladas. O artigo apresenta o algoritmo de cálculo e o método para prever a situação química após a emissão de ST ou derramamento acidental de substâncias altamente tóxicas (SAT) no ambiente. Mostra-se a sequência de cálculo da solução do problema de avaliação dos parâmetros químicos usando os dados iniciais condicionais. Um programa de computador foi desenvolvido para processar os parâmetros de contaminação química e calcular as perdas entre os funcionários e residentes que possam estar na área de acidentes de indústrias químicas ou emissões para o meio ambiente (de ST, SAT). A análise de cálculos realizados sem o uso do programa de computador para processamento dos parâmetros de contaminação química e de cálculos realizados com o seu uso confirma a confiabilidade do desenvolvimento com base no produto de software Microsoft Visual Studio (Visual C#). É proposto o método de cálculo e avaliação da situação química após acidentes e destruição nas instalações da indústria química. Descreve-se a aplicação prática do programa de computador desenvolvido, que permite que especialistas no campo da defesa civil (DC) realizem os cálculos mais rapidamente para determinar o grau de estabilidade vertical do ar, profundidade e área da nuvem química, tempo de sua chegada ao assentamento, perda de pessoal e população, para tomar decisões mais rapidamente, tanto em tempos de paz quanto em períodos especiais. O artigo apresenta as conclusões sobre os cálculos e os resultados obtidos na resolução de problemas de avaliação de situações químicas utilizando tecnologias modernas.

Palavras-chave: *exposição a substâncias perigosas, toxicidade relativa, eliminação das conseqüências de acidentes, características quantitativas da toxicidade, danos a objetos quimicamente perigosos.*

ABSTRACT

The article describes a chemical hazard that can adversely affect the environment and humans in the event of accidents at high-risk facilities, lead to man-made pollution, large casualties and deaths. The existing methods of assessment of the effects of chemical contamination were analysed. The toxic properties of poisonous substances (PSs) have been revealed. The calculation algorithm has been presented and the technique for the prediction of the chemical situation after the release of explosive or emergency spills, highly toxic substances (HTS) into the environments has been disclosed. The sequence of solution calculation of the estimation of chemical parameters problem using conditional initial data has been shown. A computer program has been developed to handle the parameters of chemical contamination and to calculate losses among working personnel and residents who may end up in the accident zone of chemical industry facilities or into the environment (PS, HTS). The analysis of the calculations without the use of a computer program for processing chemical parameters of contamination and using it confirms the reliability of its design based on the Microsoft Visual Studio software (Visual C#). The method of calculation and estimation of a chemical situation after accidents and destruction at chemical industry facilities has been offered. The practical application of the developed computer program has been described, which enables the specialists in the field of civil protection (CP) to make calculations more quickly to determine the degree of vertical stability of air, depth and area of distribution of chemical cloud, time of reaching the settlement, losses of both working personnel and population, more promptly to make decisions both in peacetime and in a special period. Conclusions were made regarding the calculations performed and the results obtained when solving the problems of chemical situation estimation using modern technologies.

Keywords: *impact of hazardous substances, relative toxicity, accident response, quantification of toxicity, damage to chemically hazardous objects.*

АНОТАЦІЯ

У статті описана хімічна небезпека, яка може негативно вплинути на оточуюче середовище та людей при виникненні аварій на об’єктах підвищеної небезпеки, призвести до техногенного забруднення, великих збитків та смертельних випадків серед людей. Проведений аналіз існуючих методик оцінки наслідків хімічного зараження. Розкриті токсичні властивості отруйних речовин (ОР). Приведений алгоритм розрахунку та розкрита методика щодо прогнозування хімічної обстановки після викиду ОР або аварійного розливу, сильнодіючих отруйних речовин (СДОР) у навколишнє природне середовище. Показана послідовність розрахунку рішення задачі оцінки хімічних параметрів з використанням умовних вихідних даних. Розроблена комп’ютерна програма обробки параметрів хімічного зараження та розрахунку втрат серед працюючого персоналу та мешканців які можуть опинитися в зоні аварій об’єктів хімічної промисловості, або викиду в навколишнє середовище (ОР, СДОР). Проведений аналіз розрахунків без застосування комп’ютерної програми обробки параметрів хімічного зараження та з її використанням підтверджує про достовірність її розробки на базі програмного продукта Microsoft Visual Studio (Visual C#). Запропонована методика розрахунку та оцінки хімічної обстановки після аварій та руйнувань на об’єктах хімічної промисловості. Описане практичне застосування розробленої комп’ютерної програми, яка дає можливість фахівцям у сфері цивільного захисту (ЦЗ) більш швидше проводити розрахунки щодо визначення ступеню вертикальної стійкості повітря, глибини та площі розповсюдження хімічної хмари, часу досягнення до населеного пункту, втрат як працюючого персоналу так і населення, оперативніше приймати рішення як в мирний час так і в особливий період. Дані висновки стосовно проведених розрахунків та отриманих результатів при розв’язуванні задач з оцінки хімічної обстановки з використанням сучасних технологій.

