

Article

Software for Hazard Zone Visualization in Case of Fire at Industrial Facility Based on Cellular Automaton Method

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Abstract

Modeling and visualizing zones within the spread of toxic clouds from fires and explosions during accidents at industrial facilities located near residential areas is of high practical value. This tool is critical for the rapid planning of population evacuation measures and emergency response. Of particular importance is the development of computer software that can quickly model the hazard zone of toxic cloud spread and superimpose it on a terrain map to determine the potential impact on residential areas. This software should be based on a mathematical model that can accurately predict the parameters of the hazard zone both near the industrial facility and beyond it, at a distance of more than 1 km. The objective of this study is to create algorithms for modeling the hazard zone during a fire or explosion at an industrial facility using a cellular automaton method and to develop a software tool for its visualization. The software must display the hazard zone for the population of a nearby residential area on a map in real time, which is necessary for assessing potential harm to residents' health and in planning their rapid evacuation. To achieve this objective, this article presents a model for determining the boundaries and main parameters of a hazard zone based on the cellular automaton method (frontal and probabilistic). The proposed model takes into account both constants (properties of chemical substances, building parameters, population size, etc.) and variables (the mass of the substance at each explosion and fire, wind speed and direction, air temperature, etc.). The FireSoft III software, developed by the authors and based on the cellular automaton model, provides more rapid calculation of the parameters and delineation of the hazard zone boundaries compared to similar software, which was tested in cases of an ammonia tank explosion and a prolonged fire in a warehouse containing polyvinyl chloride at an enterprise. This makes FireSoft III promising for use in a fire and explosion response at enterprises.

Keywords: cellular automaton; simulation modeling; computer visualization; fire hazard zone; evacuation



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1. Introduction

The location of industrial facilities in a close proximity to residential areas poses a complex threat to their residents. In addition to standard industrial risks (equipment wear, human error, fire outbreaks and explosions of special materials), there is a risk of complex accidents with multiple ignition points and detonation. In particular, the combustion of chemicals can be accompanied by the release of highly toxic reagents, and the decomposition products of building materials can turn into toxic gases. Explosions can lead to the expansion of the distribution zone of toxic substances in both gaseous and liquid form [1]. High residential density around the industrial facilities makes the population extremely vulnerable, as it facilitates the rapid spread of hazardous substances and mass casualties.

A key tool for minimizing environmental damage and ensuring safe living conditions for the population is the modeling of hazardous areas that reveals the potential spread of harmful combustion products when planning housing construction and shows the actual hazardous areas when managing evacuation measures in the event of an accident [2]. It is very important to be able to predict in advance the scale of the consequences of possible accidents, identify the most vulnerable areas and, as a result, develop scientifically based plans to protect ecosystems and the population [3,4].

Chemical process plants are traditionally among the most hazardous facilities, which activities directly threaten both people and environment [5]. This threat becomes catastrophic in the event of accidents, the likelihood of which remains high in agricultural and petroleum chemical production and related industries [6]. It is important to understand that chemically hazardous facilities include more than just specialized plants. Risks also arise from industries where toxic components are contained in raw materials, intermediates, or end products—from metallurgy and oil refining to the production of plastics, construction materials, and pharmaceuticals [7,8]. Thus, the problem is systemic: today, more than one hundred thousand industrial facilities operate worldwide, accumulating significant volumes of toxic and explosive substances [9].

Accidents at industrial facilities, which are defined as the uncontrolled release of mass (chemicals, radioactive substances) or energy (explosions), pose a threat to the respiratory tract, mucous membranes, and skin of humans and animals. The only possible way to assess quantitatively the parameters of such a hazardous source, which cannot be fully reproduced in the experiment, is mathematical modeling. To predict the spread of harmful substances during a fire, the properties of combustible materials are recorded in the model, while the boundaries and concentrations of the hazard zone are calculated as dynamic quantities. Therefore, a correct model must solve a set of interrelated problems: to describe the mechanism of hazard source formation, identify the critical conditions for the emission to begin, and calculate the intensity of toxic compound emissions into the atmosphere in fire and explosion scenarios [10]. In addition, it is necessary to visualize the spread of toxic cloud particles during an accident at an industrial enterprise, originating from point or multiple sources, and linear (pipelines) sources (Figure 1).

The atmospheric conditions of the fires shown in Figure 1 (the mass and composition of burning substances are not reliably known, since the data were taken from open sources to illustrate the scale of the cloud), according to the global weather archive (Weather and Climate, <https://www.weatherandclimate.eu>) are the following: (A) temperature +3.90 °C, wind 0–1 m/s, direction S, atmospheric pressure 998.5 Pa; (B) temperature +17.50 °C, wind 6–7 m/s, direction N, atmospheric pressure 1058.5 Pa; (C) temperature +21.10 °C, wind: 3–5 m/s, direction E, atmospheric pressure 981.5 Pa; (D) temperature +7.50 °C, wind: 6–7 m/s, direction NE, atmospheric pressure 1030.2 Pa.

