Peculiarities of Specialized Software Tools Used for Consequences Assessment of Accidents at Chemically Hazardous Facilities

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Abstract An effective response to emergencies at chemically hazardous facilities under various circumstances is only possible with software modeling tools. They allow for determining the affected area, forecasting changes in its scale, and assessing risks to public health due to such events' occurrence. The article critically analyzes the existing specialized software tools used in various countries to determine accident consequences of technogenic objects. Such objects are potential sources of emergencies associated with significant environmental pollution. The work results of these software tools are given, and their strengths and limitations in their application in solving practical problems are shown.

Keywords Accident · Chemically hazardous objects · Software tools · Modeling

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1 Introduction

The increase in capacities of technological complexes, vehicles, and energy systems leads to the accumulation of combustible, explosive, and poisonous substances in chemical industry enterprises [1, 2]. Accidents at chemically hazardous facilities are often accompanied by releasing gaseous chemically hazardous substances (CHS) into the environment. Their spread threatens the life and health of the service personnel of enterprises and the population in the surrounding area—several injured and dead, maybe thousands in particularly unfavorable cases [3–5].

Safety measures during the storage, transportation, and processing of such CHS and actions of units dealing with the localization of accidents at chemically hazardous facilities are regulated by several regulatory documents. But, the frequency of emergencies caused by chemical accidents remains the same despite the measures taken. As a result, environmental pollution occurs, and severe destruction is possible over a large area due to a chemical explosion during such accidents. Furthermore, there is a danger to all living things in the contaminated area (death of people, and animals, destruction of crops) [6–10].

Effective solution for emergency, rescue and other urgent works in the emergency zones requires the use of methodical, mathematical, and software for the rapid adoption of appropriate management decisions at all stages of the development of such situations. Therefore, we will consider the existing software used by different world countries while solving the above-described problems.

2 The Research Results

Response effectiveness to emergencies is achieved with the help of unique means and the use of various methods of forecasting such cases in the world's developed countries, such as the USA, Canada, Japan, and the countries of the European Union. Let's consider some software tools of the developed countries of the world which are used to assess the consequences of chemical accidents.

EFFECTS

The EFFECTS software [11] is developed by the Dutch organization TNO. It allows the user to predict, calculate and present the physical consequences of any accident scenario with toxic and flammable chemicals. This software offers more than 50 calculation models for emission, evaporation, fire, explosion, dispersion, and damage. Critically features of EFFECTS are:

– availability of a comprehensive chemical database containing toxic, flammable, and thermodynamic properties of more than 2000 chemical substances. The built-in editor is also available for detailed definitions of own chemicals;
– models can transfer the results of their calculations as input data to other models using the “binding” method;

- EFFECTS offers combined models in a fully automatic process in addition to the method of (manual) linking of models;
- GIS tool is included in the software. It allows you to overlay results on GIS drawings and Google Earth screenshots easily.

Strong sides of EFFECTS:

- easy to use. The user interface is suitable for experts and casual users;
- results are presented in graphs, special reports, and contours on background maps, facilitating management steps [12].

ARCHIE

ARCHIE is an automated resource for evaluating chemical hazard accidents. The US Department of Transportation developed this software in partnership with the Federal Emergency Management Association (FEMA) and the USEPA. It is an atmospheric emission and dispersion assessment tool that can be used to assess vapor dispersion, fire, and explosion effects associated with episodic releases of hazardous materials into the environment. In addition, the software can estimate emissions and duration of liquid/gas releases from tanks, pipelines, and corresponding ambient concentrations downwind of those releases [13].

ARCHIE's strong sides:

- model is straightforward to use;
- it contributes to a better understanding of the nature and sequence of events that can occur after the accident and the resulting consequences.

The software has a limitation. It takes approximately 10–15 min to run the program, including the time required to answer all questions on a typical problem (www.eng.utolefo.edu).

BREEZE

The Environmental Protection Agency, the US Military, and Coast Guard in 1987 developed this complex. It includes toxic gas dispersion, thermal radiation fire, and explosion models. BREEZE functions include 3D Analyst in its arsenal for visualization of results and export to Google Earth. In addition, it can simulate multiple sources simultaneously. The user can define this receptor/target location n and draw a base mipmap (AutoCAD DXF, ESRII Shapefile, or bitmap) using a mouse for precise placement (www.chempute.com). There is a reduced model setup and execution time with an intuitive ribbon panel interface and script templates. There is a built-in chemical database [14].

Strong sides of BREEZE:

- easy to use and quick to work;
- the intuitive interface will help the user enter the necessary and additional data related to the potential release of chemical substances (for example, the size and position of the tank rupture, the shape of the storage tank, the volume of the spill, and the presence of a reservoir) and also select the appropriate algorithms;

- results are provided in tabular and graphical formats, including 2D contour, 3D volume, and time series plot;
- operator errors are greatly minimized due to a clear list of model execution warnings.

CHARM

This software allows air transport and dispersion calculations, vapor cloud explosions, boiling liquid expanding bursts (BLEVE), jet fire, and pool fire radiation. Two versions of CHARM software are available: one for a single source on flat terrain and another for multiple origins on rough terrain. Features of CHARM include the effects of nuclear radiation. It was added to the complex version of the landscape. In addition, an intricate understanding of the terrain uses a 3D grid for modeling [15]. This software is designed for the following solutions:

- movement and concentration of air plumes from released chemicals;
- mechanical overpressure from pressure tanks and overpressure explosion from steam cloud ignition;
- traces of thermal radiation associated with jet fires, pool fires, and BLEVEs;
- impact on the population associated with any of the traces described above.

CHARM allows you to define and save a base map automatically displayed each time you start CHARM. It is done to save time in emergencies. CHARM is a Gaussian air movement model that treats any emission as a series of air flows.