Ключові слова: *вплив небезпечних речовин, відносна токсичність, ліквідація наслідків аварій, кількісна характеристика токсичності, ураження на хімічно небезпечних об’єктах.*

1. INTRODUCTION

In Ukraine, as in other industrial countries of the world, there are facilities where a large number of various chemicals, which are dangerous to the environment, toxic and harmful to human and animal health, are manufactured, recycled, disposed. Such substances are called HTS (highly toxic substances). Many of them are carried with transport, which in turn increases their risk during accidents. In addition, during a special period of state functioning, objects that store HTS may be deliberately destroyed (Bell *et al.*, 2017; Bourdrel *et al.*, 2017; Melnichuk *et al.*, 2020; Tyliszczak *et al.*, 2009; Talismanov *et al.*, 2018; Kosnik and Reif, 2019; Mo *et al.*, 2019; Krechetov *et al.*, 2018; Zavala *et al.*, 2020). In peacetime, in the event of accidents, catastrophes or other natural disasters, HTS can enter the environment and cause damage to humans, animals, plants, in particular cause fatalities. In peacetime as well as in a special period to eliminate threats to life and health, civil protection is implemented through the implementation of localisation plans and the elimination of accidents or catastrophes. There are many different methods used to calculate the parameters of chemical contamination, which take into account the toxic properties of toxic substances (Steblyuk, 1998; Williams *et al.*, 2017; New Hampshire…, 2019; NTP. National Toxicology…, 2019).

Civil protection is one of the main priorities of the activity of the central state authorities, bodies of local self-government institutions and organisations throughout Ukraine. From the foregoing, it is clear that due consideration of the post-accident chemical environment at the facilities of the chemical industry needs to be given sufficient attention, in particular to study, investigate and implement both organisational and technical measures (Manucci and Franchini, 2017).

Many well-known scientists were engaged in studying of PS and HTS, research and development of methods of chemical situation estimation at different times: V. N. Aleksandrov (Alexandrov and Emelyanov, 1990) classified the main types of poisonous substances, the nature and extent of their toxic action, V. G. Atamanyuk (Atamanyuk *et al*., 1986) described the definition of the stability of poisonous substances, A. T. Altunin (1984) described the actions of the population in the conditions of infection with highly toxic substances, G. G. Migovich (2001) listed the general analytical formulas for determining the individual components of the chemical situation estimation, P. T. Egorov (Egorov *et al*., 1977) characterised the chemical intelligence instruments, I. M. Mitsenko (Mitsenko and Mizentseva, 2004) disclosed the classification of toxic substances, A. P. Volkov (1988) highlighted the special treatment of objects after the influence of PS and HTS, M. I. Steblyuk (1998; 2006), V. I. Bukhtoyarov (1988), V. M. Shobotov (2006) proposed the calculation of the determination of the individual components of the chemical situation. The mentioned works describe the physicochemical and toxic properties of PS and HTS, give the general analytical formulas for determining the depth and area of chemical contamination, the calculations of determining the stability and time of an approach of the infected cloud from the emergency object to the settlement, but there are no algorithms of calculation starting from the initial data and ending with the projected loss of residents who will be affected by HTS. The writings of A. A. Zuikova (2006), A. V. Katkovsky (2015) consider increasing the effectiveness of decision-making in accidents with the release of chemically hazardous substances, pay attention to the use of computer technologies to solve environmental problems and industrial safety problems, draw attention to the use of information technology in the assessment of chemical environment after accidents on chemical facilities, however, the calculation using the software is not provided (Ring *et al*., 2017; Casey *et al*., 2018; Centers for Disease…, 2019; Wambaugh *et al*., 2019).

A review and analysis of the literature in the Scopus database showed that, for example, there are works (Gervich, 2016; Jordan and Abdaal, 2013; Jordan *et al*., 2009; Pashtetskiy *et al*., 2020; Konyavsky and Ross, 2019; Wang and Wang, 2014) that make a comparative characterisation of socio-economic systems for better understanding of the effects of industrial pollution on society; modern methods to support decision-making for ecological assessment of pollution in the mine territories and spatial modelling of contamination of reservoirs by processing industry have been considered; the ecological situation on water pollution after fire in chemical industry has been researched (US EPA (US Environmental…, 2018).

Currently, there are many programs for calculating chemical contamination parameters, such as ALOHA. The program is powerful, written in English. It is not adapted for the departments of the CP of Ukraine (Everything you need…, 2019; Ginsberg *et al*., 2019; Yudaev *et al*., 2019a; Yudaev *et al*., 2019b; Zykova *et al*., 2019; Rabinskiy and Tushavina, 2019). It is therefore understandable that the methodology for assessing the chemical environment should be investigated, studied, calculated and the results obtained – analysed. In order to promptly calculate the chemical situation, make timely decisions on protecting workers and residents who are affected by PS or HTS due to accidents at chemically hazardous sites, civil protection professionals need to have software that will speed up the calculation and enable them to take timely action on localisation and elimination of consequences of accidents at chemical industry facilities (Oltra *et al*., 2017; Richmond-Bryant *et al*., 2018; Jennifer, 2020).

The aim of the article – on the basis of the analysis of the existing methods of assessment of the chemical environment and the necessity to quickly respond to the consequences of accidents occurring at the facilities of the chemical industry, to develop an operational assessment of chemical contamination, to calculate the chemical situation without using software and with its use, to analyse the reliability of the results obtained.

Research objectives:

1) To analyse existing methods of calculating chemical contamination parameters.

2) To develop an algorithm for calculating the chemical post-accident assessment of a chemical facility (Figure 1).

3) To develop an operational assessment of chemical contamination.

4) To evaluate a chemical situation without the use of an operational assessment of chemical contamination and with its use, to analyse the reliability of results.

5) To analyse the results obtained using an operational assessment of chemical contamination.