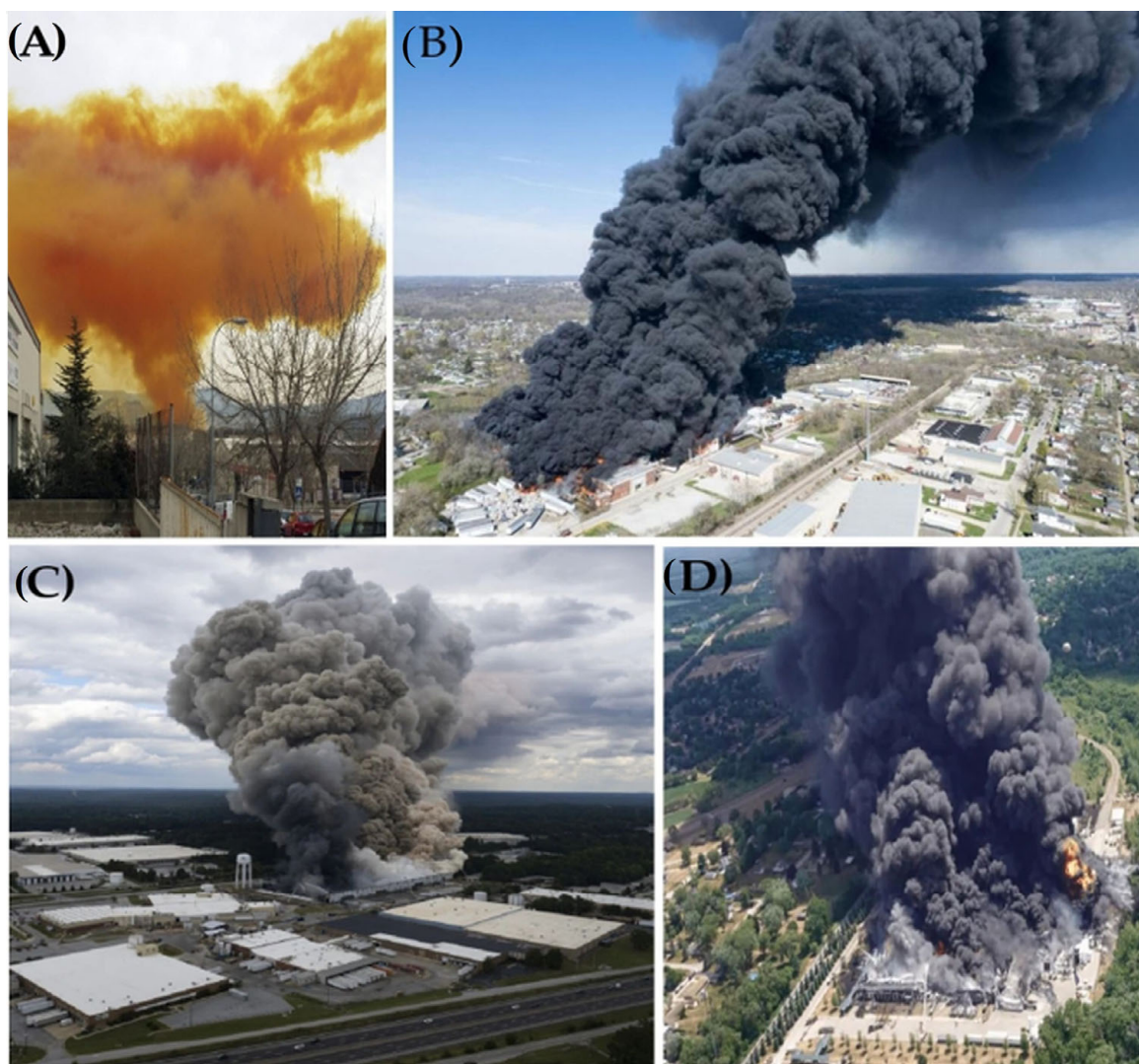


Figure 1. Examples of toxic chemical combustion cloud formation during industrial accidents: (A) An orange toxic cloud is forming after an explosion at a chemical plant in Tarragona, Spain, on 13 February 2015 [11]. (B) Toxic smoke is spewing at a recycling plant in Richmond, Indiana, on 9 May 2023 [12]. (C) Chemical smoke spewing from a Georgia factory is projected to spread toward Atlanta as winds shift on 3 October 2024 [13]. (D) Explosion at a chemical plant in Brunswick, Georgia, on 12 November 2022 [14].

Thus, effective fire and explosion risk management at enterprises requires specialized software that can quickly model the dimensions of a hazardous area, accurately redefining its visual boundaries. A step-by-step study of its development involves, first and foremost, the creation of an automated system for developing and making decisions on managing accident response processes and the evacuation of personnel and residents of nearby areas. Its key function is the simulation of emergency scenarios [15]. The resulting predictive data will serve as the basis for developing a detailed action plan, including, first and foremost, chemical monitoring to determine the contaminated zone, evacuation and search for victims, and assessment of the secondary sources hazard. In the second stage, to localize search-and-rescue operations, software for modeling hazardous areas should help in determining the final contours that show the spread of toxic substances. Finally, in the third stage, computer modeling of the hazardous area should provide data on the area of contamination by combustion products or spills from a chemical explosion for sanitary treatment, together with the collection and disposal of all resulting toxic contaminants.

The objective of this study is to develop and visualize a digital model of the spatial propagation of a toxic substance cloud, taking into account maximum permissible concentrations (MPC). This model is based on a cellular automaton model, leveraging its advantages over other models (Gaussian, Eulerian, etc.). To achieve this objective, several tasks must be completed:

1. Describe mathematically how toxic combustion products are formed and transported in the air during a fire or chemical explosion at an industrial facility, using the cellular automaton method in its probabilistic and frontal iterations.
2. Create an analytical–geometric model of the hazard zone for an accident at a typical industrial facility, based on a cellular automaton.
3. Develop and program an algorithm for calculating the hazard zone.
4. Based on the solutions obtained, create a working prototype of the hazard zone visualization software.

An existing research gap is the lack of studies that explore the possibilities of using the cellular automation method to model hazard zones during fires at industrial enterprises. Existing studies using cellular automation are related to modeling the following processes: fire spread dynamics [16], wildfires [17], fire prevention [18], pedestrian evacuation from local fire zones [19], and hazard zone spread during volcanic activity [20].