The distribution description calculated by the Source Term module is required information for the Transport/Dispersion module. Calculated distribution description data includes the following [16]:

- position X, Y, Z;
- chemical mass fraction (vapor and liquid phases);
- temperature;
- a mass of air;
- a mass of water vapor;
- exit direction and speed;
- dimensions;
- hidden energy.

The emission type determines the calculations used in the Source Term module. CHARM models the following types of emissions: container/surface description and evaporation pool/lagoon, defined by the user.

The flat terrain version of CHARM is designed to simulate release from a single source [17] (Fig. 1). Release description, meteorological parameters, and grid are the inputs required to run the scenario in the complex terrain version. This version does not require a grid. The version with rugged terrain is much more complete and can work with several sources of different types (Fig. 2).

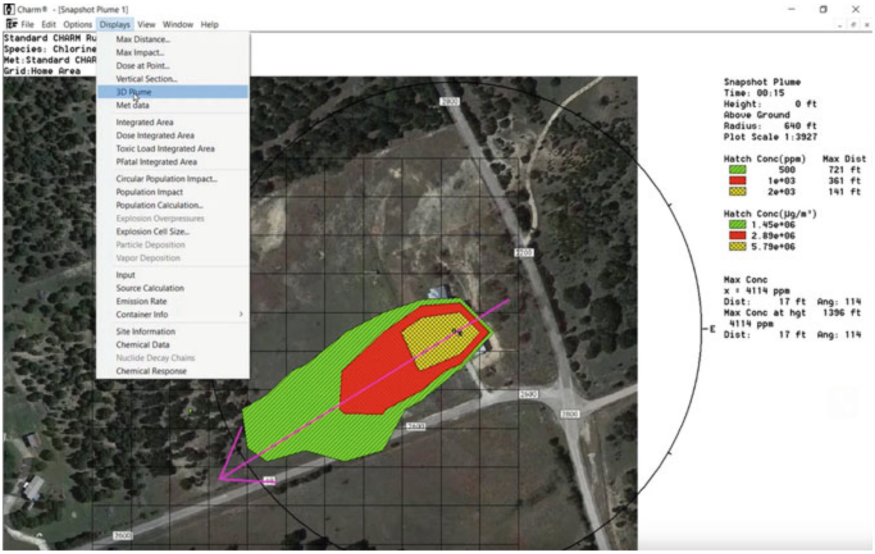

Fig. 1 Visualization of the flat terrain version [17]

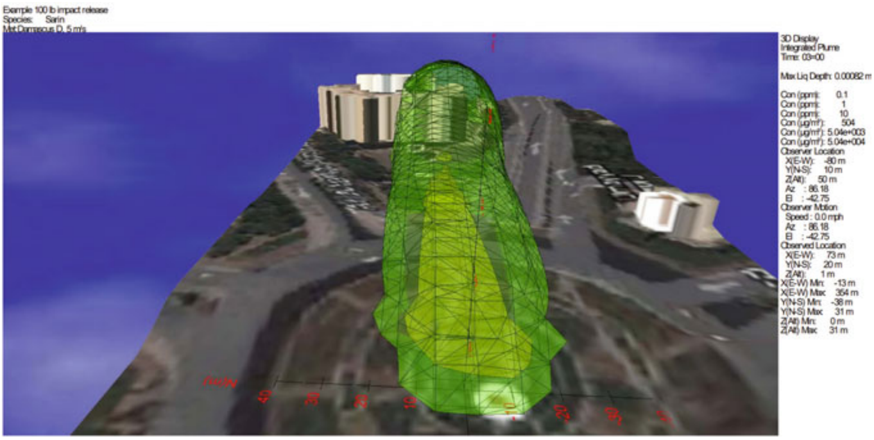

Fig. 2 Visualization of the complex terrain version [18]

Both versions include the following features:

- editor for adding/editing chemicals;
- editor for adding maps;
- the rate of emissions changing over time;
- two-phase emissions;
- shroud emissions, evaporation pools, and user-defined velocity;
- meteorology changing over time;

- real-time meteorology is available if there is a data collection system;
- automatic map import from the Internet.

The main features list of the complex terrain version:

- the influence of 3-dimensional relief on the wind field and dispersion over the area;
- averaging time is included in all concentration results;
- all results can be displayed in 3-D. This includes fires, explosions, and concentration effects;
- vertical sections can be displayed for the region along any line drawn by the user;
- effects "Probability of fatal outcome" (if probit parameters are provided), "Dose," "Toxic load," and "Thermal dose" can be displayed as any other effect;
- the editor can define grids by importing DEM and land use data available over the Internet from the USGS, the Globe Project, and other sources. Various file formats can be read, including DEM and GeoTiff;
- the height of the receptor for the plan view can be the MSL height or the height above the surface;
- maps can be superimposed on 3-D terrain;
- source location can be defined as a location on a track defined by x (longitude), y (latitude), z, and time;
- graphics program is available to display terrain, hits, and maps using DirectX for a more realistic display;
- calculation of advection/dispersion is performed on a three-dimensional grid using a finite-difference solution;
- script and its calculations can be saved in a separate set of files, so recalculation is not required;
- several release locations (each with different views) can be simulated in one run;
- each release can be at a different time in the same scenario;
- several meteorological sites;
- liquid emissions can be allowed to flow with the terrain during the formation of basins;
- source can be particles with a user-defined size distribution. Concentrations and amounts of precipitation can be displayed;
- particles can be coagulated, evaporated/condensed, and formed as a result of chemical reactions and fell to the ground;
- convective heat transfer from the surface to the torch is considered;
- chemical reactions can be calculated. The reaction rate can vary depending on temperature, solar radiation, particle size, or depends on air and water vapor;
- user can edit chemical reactions;
- three-dimensional calculation grid can contain nested grids;
- nested grids can be defined by the user or automatically created by CHARM;
- 3D grid can represent rooms, pipes, or other objects not attached to the ground;
- the ability to export grid information to ASCII and BREEZE files;
- the ability to create Google Earth files (kml/kmz) of buildings/objects, 2D and 3D effects;

- the impact of nuclear radiation from nuclides in emissions;
- possibility to specify the nuclide and mass composition of the emission;
- radiation level and dose are calculated and displayed in 2D, 3D, and tables.