2. MATERIALS AND METHODS

In order to determine the scale, nature, extent of exposure of hazardous substances to humans, animals, plants, foodstuffs, and the development of appropriate actions of the CP and the population before liquidation of chemical contamination and works on the site, chemical conditions are evaluated (Melnyk, 2013; Melnyk, 2014). The baseline data for assessing the chemical situation are:

1) the area and time of application of the HS or release into the environment of HTS;

2) type and amount of HS or HTS;

3) the degree of protection of humans, animals, food;

4) storage conditions (under pressure, without pressure) and the nature of hazardous chemicals entering the environment;

5) topographical conditions of the terrain, nature of development, presence of forest plantations on the way of spread of contaminated air. The configuration of the terrain, as well as all natural and artificial objects located on it (rivers, forests, shrubs, mountains, settlements, (closed terrain) affect the final result of the software calculation. This condition is taken into consideration upon entry of the initial data;

6) meteorological conditions: wind speed and direction in the surface layer, air and soil temperature, degree of vertical stability of air.

The degree of vertical stability of the air ground layer can be determined from the data of meteorological surveys. In addition, it can be more accurately determined by the wind speed at an altitude of 1 m and a temperature gradient (Equation 1) where t_{50} – air temperature at a height of 50 cm; t_{200} – air temperature at an altitude of 200 cm from the earth's surface. When the ratio of magnitudes $\Delta t / v^2 \leq -0.1$ there will be inversion, $-0.1 < \Delta t / v^2 < +0.1$ – isothermy, and $\Delta t / v^2 \geq +0.1$ – convection. HSs are characterised by their toxicity (toxikon – poison). It is an important characteristic of HS that determines their ability to cause pathological changes in the body that lead to severe consequences or death. The quantitative characterisation of the toxicity of HS is determined by a dose (Vozza, 2017; Sarma *et al*., 2018). The dose of a substance that causes a certain toxic effect is called the toxic dose (D). The toxic properties of HS are determined experimentally on different laboratory animals, so they are more likely to use the concept of specific toxic dose – the dose attributed to the unit of live weight of the animal and expressed in milligrams per kilogram (mg/kg). Toxic doses (Alexandrov and Emelyanov, 1990) are divided into:

1) mortal;

2) incapacitating vital activity;

3) initial.

Toxic doses of HS of skin and resorption action are divided into:

– Lethal toxic dose LD (from Lat. letalis – lethal) – is the amount of HS that causes death upon penetration into the body with a certain probability, it is denoted respectively LD_{100} or LD_{50}, (100%, 50% of wounded).

– Toxic dose that incapacitates vital activity ID (from the English “incapacitate”) – is the amount of HS that infringe vital activity both temporally or lethally of a certain percentage of wounded when penetrating a body, it is denoted respectively ID_{100} or ID_{50},(100%, 50 % of wounded).

– Initial toxic dose PD (from English “primary”) – the amount of PS that causes the initial signs of damage to an organism with a certain probability or the initial signs of damage in a certain percentage of humans and animals. Initial toxic doses are denoted PD_{100} or PD_{50}. (100%, 50% initial signs of a lesion).

It is more difficult to calculate toxic doses for PS that enters the human body as a vapour by inhalation. First of all, it is suggested that the inhalation toxic dose is directly proportional to the concentration of PS in the air, C, and the time of inhalation τ. In addition, it is necessary to take into account the intensity of breathing V, which depends on physical activity and human condition. In a calm state, a person takes about 16 breaths per minute and absorbs *8-10 l/m* of air on average. During medium exercise, the absorption of air increases to *20-30 l/m*, and during heavy physical exertion is approximately *60 l/m*. Thus, if a person weighing *G (kg)* inhales air with a concentration of PS *C(mg/l)* in it during τ *(min)* with the intensity of breathing *V (l/min)*, then the specific absorbed dose of PS (the amount of PS into the body) will be equal to Equation 2.

In (Alexandrov and Emelyanov, 1990), the German chemist F. Haber proposed to simplify this expression. He made the assumption that the relationship is constant for humans or a specific species of animals that are in the same conditions.

Divide both parts of the equation in this relation, he obtained the Equation 3.

F. Haber called $C \cdot \tau$ toxicity coefficient and assumed it as a constant. Although this product is not a specific toxic dose, it does allow comparison of different PSs by inhalation toxicity. If, for example, $C \cdot \tau$ for yperite is *1.5 mg · min/l* and for phosgene *3.2 mg · min/l*, it is clear that inhalation of yperite is about 2 times more toxic than phosgene. Notwithstanding many other factors that affect toxicity, the value $C \cdot \tau$ is used to evaluate the inhalation toxicity of PS and is referred to as relative inhalation toxicity. For the characteristics of the lethal, life-threatening and primary toxicity of the PS, which affect the human body by inhalation in the form of steam or aerosol, use the same letters and indexes as with toxic doses of skin-resorptive action. They are denoted respectively $LC\tau_{100}$ and $LC\tau_{50}$, $IC\tau_{100}$ and $IC\tau_{50}$, $PC\tau_{100}$ and $PC\tau_{50}$. The relative toxicity $C \cdot \tau$ during inhalation depends on the physical exertion on the person. For people engaged in heavy physical labour, it will be much less than for people who are at rest. With increasing respiratory rate, the rate of action of the PSs increases. For example, for GB with pulmonary ventilation, the value is *0.075 mg · min/l* and *0.025 mg · min/l*,, respectively, and if for phosgene the product $C \cdot \tau$ *3.2 mg · min/l* at respiratory rate is medium lethal, then for pulmonary ventilation *40 l/min* is absolutely lethal. Table 1 shows the toxicological characteristics of HPs.