The research hypotheses can be presented in the following way:

H1. (Hypothesis on the feasibility of mathematical modeling). *The effective prediction of spatial boundaries and concentrations of toxic combustion products during explosions and fires at industrial facilities is possible on the basis of a mathematical model based on a cellular automaton, which more adequately describes the non-stationary processes of formation and atmospheric transport of harmful substances, taking into account the variable parameters of the source and the environment.*

H2. (Hypothesis of geometric and algorithmic representation). *It is possible to develop a parametric geometric model of the hazardous area and a corresponding computational algorithm that will allow the results of the mathematical description (H1) to be transformed into a dynamic digital model with clear spatial boundaries for various concentrations of toxicants, including subthreshold (below MPC) and hazardous (above MPC) levels.*

H3. (Hypothesis on software implementation and practical significance). *The implementation of developed algorithms and models in the form of specialized software prototype will provide a clear computer visualization (2D and, in the future, 3D representation) of a toxic cloud spread, which can make it possible to use this tool for rapid risk assessment and planning protective measures, thus increasing the effectiveness of decisions in the field of fire and industrial safety.*

2. Materials and Methods

2.1. Classification of Algorithms for Modeling the Spread of a Toxic Substance Cloud

As noted in studies [21,22], an emergency at an industrial enterprise, accompanied by a fire, explosion, and release of toxic substances into the atmosphere, can be represented as a model consisting of three interconnected phases.

In the first phase, breaches in equipment or chemical containers, sparks, and oxidation processes pose a hazard to personnel in the immediate vicinity, who must follow instructions to avoid hazardous consequences. In the second phase, the fire may spread beyond the working area, and its suppression may require the efforts of specialized firefighting services. However, the spread of the toxic cloud to a distance threatening the local community is unlikely. Finally, in the third phase, the fire engulfs workshops and warehouses

containing a significant quantity of hazardous substances. The combustion will persist for a considerable period, forming a toxic cloud that spreads and can create a hazardous area.

Visualization of such a hazardous area, with the potential for an accident to progress from the first to the second and then to the third phase, overlaid on a map of urban development, taking into account the height of buildings and the distances between them, and the presence of forests, provides the optimal distribution of fire and rescue services managing the evacuation of workers and the residents. Therefore, hazardous area modeling methods and software must meet requirements related not only to the accuracy of simulating the spread of a toxic cloud, but also to the consideration of numerous parameters and the speed of calculation, along with the timely updating of data received from emergency services [23].

Key approaches to dispersion prediction include the following models [24]: Eulerian, Gaussian, box models, Lagrangian, and CFD models. The standard systematization of these approaches is recognized as the classification of E. Weber (1982) [25], which divides models into physical, statistical, and deterministic.

The most significant for us is the deterministic modeling approach, based on the physical laws of airborne pollutant transport. A special case of this approach is stationary models, which treat the environment as constant over time. The most well-known and widely used model of this type is the stationary Gaussian model.

In our previous article, we examined the well-known Gauss equation for calculating the area of a hazardous zone, based on the determination of its boundaries, derived from the calculation of the concentration in the hazardous zone (and subsequent comparison with the MPC), accounting for the continuous emission of toxic combustion products from one point and constant wind speed (1) [26].

$$C(x, y, z, p, z_0) = \frac{Q^*}{2\pi\sigma_y(x, p, z_0)\sigma_z(x, z_0)U} \cdot \exp\left[-\frac{(y-y_0)^2}{2\sigma_y^2(x, p, z_0)}\right] \cdot \left[\exp\left(-\frac{(z-h)^2}{2\sigma_z^2(x, z_0)}\right) + \exp\left(-\frac{(z+h)^2}{2\sigma_z^2(x, z_0)}\right)\right] \quad (1)$$

where $C(x, y, z, p, z_0)$ is the concentration of toxic combustion products within the hazard zone, g/m^3 ; Q is the emission intensity, g/s ; y_0 is the coordinate of the emission source; x, y, z are the coordinates of the concentration measurements; U is the average wind speed, m/s ; h is the height of the emission source of toxic substances, m ; p is the category of atmospheric stability; z_0 is the surface roughness coefficient; σ_z and σ_y are the parameters of vertical and horizontal dispersion; $Q^* = f_F \times f_W$ is a value that takes into account corrections for the depletion of the toxic cloud over time; and f_F and f_W are the coefficients of dry and wet deposition of harmful substances on the surface [26]. According to Equation (1), the concentration $C(x, y, z, p, z_0)$ depends directly on the dispersion coefficients σ_y and σ_z , which, in turn, are calculated taking into account the type of atmospheric stratification and the properties of the underlying surface [26].

Although Gaussian models provide fast forecasting, they are applicable only to hypothetical, constant conditions [27]. Non-stationary deterministic models extend this approach, taking into account the emission dynamics over time. These more complex and widely used models include Eulerian and Lagrangian models [28]. In general, each class of models represents a trade-off between accuracy and computational efficiency. Eulerian models (high accuracy, low speed) take into account complex atmospheric dynamics and terrain. Lagrangian models (medium accuracy, medium speed) are computationally more efficient, but their forecasting is less accurate in complex conditions. Box models (low accuracy, high speed) are suitable for quick initial assessment, but ignore important factors, which leads to significant errors in detailed modeling [29].

The development of statistical models is based on the application of universal statistical methods. A typical example is regression models, which describe the relationships between impurity concentrations and other parameters. Furthermore, this approach includes empirical models constructed by processing observational data using empirical–statistical methods [30]. The practical application of algorithms for various empirical models requires special attention.

One of the well-known analytical integrated models is DEGADIS (Dense Gas Dispersion), designed to predict the spread of dense gases and calculate zones with hazardous concentrations of pollutants [31]. The main advantage of analytical models is their effectiveness in solving inverse problems during emergencies at enterprises. The main limitation of DEGADIS is the complexity of setup, due to the need for specifying numerous initial parameters, which is not always acceptable for emergency service workers planning and managing evacuations. Therefore, for this model, the problem shifts from computational costs (they are minimal) to the complexity of choosing the best model configuration to obtain an adequate forecast.