So, let's summarize the main strong sides of CHARM software:

- it can be used inside and around buildings in addition to taking into account the influence of the terrain;
- results are provided in 2D, 3D and tabular format;
- it can calculate particle dynamics;
- the model can automatically set nested grids around the source to provide more detailed calculations [19].

CANARY

Quest's CANARY software is designed to assess the potential consequences of the hazardous liquid release [20]. It includes application-specific hazard models for vapor dispersion, fire emission, and vapor cloud explosions. CANARY has supporting models to generate the source terms required for consequence models: multicomponent thermodynamic calculation, liquid evaporation calculation, and release rate calculation. CANARY allows the user to define hazard endpoints (e.g., gas concentration, radiation flux, overpressure) that determine the extent of the toxic or flammable gas cloud, radiation from multiple types of fire, or overpressure from an explosion.

It provides thermodynamic calculations for mixtures of up to 10 components. In addition, it has a database of over 250 members. The component database and thermodynamic model allow CANARY to process many mixtures and materials, including light hydrocarbons, heavy hydrocarbons, aromatics, toxins, refrigerants, and liquefied gases. The complete list of these substances is presented in [21].

CANARY integrates multicomponent thermodynamics into time-varying fluid release simulations. These simulations account for two-phase flow, flash evaporation, aerosol formation, and liquid rain. In addition, evaporation from liquid pools takes into account pool dispersion, heat transfer effects, and neutralization. The information generated by these models forms the input term(s) for hazard models.

CANARY includes application-specific hazard models: vapor dispersion, fire radiation, and vapor cloud explosions. In addition, CANARY allows users to define hazard endpoints: gas concentration, radiation flux, overpressure, and hazard of flammable and toxic vapor clouds as a result of emissions: pressurized gases, liquefied gases, superheated liquids, supercooled liquids, and volatile liquids. An example of modeling in the software is presented in Fig. 3.

Strong sides of CANARY:

- It accepts a wide range of user input.
- It has a complex character, valid for any project that requires the calculation of process hazards.

Fig. 3 Example of modeling in the CANARY software

Analysis of the consequences begins with calculating the liquid release rate and its thermodynamic state after depressurization into the atmosphere. The amount of material spilled into the ground or became a vapor or aerosol is determined if the release starts as a liquid. Dispersion of the released material in the atmosphere is predicted for the vapor clouds hazard. The release model provides information to fire radiation models to determine thermal radiation effects if the ignition of flammable material is assumed vapor cloud explosion (VCE) model can be used to assess the impact of overpressure if a combustible vapor cloud ignites. Several other models of consequences for specific purposes are also used. These include using publicly available consequence models (e.g., DEGADIS or LNGFIRE for LNG), computational fluid dynamics models to solve complex problems, or models built to solve specific consequences analysis tasks [22].

The models used in this software are taken from open scientific sources (published scientific articles), and individual data included in the models are obtained from internal tests conducted by Quest. Hazardous liquids were released into the atmosphere during these tests. At the same time, most of the received data are unavailable.

PHAST

PHAST is a comprehensive hazard analysis software for all process design and operation phases. PHAST contains models developed for hazard analysis of scenarios: emissions and dispersion, jet fires, pool fires, fireballs, and toxic emission hazards, including indoor harmful dose calculations. Its features include the use of a geographic information system (GIS) to display the results of consequences on maps and site plans (Figs. 4, 5, 6 and 7) [23]. In addition, this software may conduct sensitivity studies to assess the need for mitigation measures such as design, operational, or response changes.

Strong sides of PHAST:

- Ease of use is achieved due to the predefined relationship of emission, dispersion, pool, flammability, and toxicity calculations.
- Quick and accurate results.
- Comprehensive reports and charts for the easy and intuitive display of results.
- It considers emissions from leaks, pipe breaks, safety devices, vessel breaks, and ventilation.