Tabular values of skin resorptive PS are valid only for infinitely large exposure, that is, for cases where PSs, that hit the skin surface, are not removed or degassed. In fact, for the manifestation of one or another toxic effect on the surface of the skin, there must be a greater amount of poison than the toxicity of toxic substances given in the table. This amount and the time during which PS is on the surface of the skin during absorption, in addition to toxicity, is largely due to the rate of absorption of the PS through the skin. Thus, according to US specialists, a substance VX characterised by a skin-resorptive toxic dose *LD_{50} 6-7mg* per humans will enter the human body if the droplet-liquid VX amounted at *200mg* is on the surface of the skin for 1 hour, or approximately *10mg* – for 8 hours. Due to the protective properties of the clothing, this amount is increased, and in the summer for 8 hours exposure will be approximately *95mg*.

It should be noted that the table values of the constant $C \cdot \tau$ are valid for short exposures, which differ significantly for different poisonous substances depending on their physical, physicochemical and chemical properties. For AC this value is valid if τ – several minutes, and for CG – within one hour. The extent of damage caused by accidents at chemically hazardous sites depends first of all on the number of PSs, meteorological and topographic conditions of the area, the type of storage of HTSs (under pressure, without pressure). From the above it can be concluded: protective measures and, above all, the forecasting, detection and periodic monitoring of the chemical situation, alerting the personnel of the enterprise, the population and the CA forces, should be carried out with extremely high speed.

To create an operational assessment of chemical contamination and enable timely decision-making on taking measures to localise and eliminate the consequences of accidents at chemical industry facilities, it is necessary to develop an algorithm for civil protection professionals to evaluate chemical contamination parameters. It must start from the moment of receipt of the initial data on an object at which an accident occurred, its location, settlement, if any, the number of residents who live in it, ending with calculations of the consequences of chemical contamination, possible loss of working staff at this facility, a population that is projected to fall into the zone of chemical contamination.

1) Develop an algorithm for calculating the chemical post-accident assessment of a chemical facility (Figure 1).

2) Develop an operational assessment of chemical contamination.

a) Create a new project "Windows Form Application".

b) Add software elements.

c) Write the program code.

d) Add reference material.

e) Run the program and enter the corresponding output data.

f) Calculate the problem.

g) Obtain the results of the calculation.

The program works in accordance with the algorithm provided in (Figure 1). Let us enter the source data. In accordance with the input data, the software determines the degree of vertical stability of the air (inversion, convection, isothermy). Considering the topographic conditions of the area (source data), the Depth (D) and the area (S) of chemical contamination are calculated (Figure 1).

The next step is the time it takes to reach and the time it takes to affect people with toxic substances. Further, the software calculates population losses by degrees of severity, taking into consideration the availability of personal protective gear. The software interface is as follows (Figure 2).

Table 2 provides statistics on past accidents. Table 2 was developed with the use of software modelling of data.

3. RESULTS AND DISCUSSION:

The study was conducted on the following input data (Melnyk, 2014):

1. An emergency object: Kind of HTS – chlorine; Quantity of HTS – 10 t; Type of container – unbuttoned; Number of employees – 600 people; Gas supply is 70%.

2. Settlement: Distance to the village R-3 km; Number of inhabitants 1000 persons; Gas mask security – 90%; Terrain – open; Meteorological conditions – V_w = 2 m/s, $\Delta t°C$ = 70.1

Calculation sequence:

1. Determine the degree of vertical stability of the air: Wind velocity V_w = 2 m/s and Δt^0C = 0,1 – isothermy.

2. Determine the depth of CCZ: D = 7 km. Take into account the correction coefficient of wind speed: D = 7 km · 0.7 = 4.9 km; D = 4.9 km.

3. Determine the width of CCZ: W = 0.15 · G – isothermy. W = 0.15 · 4.9 km = 0.74 km. W = 0.74 km.

4. Determine the area of CCZ: S = 1/2 · G · W. S = 1/2 · 4.9 km · 0.74 km = 1.8 km2; S = 1.8 km^2

5. Map the predicted CCZ (Figure 1).

6. Determine the t_{reach} of contaminated air to the locality: t_{reach} = 3000 m/(3 m/s 60) = 16.66 minutes.

7. Determine the HTS $t_{affection}$: affection = 1.3 h · 0.7 = 0.91 h.

8. Calculate the possible losses of employees:

600 · 18%/100% = 108 persons – total losses (t.l.);

108 · 25%/100% = 27 persons with lesions of mild degree (m.d.);

108 · 40%/100% = 43 persons of moderate and severe degree (m.s.d);

108 · 35%/100% = 38 persons – fatalities (f.).

9. Calculate the possible population loss:

1000 · 9%/100% = 90 persons t.l.;

108 · 25%/100% = 23 persons m.s.d.;

108 · 40%/100% = 36 persons m.d.;

108 · 35%/100% = 31 persons f.

The results of the calculation are shown in Table 3.

4. CONCLUSIONS:

Comparative analysis of the results obtained from the solution of the problem of chemical post-accident assessment at a chemical industry facility conducted in two ways: without using an operational assessment of chemical contamination and with its use testify to the correctness of the developed an operational assessment of chemical contamination software product in accordance with the proposed methodology. The novelty of the obtained results is that a methodology for the assessment of the chemical situation after accidents at the chemical industry facilities is improved and an operational assessment of the parameters of chemical contamination is developed.