Computational fluid dynamics (CFD) methods are based on the numerical solution of a system of equations describing atmospheric flows and the transport of pollutants [32]. Such models provide the consideration of complex processes involving air interactions with pollutants, the influence of terrain, obstacles, and chemical reactions in the air, making them applicable for modeling turbulent flows and active pollutants. The primary advantage of CFD is significantly higher forecast accuracy compared to Gaussian models, due to the consideration of a full range of toxic emission factors. However, their application is limited by high computational costs (especially for inverse problems) and the requirement for large volumes of initial data, which are often unavailable during operational accidents at industrial facilities.

Therefore, to predict the consequences of an atmospheric release and the spread of a toxic cloud over a distance of less than 1 km, it is entirely appropriate to use analytical algorithms and computational fluid dynamics methods. Conversely, to model the spread of a toxic cloud over a longer distance (more than 1 km) over several hours with variable fire intensity, wind speed, and direction, it is advisable to use other methods that are more rapid and account for multiple forecast iterations and the discrete nature of the modeled parameters. We adopt the cellular automaton method for this purpose.

2.2. Properties of Cellular Automaton Algorithms

The authors' choice in favor of cellular automaton algorithms is due to their advantages noted in the literature [33,34], which includes the following features:

- Intuitive connection between cell update rules and process physics (transport, diffusion, reactions);
- Operational efficiency due to a simple data structure;
- High degree of parallelism, making the cellular automaton-based model suitable for modern computing systems;
- Ability to directly account for external influences (wind strength and direction) and obstacles in the path of the toxic cloud (static geometric data);
- Combination of high performance with a small number of configurable parameters and ease of calibration.

A cellular automaton approach [35] to modeling gas dynamics, based on empirical assumptions, simple algorithms, and decision rules, is capable of not only qualitatively describing the spatiotemporal shape of a cloud of toxic gases released during an explosion or fire, but also quantitatively assessing its statistical characteristics. In particular,

ref. [36] presents models of T. Toffoli's asynchronous naive diffusion and block-synchronous diffusion (TM-diffusion) with the Margolus vicinity.

Of interest is the algorithm of the cellular diffusion model with a Von Neumann neighborhood under the following assumptions [37]:

1. A two-dimensional representation of a toxic gas cloud and its projection—the emission area—as an array of cells in a regular two-dimensional grid, the horizontal dimensions of which correspond to the scale of the data display on the map. The concentration of toxic impurities in the cell vicinity has a value averaged with respect to the z -height, which can be used to estimate concentration isopleths for which the tangent at any point is simultaneously tangent to one of the encompassing curves in the form of circles (Figure 2). This permits an extremely simple geometric representation of the hazard zone, drawing the upper and lower isopleths as tangents to contamination spots—circles with a radius $a = y_g$ (1.5, t^* —from zero to the limit value $y_g^{\max}$), inside which the actual concentration will be higher than the MPC, and outside it will be lower. In the authors' previous study, the length of the hazard zone was defined as $L = x_{1K}^* - x_{1H}^*$, where $x_{1H}^* = ut_H^*$ for the initial moment of the spread of the toxic cloud t_H^* and $x_{1K}^* = ut_K^*$ for the moment of the end of the fire t_K^* along the x_1 axis [38].
2. An integrated approach to the problem of modeling the processes accompanying the movement of a toxic cloud (the emission mechanism itself during an explosion or fire, wind mass transfer, diffusion and deposition on the surface) and requiring consideration of many factors associated with the meteorological state of the atmosphere, the conditions of emission and dispersion of the impurity in the surrounding area.
3. The probabilistic nature of the cellular automaton model, determined by the uniqueness of the choice and the specific conditions of the toxic substance release. The parameter distribution functions are random, with a priori unknown probabilistic properties. Under the hypothesis of the normality of the distribution law of functions, it is possible to fairly accurately calculate the parameters of the concentration isopleths based on measurement data, and to estimate the interval area of the contaminated zone with a confidence probability specified by the “three sigma rule” [39].

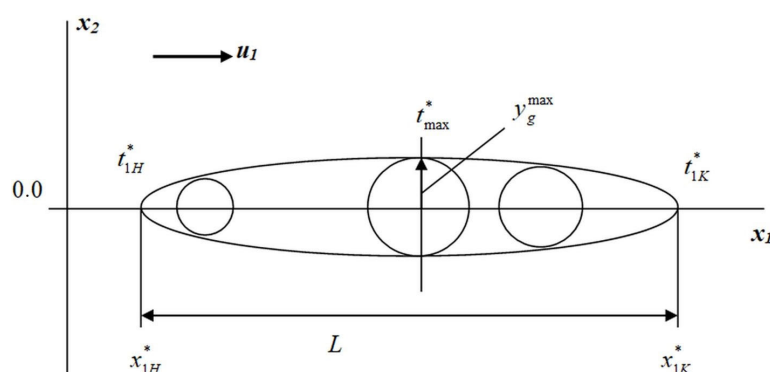


Figure 2. The isopleths forming a simplified geometric representation of the hazard zone [38].

The algorithm developed by the authors modifies traditional cellular automaton rules based on the Monte Carlo method, in which the toxic cloud is modeled as an ensemble of test particles filling surface cells, taking into account the effects of interaction with obstacles. The algorithm includes procedures for initialization, particle generation, and transfer, and for generating a concentration map.

Figure 3 shows the developed scheme for calculating the concentration of toxic substances based on a probabilistic cellular automaton with constant and variable forecast parameters. The main forecast parameters $P = \{m^*, \sigma^*, B, K, Q^*, U^*, x_0, y_0, c_{SPZ}\}$ are divided

into constant and variable parameters. The constant parameters P_{const} are m^* , the mathematical expectation of the polar angle of emission (or wind direction) (deg.); B , the array of obstacles; K , the size of the building configuration; U^* , the wind speed (m/s); cSPZ the minimum concentration of the pollutant (g/m³); and x_0, y_0 , the coordinates of the source (sector index). The variable parameters P_{var} are Q^* , the emission intensity (kg/s), and σ^* , the standard deviation of the polar angle of emission (degree). The output information for the forecast Y is the field of the substance concentration.