Fig. 4 Thermal radiation contours

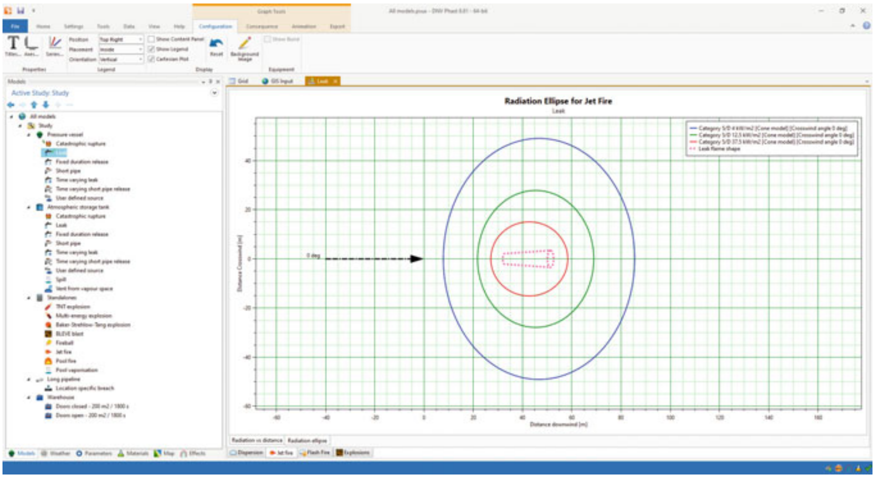

Fig. 5 List of scenarios for simulation

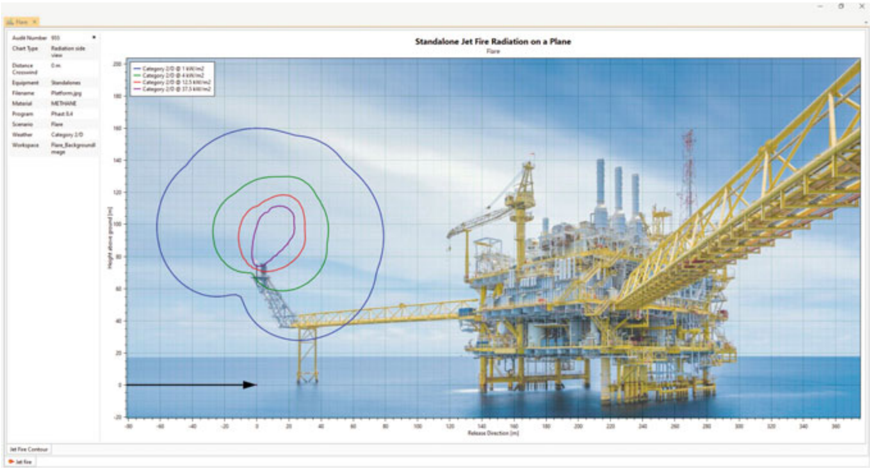

Fig. 6 Results of modeling on an artificial object

KAMELEON FIREX

This software tool was developed by Comput IT together with partners Statoil, ENI-group, ConocoPhillips, Gaz de France, Ruhrgas, and Sandia National Laboratories. KAMELEON FIREEX is an advanced Computational Fluid Dynamics (CFD) tool for 3D transient modeling of flares, gas dispersion, fire development, and fire mitigation. Features of this tool include efficient and user-friendly pre- and post-processing capabilities. In addition, it has options for animating simulation results and "moving cameras" through the simulation [24].

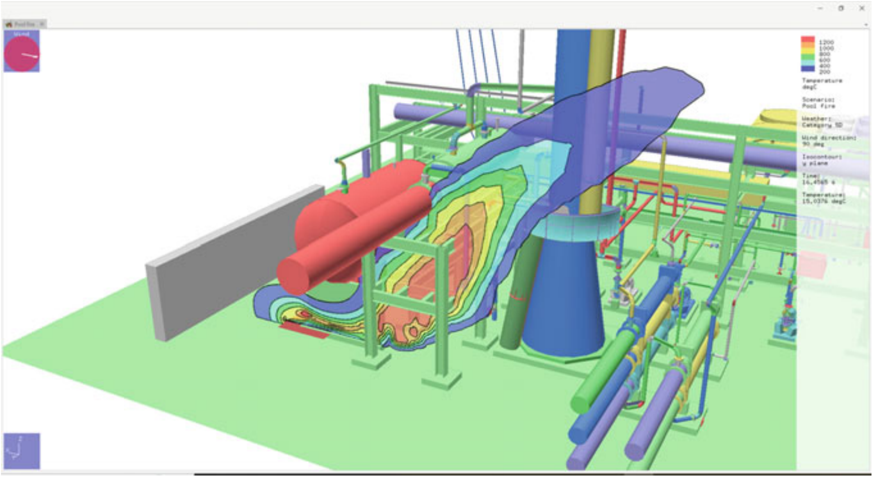

Fig. 7 Pool fire modeled by Phast CFD extension

This software has CAD import capabilities where CAD geometries are automatically converted to solid structures or surface/volume porosity used by the KFX calculation model. In addition, its models can pass the results of their calculations as input data to other models.

Strong sides of KAMELEON FIREX: it gives quick and accurate results; a clear list of model launch warnings greatly minimizes operator error.

FLACS

This is a CFD tool developed by GEXCON. It is widely used in the explosion and atmospheric dispersion modeling [25]. It has special modules for modeling gas, dust, and explosions using chemical explosives such as TNT. Its features include integrated explosion and dispersion modeling capabilities. This allows modeling consequences in Full-3D with an assessment of mitigation effects and preventive measures. In addition, it has a porosity distribution model for obstacles at a small subgrid-scale, a semi-automatic process for generating complex flow geometries, and a simple Cartesian grid that allows fast simulations compared to other general-purpose CFD codes (Figs. 8, 9) [26].

This software allows you to choose modules for individual needs [27]:

– FLACS-Dispersion can simulate natural, forced ventilation and loss of tightness due to leaks and dispersion of hazardous substances;
– FLACS-GasEx can simulate steam cloud explosions;
– FLACS-Fire module has jet and basin fire modeling;
– FLACS-Hydrogen is a tool for assessing the risk associated with the use of hydrogen as an energy carrier;
– FLACS-Blast simulates the propagation of blast waves arising from the detonation of condensed-phase explosives;