The existing methods of calculation of chemical contamination parameters were analysed. The algorithm of calculation of chemical contamination parameters was given. An operational assessment of chemical contamination using Microsoft Visual Studio (Visual C#) was developed. The software can be downloaded from https://visualstudio.microsoft.com/ru/vs/express/ for calculation and estimation of a chemical situation after accidents and destruction at chemical industry facilities. The chemical situation without using an operational assessment of chemical contamination and with its use was estimated, the reliability of the obtained results was analysed. The developed operational assessment of chemical contamination will enable the specialists of city and district departments of civil protection and defence-mobilisation work to make calculations on chemical situation more promptly, to take timely measures of protection of workers, population and territories that will be under the influence of HS and HTS.

5. REFERENCES:

1. Alexandrov, V. N., and Emelyanov, V. I. (1990). *Poisonous substances*. Moscow, Russian Federation: Voenizdat.
2. Altunin, A. T. (Ed.). (1984). *Civil defence*. Moscow, Russian Federation: Voenizdat.
3. Atamanyuk, V. G., Shirshev, L. G., and Ekimov, N. I. (1986). *Civil defence*. Moscow, Russian Federation: Vysshaya Shkola.
4. Bell, S. M., Phillips, J., Sedykh, A., Tandon, A., Sprankle, C., Morefield, S.Q., Shapiro, A., Allen, D., Shah, R., Maull, E.A., Casey, W.M., and Kleinstreuer, N.C. (2017). An integrated chemical environment to support 21st-century toxicology. *Environmental Health Perspectives, 125*, Article number 054501. doi:10.1289/EHP1759.
5. Bourdrel, T, Bind, M.-A, Béjot, Y., Morel, O., and Argacha, J.-F. (2017). Cardiovascular effects of air pollution. *Archives of Cardiovascular Diseases, 110*, 634–642. doi:10.1016/j.acvd.2017.05.003.
6. Bukhtoyarov, V. I. (Ed.). (1988). *Textbook of a sergeant of chemical troops*. Moscow, Russian Federation: Voenizdat.
7. Casey, W. M., Chang, X., Allen, D. G., Ceger, P. C., Choksi, N. Y., Hsieh, J.-H., Wetmore, B.A., Ferguson, S.S., DeVito, M.J. , Sprankle, C.S., Kleinstreuer, N.C. (2018). Evaluation and optimization of pharmacokinetic models for in vitro to in vivo extrapolation of estrogenic activity for environmental chemicals. *Environmental Health Perspectives, 126*, Article number 97001. doi:10.1289/EHP1655.
8. Centers for Disease Control and Prevention. (2019). National Health and Nutrition Examination Survey. Retrieved from https://www.cdc.gov/nchs/nhanes/index.htm
9. Egorov, P. T., Shlyakhov, I. A., and Alabin, N. I. (1977). *Civil defence*. Moscow, Russian Federation: Vysshaya Shkola.
10. Everything you need to know about aerosols and air pollution. (2019). Retrieved from https://ethicalunicorn.com/2019/04/29/everything-you-need-to-know-about-aerosols-air-pollution/.
11. Gervich, C. (2016). Social-ecological systems mapping to enhance students' understanding of community-scale conflicts related to industrial pollution. *Learner-Centered Teaching Activities for Environmental and Sustainability Studies, 1*, 233-238.
12. Ginsberg, G. L., Fedinick, K. P., Solomon, G. M., Elliott, K. C., Vandenberg, J. J., Barone, S., and Bucher, J. R. (2019). New toxicology tools and the emerging paradigm shift in environmental health decision-making. *Environmental Health Perspectives*, *127*(12), Article number 125002-1-125002-7. doi:10.1289/EHP4745.
13. Jennifer, A.L. (2020). Assessment of exposures in vulnerable populations: exposure and response modelling for environmental contaminants through a lifetime. In *Good health and well-being* (pp. 38-50). Cham, Switzerland: Springer International Publishing AG. doi:10.1007/978-3-319-95681-7_73.
14. Jordan, G., and Abdaal, A. (2013). Decision support methods for the environmental assessment of contamination at mining sites. *Environmental Monitoring and Assessment, 185*, 7809-7832.
15. Jordan, G., Van Rompaey, A., Somody, A., Fügedi, U., and Farsang, A. (2009). Spatial modelling of contamination in a catchment area impacted by mining: A case study of the Recsk copper mine, Hungary. *Land Contamination and Reclamation, 17*(3-4), 413-421.
16. Katkovsky, A. V. (2015). Use of information technology in the process of studying the discipline "Civil Protection". *Collection of the NA of Border Guard Service of Ukraine. Series: Pedagogical and Psychological Sciences, 1*(74), 111-120.
17. Konyavsky, V.A., and Ross, G.V. (2019). Secure computers of the new Harvard architecture. *Asia Life Sciences, 28*(1), 33-53.
18. Kosnik, M. B., and Reif, D. M. (2019). Determination of chemical-disease risk values to prioritize connections between environmental factors, genetic variants, and human diseases. *Toxicology and Applied Pharmacology, 379,* Article 114674. doi:10.1016/j.taap.2019.114674.
19. Krechetov, I.V., Skvortsov, A.A., Poselsky, I.A., Paltsev, S.A., Lavrikov, P.S., and Korotkovs, V. (2018). Implementation of automated lines for sorting and recycling household waste as an important goal of environmental protection. *Journal of Environmental Management and Tourism, 9*(8), 1805-1812.
20. Manucci, P. M., and Franchini, M. (2017). Health effects of ambient air pollution in

developing countries. *International Journal of Environmental Research and Public Health*, *14*(9), Article 1048. doi:10.3390/ijerph14091048.