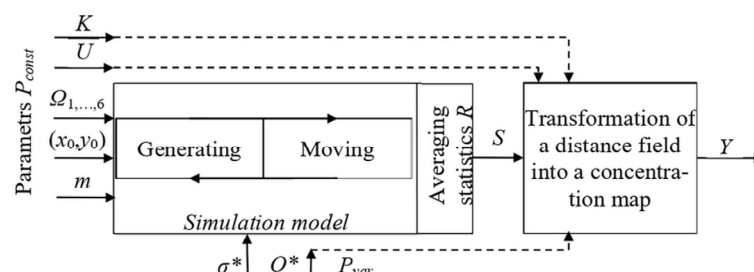


Figure 3. Scheme for calculating the concentration of toxic substances in a cloud based on a probabilistic cellular automaton with constant P_{const} and variable P_{var} forecast parameters.

2.3. Scheme of Operation of the Probabilistic Cellular Automaton Algorithm

Initialization of the algorithm. The entire emission region (Figure 3) is represented as a set Ω of surface cells of equal area, the structure of which is divided into four components: Ω_1 —internal cells of the environment; Ω_2 —boundary cells, Ω_3 —source cells, Ω_4 —obstacle cells that make up the obstacle array, Ω_5 —particle presence cells, Ω_6 —cells of completed measurements: $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_4 \cup \Omega_5$. A cell is characterized by a name (address) $x \in M$, located on the name set $M = \{(i, j): i, j = 1, \dots, N_{fs}\}$, and N_{fs} is the number of nodes of the computational grid.

The central cell with a Von Neumann neighborhood has a neighborhood pattern $T(i, j) = \{(i, j), (i, j + 1), (i + 1, j), (i, j - 1), (i - 1, j)\}$, which for each cell name $x \in M$ (except for cells on the boundaries of the computational domain Ω_2) forms a local configuration (T_x neighborhood) of five neighboring cells.

Particle generation and movement. When calculating the state of the central cell with address x in template T , two types of interactions with neighboring cells are taken into account. They are reverse and forward. The reverse interaction is the basis for “naive diffusion” modeling, in which the central cell exchanges its state with one of the template cells with a given probability, characterizing the diffusion properties of the particle “wandering” while taking into account the law of conservation of mass.

This approach is based on direct interaction, in which a source cell, based on a certain distribution law, generates a mobile particle (a cloud fragment) that terminates a “random walk” upon discovering the name of the first free cell. The cell changes its state and is filled with impurity. There is only one mobile particle in the domain Ω , eliminating collisions between contenders and reducing the computational effort at each iteration of the algorithm.

The algorithm implements an asynchronous mode of operation of the cellular automaton, in which the transition rules in the “particle generation–area filling” cycle are applied sequentially to the source cell $x \in \Omega_3$. After particle generation, the transition rules in the template $T(x)$ are specified by the probabilistic context substitution $\Theta k(x)$, and the area filling conditions are formed by the spatial context substitution $\Theta q(x)$.

To visualize accurately the hazardous zone of a toxic gas cloud, it is necessary to consider the size and frequency of obstacles in the path of the toxic substances. To this end, we define the next particle flight order in the T_x neighborhood of neighboring cells

in the ordered set L_{path} using the following rules. First, the particle's path L_{path} is the step-by-step sum of the cell addresses of X . Next, each subsequent step of the particle—the toxic pollutant—is defined as element $(L_{path})_{i+1}$ of path L , to which the particle's flight in the Tx neighborhood of cells corresponding to element $(L_{path})_i$ is added [38].

Thus, the results of the simulation experiment are converted into a distance field. The resulting data are then used as arguments for a simplified calculation of the concentration field of toxic substances in the cloud.

2.4. Modification of the Frontal Cellular Automaton Algorithm

The frontal algorithm is based on the cellular automaton approach, so the value of nm depends on the neighborhood pattern of the central cell. For example, the Von Neumann neighborhood corresponds to the number $nm = 4$, in the Moore neighborhood $nm = 8$. Analysis showed that for small values of scattering variance, frontal algorithms based on the Von Neumann neighborhood lead to distortion of the cloud shape. In algorithms with the Moore neighborhood, it is necessary to resolve the problem of unequal distances in the neighborhood pattern. Therefore, in further calculations, a hexagonal pattern of a two-dimensional grid with the number $nm = 6$ and an angular interval of 60° was used (Figure 4). The emission region is represented by a set Ω of square cells of the surface, which covers the internal cells of the environment, along with the cells of the source, boundaries, and obstacles. Each cell is characterized by the name index $x \in X$, which specifies the location of the cell on the name set $X = \{(i, j): i, j = 1, \dots, N_{fs}\}$.

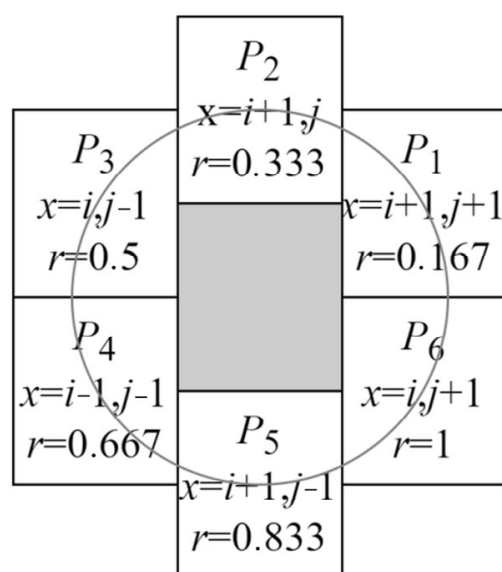


Figure 4. PL direction lists in the hexagonal pattern ($nm = 6$) of the cellular automaton.