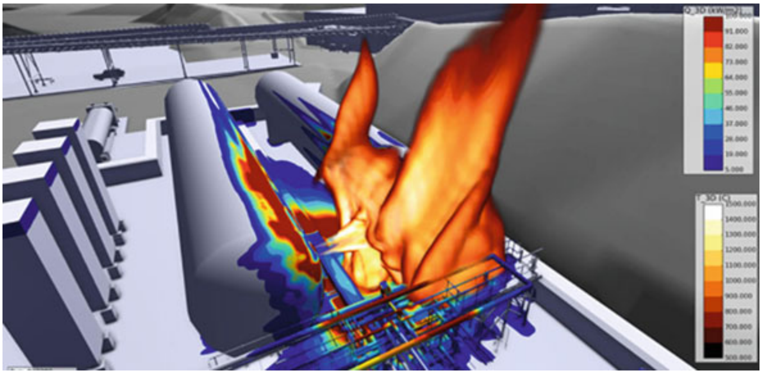

Fig. 8 Modeling the consequences

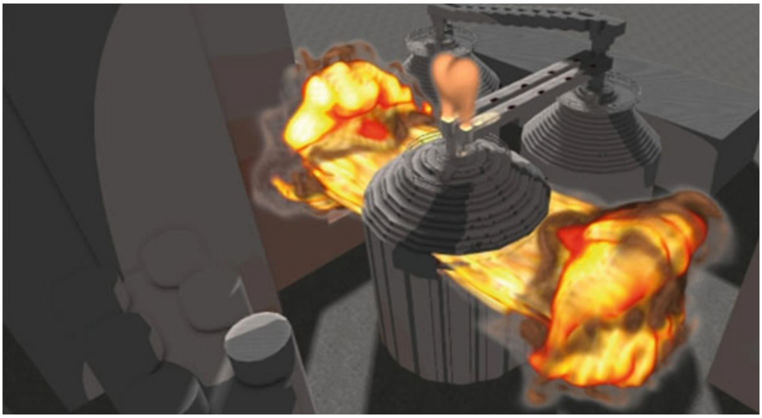

Fig. 9 Simulation of various geometry and texture

– FLACS-Risk can model and visualize 3D CFD risks.

Strong sides of FLACS:

– it has various options for viewing results in 2D, 3D, animation, and text files. It provides a better understanding of phenomena and results;
– atmospheric conditions at the entrance can be determined by taking into account the roughness of the surface and stability of the atmosphere;
– the wide application can perform both dispersion and explosion with the same installation.

Limitations of FLACS:

– many of the validation studies reported that FLACS do not provide enough detail to give confidence in the reproducibility of the results;

- often, results are shown for only one grid, and grid sensitivity tests are not reported;
- FLACS uses a one-block Cartesian grid. This can lead to unreliable predictions of dense gas scattering over sloping or undulating terrain due to too high momentum dissipation from the stepped surface simulation. Modeling such flows requires a curvilinear, unstructured grid or a cut-cell approach. The single-block Cartesian grid also introduces limitations to the approach that can be used to model gas jets. Grids cannot contain vast numbers of cells. Code is not yet parallelized;
- FLACS has no submodel selection. Only one turbulence model is provided, which is well established. But has some limitations, and the code lacks a Lagrangian or inhomogeneous Euler model for splash or particle modeling.

TRACE

TRACE is an engineering analysis tool for dispersion modeling [28]. It provides simulations of accidental releases of toxic substances caused by pipe/flange leaks, water spills, hydrogen fluoride, acid spills, pipe emissions, or elevated dense gas emissions [29]. In addition, simulation capabilities for scenarios such as vapor cloud explosions, solid explosives, pool fires, and flares are updated. Its key features include a comprehensive chemical database of over 600 pure constituents of substances as well as liquid mixtures. The sequential process prompts the user and leads to a set of models to solve the problem.

WHAZAN

Technica International Ltd., in collaboration with the World Bank, develops WHAZAN (World Bank Hazard Analysis). It is an impact analysis package. This package calculates consequences and hazard zones resulting from incidents involving toxic and flammable chemicals. It contains models of the dispersion of harmful substances, fire, and explosion [30]. WHAZAN has an extensive chemical library that the user can expand. The software can run models separately or link two or three models so that the output of one model can be automatically used as input to another model [31]. All models included in AST are semi-empirical and subject to constraints. The accuracy of the results depends on the assumptions made by the model and the accuracy of the input data.

Strong sides of WHAZEN:

- product is easy to use and quick to work;
- the user interface is designed to minimize operator errors.

SCIA

SCIA software [32] is designed to assess and analyze all possible hazards from industrial accidents. It includes models for fire, explosion, and toxic release assessment. These models can be used to study radiation, overpressure, and toxic spill hazards in various scenarios.

SCIA features include GIS for scenario screening/evaluation. It contains MSDS.

The strong sides of SCIA are:

- Simulation quickly and reliably assesses the consequences of possible accidents.
- A convenient and effective tool for assessing the consequences of significant chemical accident decision-making processes for land use planning.
- Results can be saved in various formats, exported to Microsoft Excel, and then plotted using Microsoft Excel or VB.
- A clear list of model execution warnings greatly minimizes operator error.

HAZDIG

HAZDIG (HAZardous Dispersion of Gases) is a tool for studying the accidental release of hazardous chemicals and their consequences [33]. HAZDIG consists of five main modules for data, emission scenario generation, dispersion, characterization, and graphics. In addition, it includes the latest models for estimating atmospheric stability and distribution.

HAZDIG has unique features. The database contains various proportionality constants, and complex empirical data is built into the system. Moreover, it has a modular structure that ensures fast data processing and calculation of the result.

Strong sides of HAZDIG:

- graphic module provides a presentation of the results in an easy-to-understand and visually attractive form;
- output data of the software is formatted in such a way that it can be directly used for reporting results without the need for editing;
- broader applicability: it includes more models than existing accident simulation packages to handle more situations with minimal input data;
- higher accuracy: it contains more accurate and newer models than those processed by existing packages;
- convenience for the user.

MAXCRED

MAXCRED software allows you to simulate an accident and assess potential damage. This software includes various explosion and fire models: confined vapor cloud explosion, unconfined vapor cloud explosion, BLEVE, pool fires, flares, and fireballs. A unique feature of MAXCRED is that it can handle the dispersion of heavier-than-air and lighter-than-air gases. In addition, the software can check the plausibility of the proposed scenario [34].