21. Melnichuk, T.N., Abdurashytov, S.F., Andronov, E.E., Abdurashytova, E.R., Egovtseva, A.Y., Gongalo, A.A., Turin, E.N., and Pashtetskiy, V.S. (2020). The taxonomic structure of southern chernozem at the genus level influenced by microbial preparations and farming systems. *IOP Conference Series: Earth and Environmental Science, 422*(1), Article number 012101.
22. Melnyk, O. V. (2013). *Methods of estimation of radiation and chemical situation in peacetime and wartime in case of emergencies at the facilities of nuclear power plants and chemical industry.* Uman, Ukraine: FOP Yellow O.O.
23. Melnyk, O. V. (2014). *Civil defence*. Uman, Ukraine: Pavlo Tychyna Uman State Pedagogical University.
24. Migovich, G. G. (2001). *Handbook of Civil defence*. Kyiv, Ukraine: Ukrainian Technology Group.
25. Mitsenko, I. M., and Mizentseva, O. M. (2004). *Civil defense*. Chernivtsi, Ukraine: Knyga – XXI.
26. Mo, Z., Fu, Q., Lyu, D., Zhang, L., Qin, Z., Tang, Q., Yao, K. (2019). Impacts of air pollution on dry eye disease among residents in Hangzhou, China: a case-crossover study. *Environmental Pollution, 246*, 183–189. doi:10.1016/j.envpol.2018.11.109.
27. New Hampshire Department of Environmental Services Current and Forecasted Air Quality in New Hampshire. Environmental Fact Sheet (2019). Retrieved from https://www.des.nh.gov/organization/commissioner/pip/factsheets/ard/documents/ard-16.pdf.
28. NTP. National Toxicology Program. National Institute of Environmental Health Sciences (2019) Chemical Effects in Biological Systems. Retrieved from https://manticore.niehs.nih.gov/cebssearch/.
29. Oltra, C., Sala, R., Boso, A., and Asensio, S. L. (2017). Public engagement on urban air pollution: an exploratory study of two interventions. *Environmental Monitoring and Assessment, 189*(6), Article 296.
30. Pashtetskiy, V.S., Turin, E.N., Izotov, A.M., Abdurashytov, S.F., Gongalo, A.A., and Zhenchenko, K.G. (2020). Effect of Pisum sativum L. seed treatment with the complex of microbiological preparation on the plants' growth and development under direct sowing. *IOP Conference Series: Earth and Environmental Science, 422*(1), Article number 012012.
31. Rabinskiy, L.N., and Tushavina, O.V. (2019). Problems of land reclamation and heat protection of biological objects against contamination by the aviation and rocket launch site. *Journal of Environmental Management and Tourism, 10*(5), 967-973.
32. Richmond-Bryant, J., Snyder, M.G., Owen, R.C., and Kimbrough, S. (2018). Factors associated with NO_2 and NOX concentration gradients near a highway. *Atmospheric Environment, 174*, 214-226. doi:10.1016/j.atmosenv.2017.11.026.
33. Ring, C.L., Pearce, R. G., Setzer, R. W., Wetmore, B. A., and Wambaugh, J. F. (2017). Identifying populations sensitive to environmental chemicals by simulating toxicokinetic variability. *Environment International, 106*, 105–118. doi:10.1016/j.envint.2017.06.004.
34. Sarma, A. K., Singh, V. P., Bhattacharjya, R. and Kartha, S. A. (2018). *Urban Ecology, Water Quality and Climate Change.* Dordrecht, The Netherlands: Springer Science.
35. Shobotov, V. M. (2006). *Civil defence*. Kyiv, Ukraine: Center for educational literature.
36. Steblyuk, M. I. (1998). *Methods of evaluation of radiation, chemical and fire conditions*. Kiev, Ukraine: UVK Printing Station.
37. Steblyuk, M. I. (2006). *Civil defence*. Kiev, Ukraine: Znannya.
38. Talismanov, V.S., Popkov, S.V., Zykova, S.S., Karmanova, O.G., and Bondarenko, S.A. (2018). Synthesis and cytotoxic activities of substituted N-4-[4-(1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-2-yl]phenyl-N′-arylureas. *Journal of Pharmaceutical Sciences and Research*, *10*(1), 152-155.
39. Tyliszczak, B., Polaczek, J., Pielichowski, J., and Pielichowski, K. (2009). Preparation and properties of biodegradable slow-release PAA superabsorbent matrixes for phosphorus

fertilizers. *Macromolecular Symposia*, *279*(1), 236-242.

40. US EPA (US Environmental Protection Agency). (2018). Retrieved from https://www.epa.gov/pm-pollution/particulate-matter-pm-basics.

41. Volkov, A. P. (1988). *A guide to special cleaning*. Moscow, Russian Federation: Voenizdat.

42. Vozza, D. (2017). Historical pollution and human rights violations: is there a role for criminal law? *Historical Pollution: Comparative Legal Responses to Environmental Crimes, 1*, 385-421. doi:10.1007/978-3-319-56937-6_13.

43. Wambaugh, J. F., Wetmore, B. A., Ring, C. L., Nicolas, C. I., Pearce, R. G., Honda, G. S., Dinallo R., Angus D., Gilbert J., Sierra T., Badrinarayanan A., Snodgrass B., Brockman A., Strock Ch., Setzer, R.W. (2019). Assessing Toxicokinetic Uncertainty and Variability in Risk Prioritization. *Toxicological Sciences*, *172*(2), 235-251. doi:10.1093/toxsci/kfz205.

44. Wang, Y. Y., and Wang, B. Q. (2014). Study on countermeasures of water pollution accident after chemical industry fire. *Advanced Materials Research,* 886, 219-222.