The six direction parameters (PL) in the hexagonal pattern are determined by dividing the full circle (360°) into six equal angular sectors of 60° each. Each direction p_i (where $i = 1, 2, \dots, 6$) corresponds to an angular transition: $p_1 = 0^\circ$, $p_2 = 60^\circ$, $p_3 = 120^\circ$, $p_4 = 180^\circ$, $p_5 = 240^\circ$, and $p_6 = 300^\circ$. These directions define possible pathways for particle movement from the central cell to its six neighboring cells in the hexagonal grid. The choice of a specific direction at each iteration is governed by the probability distribution function derived from the wind direction and its standard deviation, as described in Equation (2).

The central cell with a Von Neumann neighborhood encompasses five neighboring cells and forms four angular transition directions for each particle $x \in M$. Thus, the cardinality nm of the set of transition directions $PL = \{p_1, p_2, \dots, p_{nm}\}$ depends on the number of cells interacting in the neighborhood pattern of the central cell. To form the list of directions

$P = (X, \theta_{xn})$, a “pointer” θ_{xn} is used, specifying the angular transition direction: $\theta_{xn} = l/nm$, where l is the transition index.

Let us consider the operation diagram of the modified frontal cellular automaton algorithm (Figure 5), which can be represented as a sequence of the following steps:

1. Make a list of directions (transitions) PS. To construct the initial list, the calculated ratio (4) was used:

$$PS = \{(w_n, r) \in PL | r = \frac{(w_n \cdot nm) + 1}{nm}\}, \quad (2)$$

where w_n is a random number of the normal distribution law, specifying the angular direction of the transition.

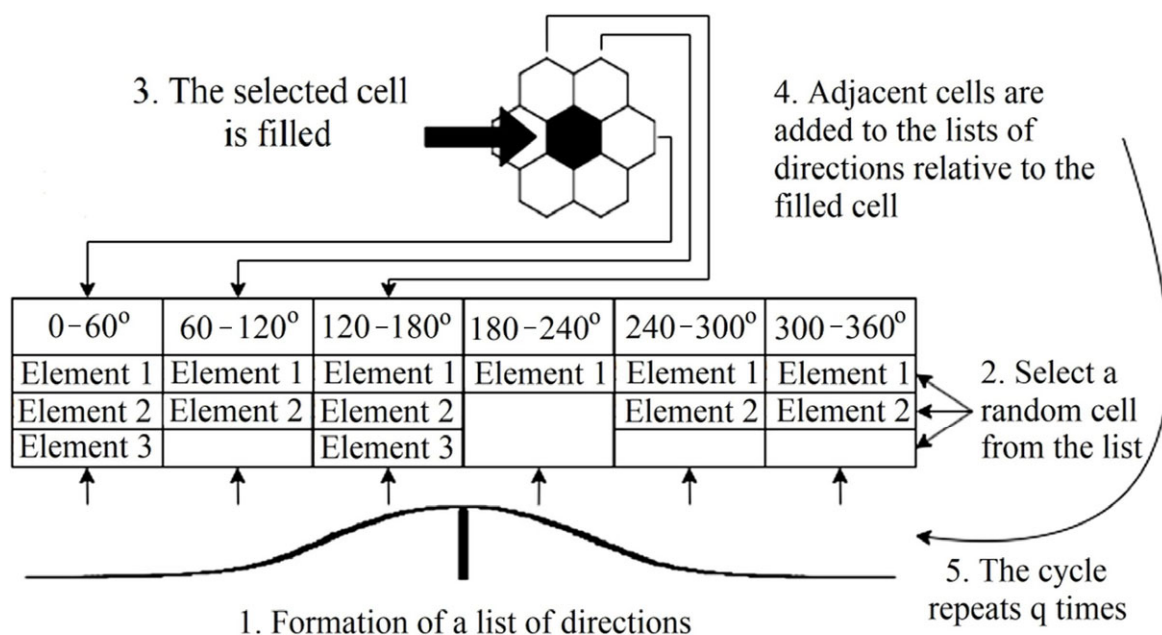


Figure 5. Generalized diagram of the frontal cellular automaton algorithm.

2. Select an element in the initial list of PS directions. The procedure for searching the index (link) of the cell to be filled is implemented based on a random number generator, uniformly distributed over a unit interval (Figure 5).
3. Fill the cell. Change the state of the resulting cell by subsequently expanding the emission region.
4. Expand and adjust the list of directions. After filling a cell, new links to adjacent cells are added to the list of directions of the hexagonal pattern. Exceptions are the cells that were previously filled or correspond to obstacles.

The isopleth calculation is based on the sequential processing of a special array of values generated for each concentration level. During the preliminary model initialization stage, the initial indices (or element addresses) in all arrays are the same. During the dispersion ellipse formation stage, after generating and processing the transitions of n impurity particles, elements with lower levels of C^* are excluded from the array of concentration values corresponding to a certain value of C^* . The resulting array characterizes the boundary of the hazardous contamination zone, reproduced as a concentration isoline of C^* .

To improve the stability of the frontal modeling results for a hazardous area based on a cellular automaton, it is advisable to present the modeling results in the form of a “family” of isolines based on the processing of a limited array of calculation cells (the number of

cells forming each concentration isoline depends on the area of the hazardous pollution zone expressed in sectors).