The strong sides of MAXCRED are the following:

- it is capable of simulating accidents of the second and higher order;
- broader applicability: it includes more models than existing accident simulation packages to handle more situations with a minimum amount of data;
- it contains more accurate and newer models than those processed by existing packages;

– convenience for the user.

ALOHA

ALOHA (Areal Locations of Hazardous Atmospheres) is a computer program designed specifically for use by emergency responders for emergency planning and training [35, 36]. ALOHA models the critical hazards—toxicity, flammability, thermal radiation (heat), and overpressure (explosive force). These issues are associated with chemical releases that result in toxic gas releases, fires, and explosions. In versions before 5.4, ALOHA only models a harmful threat: how the cloud of poisonous gas may dissipate in the atmosphere after an accidental chemical release. This software dashes on small computers that are easy to transport and affordable to most users [37].

This program's chemical library contains information on the physical properties of approximately 1,000 common hazardous chemicals. Calculations performed by the program represent a compromise between accuracy and speed; ALOHA was designed to get results quickly and minimize operator error. The program checks the information you enter and warns you of mistakes. ALOHA was developed jointly by the National Oceanic and Atmospheric Administration (NOAA) and the Environmental Protection Agency (EPA).

ALHOA models three hazard categories: toxic gas release, fire, and explosion. This program uses several different models, including the air dispersion model. This model estimates the movement and dispersion of chemical gas clouds. ALOHA can estimate toxic gas dispersion, overpressure values from a vapor cloud explosion, or flammable vapor cloud regions using the given model. ALOHA uses additional models to assess hazards associated with other fires and explosions. As a result, ALOHA can quickly solve problems and provide results in a graphical and easy-to-use format.

ALOHA allows the modeling of chemical emissions from four sources (Direct, Spill, Tank, and Gas pipe) (Table 1).

ALOHA can model the dispersion of pollutant gas clouds in the atmosphere. It also displays a diagram showing a top view of regions or threat zones where it predicts exceeding key hazard levels (LOCs). ALOHA uses the Gaussian model to predict how gases with roughly the same buoyancy as air disperse in the atmosphere (Fig. 10). This software uses weather data that can be entered by the user or directly from a weather station.

Heavy gas dispersion calculations used in ALOHA are based on the same as in the DEGADIS model. The last is one of several known heavy gas models. This model was chosen due to its general acceptance and extensive testing by the authors.

ALOHA allows simulating fire and explosion scenarios and toxic gas dispersion scenarios starting with version 5.4.

ALOHA has an easy-to-use graphical interface and display. It also includes a mapping program called MARPLOT that allows you to customize overlays showing local features and vulnerable populations.

Table 1 ALOHA sources and scenarios

Source	Poisoning scenarios	Fire scenarios	Explosion scenarios
Direct			
Direct emission	Cloud of toxic vapor	Flammable zone (fire flare)	Vapor cloud explosion
Spill			
Evaporation	Cloud of toxic vapor	Flammable zone (fire flare)	Vapor cloud explosion
Burning (spill fire)		Spill fire	
Tank			
Not flammable	Cloud of toxic vapor	Flammable zone (fire flare)	Vapor cloud explosion
Combustion		Jet fire, spill fire	
The explosion of boiling, expanding liquid		The explosion of expanding boiling liquid (fireball and spill fire)	
Gas pipe			
Not flammable	Cloud of toxic vapor	Flammable zone (fire flare)	Vapor cloud explosion
Combustion		Jet fire	

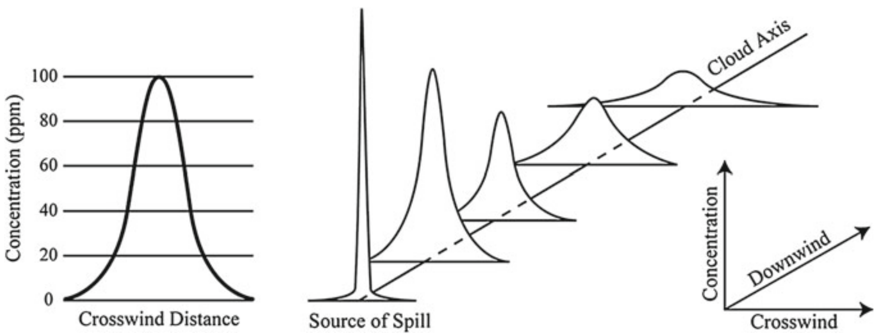

Fig. 10 Gaussian distribution

ALOHA system has a limitation–e input should be corrected, and a new hazard zone chart created if any atmospheric conditions (such as wind speed) change significantly during the response. In another case, the old chart may need to be revised even if you can provide accurate data.

ALOHA results can be unreliable under certain conditions. There are some effects that ALOHA does not a model at all. ALOHA results may be unpredictable under the following conditions:

– deficient wind speed;

- very stable atmospheric conditions;
- wind movement and terrain effects;
- concentration unevenness, especially near the emission source.

ALOHA does not consider the accumulation of high gas concentrations in low-lying areas.

ALOHA allows you to enter only individual wind speed and wind direction values. The wind speed and direction are assumed to remain constant (at any given height) throughout the area downwind of the chemical release. ALOHA does not consider terrain, the presence of various structures, or other obstacles (Fig. 11).

Wind creates vortices and changes direction and speed in cities with the flow around large buildings. As a result, it significantly changes the shape and movement of the cloud, as shown in Fig. 12. Streets bordering large buildings can create a street canyon pattern that intercepts and directs dissipating clouds. ALOHA ignores these effects when making a threat zone graph; the threat area will appear to pass over or through obstacles such as buildings.

ALOHA's performance is limited because wind can change direction and speed both over distance and over time. As a result, ALOHA will not make predictions more than an hour after the start of the release of more than 10 km (6.2 miles) from the release point (it truncates threat zones longer than 10 km).