45. Williams, A. J., Grulke, C. M., Edwards, J., McEachran, A. D., Mansouri, K., Baker, N.C., Patlewicz, G., Shah, I., Wambaugh, J.F., Judson, R.S. (2017). The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. *Journal of Cheminformatics, 9*, Article 61. doi:10.1186/s13321-017-0247-6.

46. Yudaev, I., Ivushkin, D., Belitskaya, M., and Gribust, I. (2019b). Pre-sowing treatment of *Robinia Pseudoacacia L*. seeds with electric field of high voltage. *IOP Conference Series: Earth and Environmental Science, 403*(1), Article number 012078.

47. Yudaev, I., Stepanchuk, G., Kaun, O., Ukraitsev, M., and Ponamareva, N. (2019a). Small-sized irradiation structures for intensive year-round cultivation of green vegetable crops. *IOP Conference Series: Earth and Environmental Science, 403*(1), Article number 012084.

48. Zavala, J., Freedman, A. N., Szilagyi, J. T., Jaspers, I., Wambaugh, J. F., Higuchi, M., and Rager, J. E. (2020). New approach methods to evaluate health risks of air pollutants: Critical design considerations for in vitro exposure testing. *International Journal of Environmental Research and Public Health, 17*(6), Article number 2124. doi:10.3390/ijerph17062124.

49. Zuikova, A.A. (2006). *Increasing the effectiveness of decision-making in accidents with the release of hazardous chemical substances*. Tula, Russian Federation: Tula State University.

50. Zykova S.S., Talismanov V.S., Tsaplin G.V., Bulatov I.P., Popkov S.V., Karmanova O.G., and Savinkov A.V. (2019). Study of acute toxicity and antihypoxic activity of N4-substituted 5-(1,2,4-triazole-1-ylmethyl)-1,2,4- triazole-3-thiones. *International Journal of Pharmaceutical Research, 11*(3), 1189-1192.

$$\Delta t = t_{50} - t_{200}, \quad \text{(Eq. 1)}$$

$$D = \frac{C \cdot \tau \cdot V}{G} = \frac{\frac{mg}{l} \cdot \min \cdot \frac{l}{min}}{kg} = \frac{mg}{kg} \quad \text{(Eq. 2)}$$

$$T = C \cdot \tau = \frac{mg \cdot min}{l} \quad \text{(Eq. 3)}$$

__Table 1.__ Toxicological characteristics of HP. Source: the author

Name of poisonous substances and their code	**Lesion through the respiratory system**		**Lesion through skin**
	$LC\tau_{50}$ (mg·min)/l	***$IC\tau_{50}$ (mg·min)/l***	***LD_{50} mg/person***
Sarin (GB)	0.075	0.055	1480
Soman (GD)	0.05	0.025	100
VX (VX)	0.01	0.005	7
Yperite (AD)	1.50	0.200	–
Nitrous yprete (HN)	1.00	0.100	5000
Hydrogen cyanide (AC)	2.00	0.300	1000
Cholorocyan (CK)	11.00	7.000	–
Phosgene (CG)	3.20	1.600	–
Bi-et (BZ)	110.00	0.110	–
Chloroacetophenone (CN)	85.00	0.030	–
Adamsite (DM)	30.00	0.030	–
CS (CS)	25.00	0.020	–
CR (CR)	–	0.001	–

__Table 2.__ Comparative analysis of accident development scenarios

The statistics of accidents at chemical facilities						Data calculated with the use of software		
Accident location	HHC type	The amount of HHC (tonnes)	Depth of affection (km)	Area of affection (km^2)	The number of people affected	Depth of affection (km)	Area of affection (km^2)	The number of people affected
1934, Niagara Falls, (USA).	chlorine	15	-	-	1	10	4.5	30
1989, Jonava (Lithuania)	ammonia	7000	30	37	36	35	43.3	50
1991, Mexico	chlorine	300	-	-	500	30	37.1	700
2008, Balakovo (Russia)	ammonia	0.6	-	-	2	0.4	0.007	10

Table 3. *Calculation of chemical contamination parameters. Source: the author*

	List of tasks	**Without an operational assessment of chemical contamination**	**With an operational assessment of chemical contamination**
1	Determination of degree of vertical stability of air	isothermy	isothermy
2	Determination of depth of chemical contamination zone	4.9 km	4.93 km
3	Determination of the width of the chemical contamination zone	0.74 км	0.75 km
4	Determination of the area of the chemical contamination zone	1.8 km^2	1.8 km^2
5	Mapping the predicted CCZ		
6	Determination the time of reaching the contaminated air to the settlement	16.66 min.	16.8 min.
7	Determination the time of HTS lesion	0.91 h.	0.91 h.
8	Calculation of possible losses of employees	108 person t.l. 27 persons m.d. 43 persons m.s.d. 38 persons f.	108 person t.l. 27 persons m.d. 43 persons m.s.d. 38 persons f.
9	Calculation of possible population losses	90 persons t.l. 23 persons m.s.d. 36 persons m.d. 31 persons f.	90 persons t.l. 23 persons m.s.d. 36 persons m.d. 31 persons f.