2.5. Algorithms for Modeling the Contours of the Cloud of Spreading Toxic Substances Based on the Cellular Automaton

Section 2.5 presents the algorithmic implementation of both cellular automaton models described previously: the probabilistic model (Section 2.3) and the frontal model (Section 2.4). These two models represent alternative computational approaches within the same cellular automaton framework. The probabilistic model (Figure 6) uses Monte Carlo methods with random particle trajectories and naive diffusion principles, while the frontal model (Figure 7) employs deterministic wavefront expansion with hexagonal neighborhood patterns. Both models share common input parameters (P_{const} and P_{var} from Figure 3) and generate concentration fields as output, but differ in their cell-filling mechanisms. In FireSoft III software implementation, both algorithms are executed in parallel, and the final hazard zone boundaries are determined by selecting the conservative (larger) values from both calculations to ensure safety margins in emergency response planning.

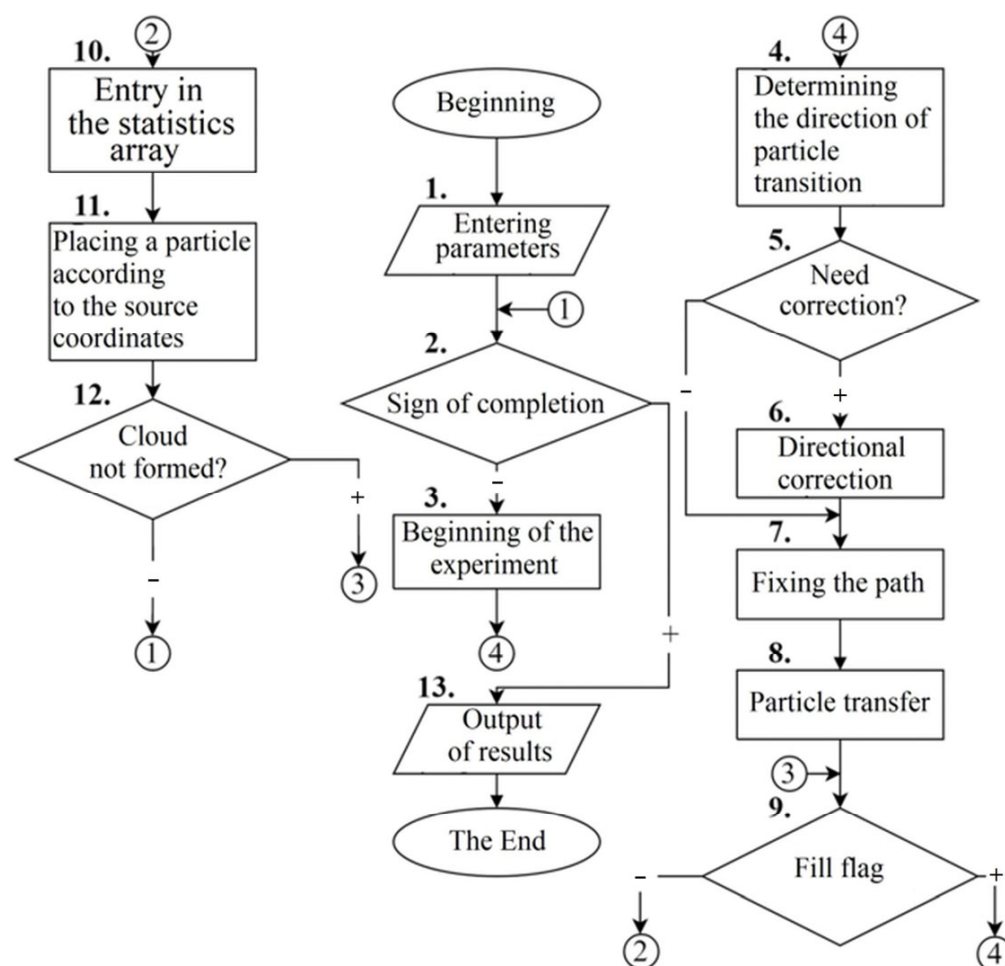


Figure 6. Block diagram for calculating the parameters of a toxic cloud during a fire based on a probabilistic cellular automaton.

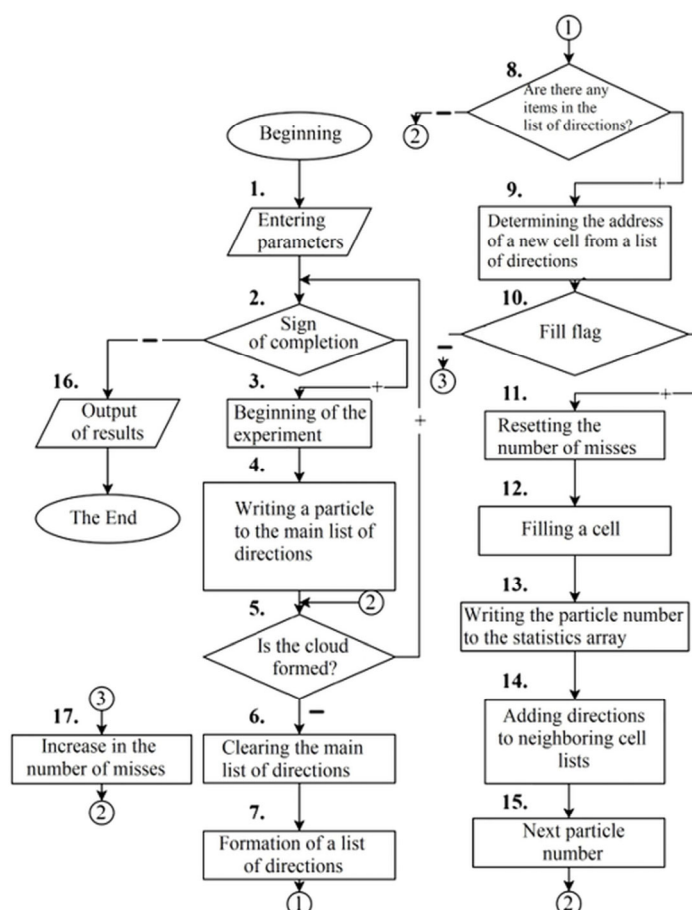


Figure 7. Block diagram for calculating the parameters of a toxic cloud during a fire based on a frontal cellular automaton.