ALOHA does not take into account the following issues during simulation:

- by-products of fires, explosions, or chemical reactions;
- shares;
- chemical mixtures;
- topography of the area;
- dangerous fragments.

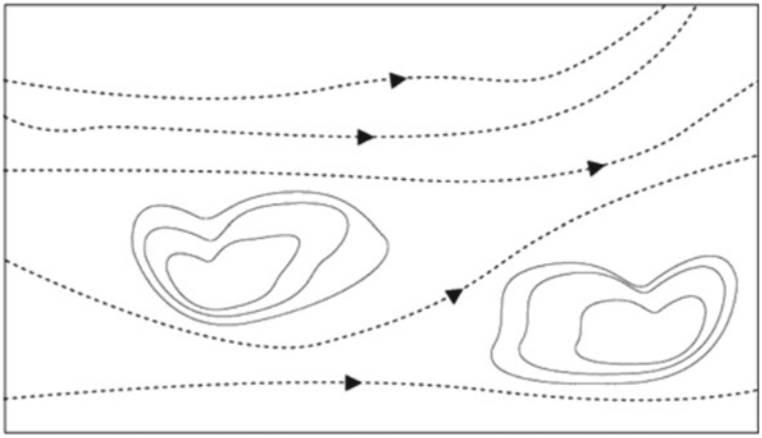

Fig. 11 Change in wind movement depending on the topography of the area

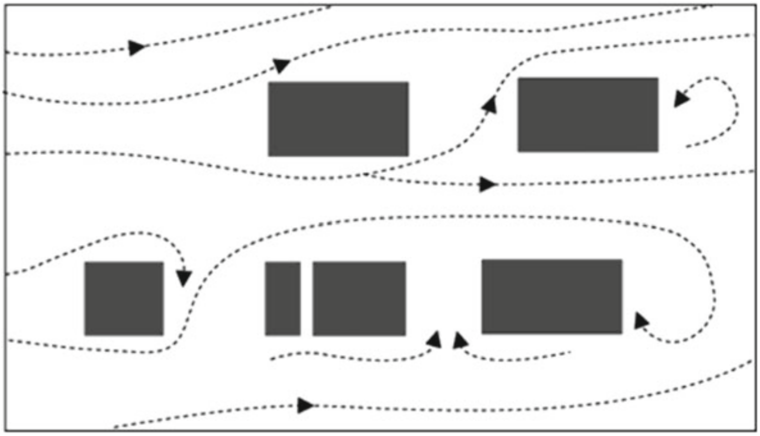

Fig. 12 Small-scale fluctuations in wind direction

ALOHA assumes that dissipating chemical cloud does not react with the atmosphere gases (oxygen and water vapor). Therefore, ALOHA does not consider processes that affect the dispersion of particles (including radioactive particles).

ALOHA is designed to simulate the release of pure chemicals and some chemical solutions. ALOHA is not intended for use with radioactive chemical releases.

This software does not consider the accumulation of discharge in depressions or liquid flow down the slope.

ALOHA does not simulate the trajectories of dangerous fragments that can occur in explosions.

3 Conclusions

Accidents at chemically hazardous facilities are often accompanied by releasing dangerous chemicals into the environment. Their spread threatens the life and health of the service personnel of enterprises and the surrounding area population.

Methodical software is used to quickly make appropriate management decisions at all stages of such situations to assess the consequences of accidents at chemically hazardous facilities and to effectively solve emergency rescue and other urgent work in emergency zones.

It was established that the following software tools are the most effective due to their advantages and features: EFFECTS, ARCHIE, CHARM, CANARY, PHAST, KAMELEON FIREX, FLACS, TRACE, WHAZAN, SCIA, HAZDIG, MAXCRED, and ALOHA. Such an assumption was made due to a critical analysis of specialized computer systems for assessing the consequences of accidents at chemically hazardous facilities. Their use allows simulation of results of the release (spill) of dangerous substances during accidents using geoinformation technologies; investigation of the influence characteristics of input factors on the process of distribution of hazardous chemicals in the environment; increasing visibility of the forecasting process of consequences of accidents at chemically hazardous objects and transport by visualizing the calculation process and forecasting results; forming skills and abilities to systematize information about chemically dangerous substances, methods of protection and procedures for dealing with them.