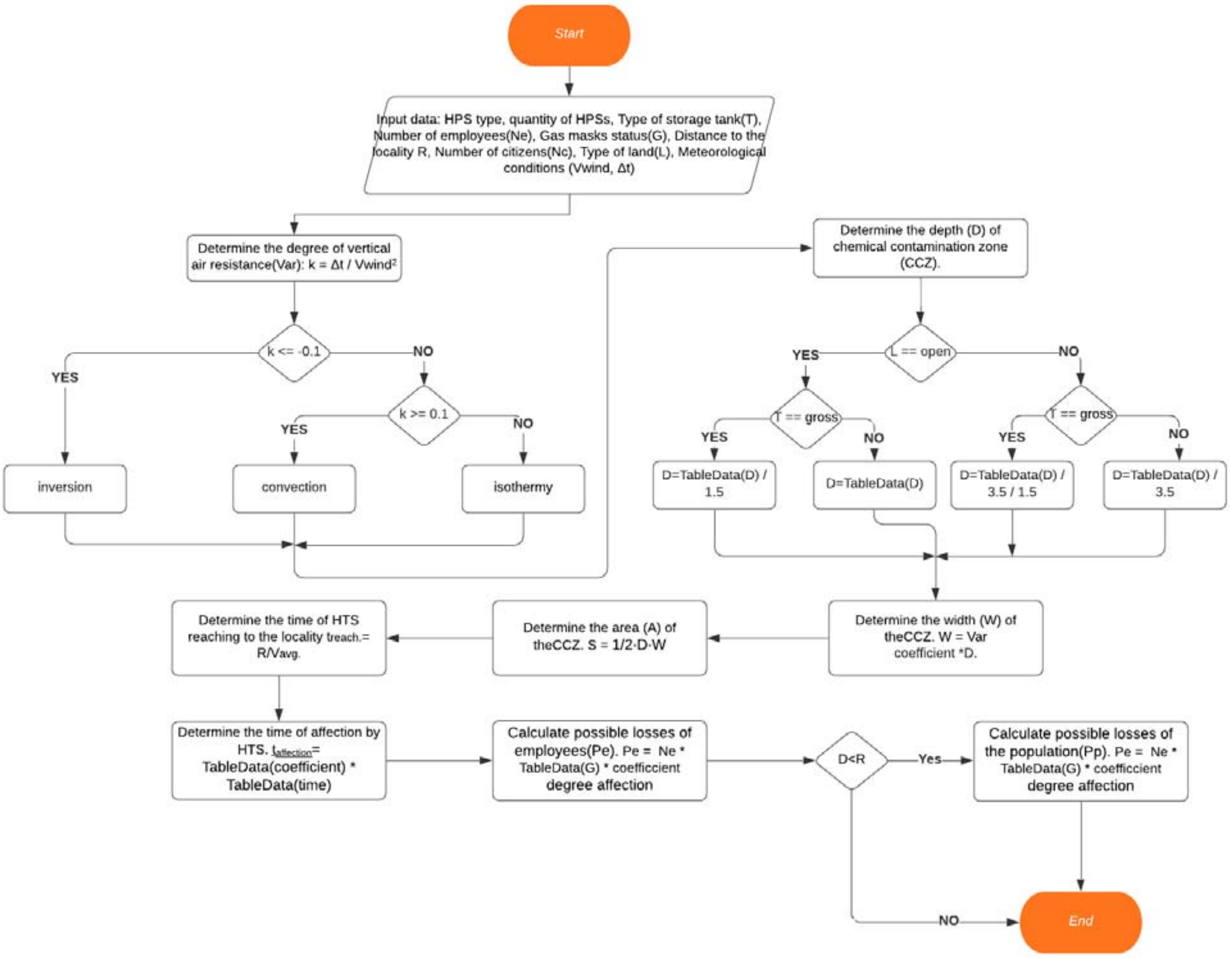

Figure 1. *Algorithm for calculating the chemical situation evaluation after accidents at chemical facilities*

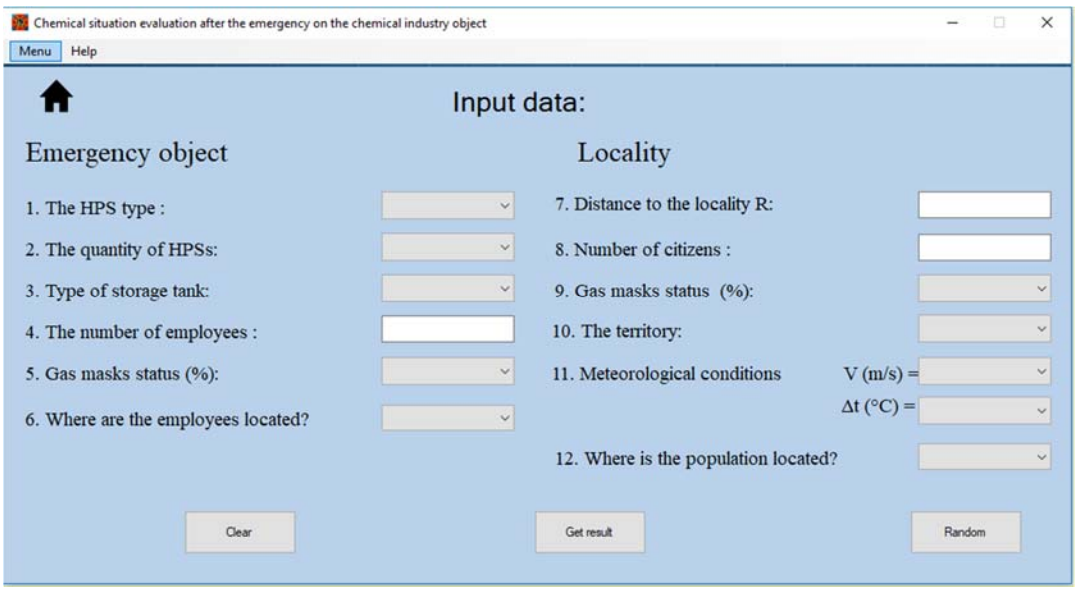

Figure 2. *Software Interface*