References

1. Popov, O.O., et al.: Approaches to assessing consequences of accidents during transportation of hazardous substances by road. In: Studies in Systems, Decision and Control. Systems, Decision and Control in Energy IV (2023, in press)
2. Anpilova, Y., Yakovliev, Y., Trofymchuk, O., Myrontsov, M., Karpenko, O.: Environmental hazards of the Donbas hydrosphere at the final stage of the coal mines flooding. In: Systems, decision and control in energy III. Studies in systems. Decision and Control. Springer, Cham (2021). https://doi.org/10.1007/978-3-030-87675-3_19
3. Yatsyshyn, T., Shkitsa, L., Popov, O., Liakh, M.: Development of mathematical models of gas leakage and its propagation in atmospheric air at an emergency gas well gushing. East. Eur. J. Enterp. Technol. **5/10**(101), 49–59 (2019). https://doi.org/10.15587/1729-4061.2019.179097
4. Kotsiuba, I.G., Skyba, G.V., Skuratovskaya, I.A., Lyko, S.M.: Ecological monitoring of small water systems: algorithm, software package, the results of application to the uzh river basin (Ukraine). Methods Objects Chem. Anal. **14**(4), 200–207 (2019). https://doi.org/10.17721/moca.2019.200-207
5. Skurativska, I., Skurativskyi, S., Popov, O., Mykhliuk, E., Dement, M.: Complex oxygen regimes of water objects under the anthropogenic loading. In: Studies in Systems, Decision and Control. Systems, Decision and Control in Energy III, vol. 399. pp. 317–334. (2022). https://doi.org/10.1007/978-3-030-87675-3_20
6. Popov, O.O., et al.: Software and modeling tools for assessment of environmental consequences of open flowing of oil wells. In: Studies in Systems, Decision and Control. Systems, Decision and Control in Energy IV (2023, in press).
7. Semerikov, S., et al.: Our sustainable pandemic future. E3S Web Conf. **280**, 00001 (2021). https://doi.org/10.1051/e3sconf/202128000001
8. Semerikov S.O., et al.: 3rd International Conference on Sustainable Futures: Environmental, Technological, Social and Economic Matters. In: *IOP Conference Series: Earth and Environmental Science*, vol. 1049, p. 011001 (2022). https://doi.org/10.1088/1755-1315/1049/1/011001
9. Myrontsov, M., Karpenko, O., Trofymchuk, O., Okhariev, V., Anpilova, Y.: Increasing vertical resolution in electrometry of oil and gas wells. In: Systems, Decision and Control in Energy II. Studies in Systems, Decision and Control, vol. 346. pp. 101–117 (2021). https://doi.org/10.1007/978-3-030-69189-9_6
10. Hovalenkov, S.S.: Emergency prevention caused by man-made emissions of hazardous light gaseous chemicals. National University of Civil Defence of Ukraine, State Emergency Service of Ukraine, Kharkiv (2020)
11. TNO: Effects Advanced, easy-to-use consequence analysis: Software that streamlines safety analysis. (2017). http://resolver.tudelft.nl/uuid:0dac0288-8862-4d9e-91d3-38a8fcd42589
12. Suganya, R., Abbasi, S.A.: A critical assessment of available software for forecasting the impact of accidents in chemical process industry. Int. J. Eng. Sci. Math. **6**(7), 269–289 (2017)
13. Early, I.I., Livingston, M.C, Newsom, D.E.: A pilot program for introduction of (ARCHIE) automated resource for chemical hazard incident evaluation. United States (1990)

14. SAFETY & QUALITY (2022). https://www.chempute.com/safety.html
15. CHARM® Software–When Realism Counts (2022). https://www.charmmodel.com/
16. Eltgroth, M.W.: Complex hazardous air release model (CHARM®) technical reference manual. https://www.charmmodel.com/doc/TechRef_09.pdf
17. CHARM Trial–Flat Terrain (2022). https://www.charmmodel.com/charmtrial-flatterrain.aspx
18. CHARM Trial–Complex Terrain (2022). https://www.charmmodel.com/charmtrial-complexterrain.aspx
19. CHARM User's Manual CHARM User's Manual. Mark Eltgroth LLC, Lometa, Texas. https://www.charmmodel.com/doc/UserMan_09.pdf
20. CANARY by Quest—Consequence Analysis Software (2022). https://www.questconsult.com/software/canary/
21. CANARY Materials (2022). https://www.questconsult.com/pdf/CANARY_Materials.pdf
22. Consequence Analysis (2022). https://www.questconsult.com/services/consequence-analysis/
23. Control your hazards by knowing the consequences (2022). https://www.dnv.com/software/services/plant/consequence-analysis-phast.html#Software
24. Fire simulation software–CFD simulation - Kameleon FireEx–KFX (2022). https://www.dnv.com/services/fire-simulation-software-cfd-simulation-kameleon-fireex-kfx-110598
25. FLACS-CFD (2022). https://www.gexcon.com/software/flacs-cfd/
26. FLACS-CFD Features & Benefits (2022). https://www.gexcon.com/software/flacs-cfd/features-benefits/
27. FLACS-CFD Solvers (2022). https://www.gexcon.com/software/flacs-cfd/solvers/
28. SAFER Systems Safer Trace assessment tool for toxic chemicals (2022). https://www.thebigredguide.com/safer-systems-safer-trace-software-technical-details.html#more-info
29. Popov, O.O., et al.: The use of specialized software for liquid radioactive material spills simulation to teach students and postgraduate students. CEUR Workshop Proc. **3085**, 306–322 (2022). http://ceur-ws.org/Vol-3085/paper05.pdf
30. Kiranoudis, C., Kourniotis, S.P., Christolis, M.N., Markatos, N.C.: An operational centre for managing major chemical industrial accidents. J. Hazard. Mater. **289**(2–3), 141–161 (2002). https://doi.org/10.1016/S0304-3894(01)00299-0
31. Kumar, A., Agarwal, S.: Whazan: A software for chemical hazards analysis. Environ. Prog. **8**(3), A6–A7 (1989). https://doi.org/10.1002/EP.3300080305
32. SCIA ENGINEER (2022). https://www.scia.net/en/scia-engineer
33. Khan, F.I., Abbasi, S.: HAZDIG: a new software package for assessing the risks of accidental release of toxic chemicals. J. Loss Prev. Process Ind. **12**(2), 167–181 (1999). https://doi.org/10.1016/s0950-4230(97)00043-0
34. Khan, F.I., Abbasi, S.A.: MAXCRED—a new software package for rapid risk assessment in chemical process industries. Environ. Model. Softw. **14**(1), 11–25 (1998). https://doi.org/10.1016/S1364-8152(97)00031-5
35. ALOHA Software (2021). https://www.epa.gov/cameo/aloha-software
36. Zinovieva, I.S., et al.: The use of GIS in renewable energy specialist's learning. CEUR Workshop Proc. (2023, in press)
37. ALOHA.: USER'S MANUAL. February 2007. National Oceanic and Atmospheric Administration (NOAA) and the Environmental Protection Agency (EPA), Washington (2007). https://nepis.epa.gov/Exe/ZyPDF.cgi/P1003UZB.PDF?Dockey=P1003UZB.PDF