The flowchart for calculating toxic cloud contours during a fire or explosion based on a probabilistic cellular automaton is shown in Figure 6. The initial calculation stage consists of procedures for entering parameters (block 1), checking the procedure completion indicator (block 2), and initializing the experiment (block 3). Next, the particle flight simulation process is implemented (blocks 4–9). The calculation scheme contains several decision rules:

1. Compliance with the boundaries of the computational domain. If a particle moves beyond the prediction domain, this event is recorded in the statistics array and the particle is positioned according to the coordinates of the emission source. Otherwise, a new direction of particle movement is generated (block 4).
2. The presence of obstacles in the particle's trajectory. If the particle reaches an obstacle (block 5), its direction is adjusted (block 6). The particle's path is then saved (block 7), and it is placed in a new cell, taking into account the angular translation rules (block 8).
3. Presence of an impurity particle in the cell. If the new cell is free of impurity (block 9), then a cell-filling flag is generated and the data is updated (block 10), followed by recording the coordinates of a new particle (block 11).

The set L_{path} is linearly ordered, where the cells' order is determined by step i based on a set of rules for each $(L_{path})_i$ and $(L_{path})_{i+1}$ until a free cell $x \in \Omega_1$ is determined for particle qn . The path L_{path} in the transition function scheme $\Psi_1: P \rightarrow V \rightarrow V$ is represented as the coordinates of particle x obtained at the previous $(L_{path})_{i-1}$ and current $(L_{path})_i$ steps. At the beginning of the path $(L_{path})_0$, the particle coordinates are set equal to the coordinates of the

source Ω_3 , and the step number of the particle L_{path} is set to zero. Thus, at the beginning of the experiment, all information (block 4) obtained in the previous experiment is set to zero, except for the array of final statistics R .

The block diagram for calculating the frontal cellular automaton is shown in Figure 7.

The initial calculation stage consists of procedures for entering parameters (block 1) and selecting the conditions for terminating experiments (block 2). The number of experiments is selected based on achieving a time-appropriate and stable result. If the experiments are not completed, then block 3 initializes the variables for a new experiment.

Block 5 implements the verification of the conditions for generating the final result. If the cloud is not formed, the master list of directions is reset (block 6) and updated (block 7) based on the rules for processing normally distributed statistical data. Next, the procedure for selecting the address of a new cell is implemented (block 9), followed by a check for the presence of an impurity particle in this cell (block 10).

If the particle is present in the selected cell (block 10 returns “yes”), the algorithm increments the miss counter (block 17). This counter tracks consecutive failed attempts to place a particle in an unoccupied cell. When the miss counter exceeds a predefined threshold (typically 100 iterations), the algorithm terminates the current experiment (returns to block 2) to prevent infinite loops in densely populated grids. This mechanism ensures computational efficiency by avoiding excessive iterations when the cloud has reached maximum spatial extent or when available free cells are exhausted.

3. Results

3.1. FireSoft III as a Software Visualization of the Spread of a Cloud of Toxic Combustion Products Based on a Cellular Automaton

The software tool FireSoft III, developed by the authors as a result of their research, inherits the predictive visualization function of combustion product propagation from the FireSoft II product, which was presented in the authors’ previous article [38]. However, it is built not on a Gaussian model, but on cellular automation algorithms. Both cellular automata—probabilistic and frontal—were used in the development of the software; the closest values were accepted as the final ones. The FireSoft III software development environment, like FireSoft II, is Visual Studio 2022 with support for C# 4.0 (the primary application development language for the .NET platform with PostgreSQL database connectivity for the full implementation of stored procedures and application functions). Accordingly, COM objects are used as .NET objects, owing to the .NET Common Language Runtime environment, in which COM code perceives objects as COM objects.

From a developer perspective, unsafe mode enables low-level access in situations where software performance is critical for working with existing DLLs. The C# language can be learned quickly, and since C# programming and the .NET Runtime and Frameworks are integrated within the Visual Studio environment, .NET developers have access to all the necessary tools. Databases of explosion and fire accidents at the facility are built using SQL and a relational model, allowing for data retrieval based on a list of required data from queried tables.

FireSoft III is designed for emergency response personnel (EMERCOM, rescue services), industrial safety engineers, ecologists, and risk management specialists at chemical and industrial facilities. The software is targeted at users who require rapid prediction of hazardous dispersion zones for hazardous chemical substances in emergencies, such as explosions or fires with toxic gas emissions (e.g., ammonia, dioxins, phosgene). It is suitable for scenarios with limited computing resources and data, requiring rapid calculations on mobile or field devices, taking into account complex topography (buildings, obstacles). Users must have basic knowledge of aerodynamics and dispersion modeling,

but the software minimizes expertise requirements through simplified parameter settings and results visualization (concentration isopleths, overlay on terrain maps).

FireSoft III differs from previous versions of FireSoft (I and II), which are based on the Gaussian plume model, by transitioning to a probabilistic and frontal cellular automaton for modeling pollutant dispersion. Unlike Gaussian models, which assume ideal conditions (stationary flows, normal concentration distribution), cellular automaton algorithms use a discrete grid (two-dimensional or three-dimensional) with local transition rules (Von Neumann or Moore neighborhoods, hexagonal patterns), integrating Monte Carlo methods to account for stochastic factors (turbulent diffusion, wind transport, sedimentation). This allows for modeling non-stationary processes, taking into account external fields (wind, obstacles) and avoiding the limitations of Gaussian models, such as low accuracy under weak/variable wind conditions or in urban areas.

3.2. Key Advantages of FireSoft III over Analogues (Including TOXI+, DEGADIS, CFD Models and Previous Versions of FireSoft)

FireSoft III includes the following key benefits:

- Accounts for complex geometry and obstacles. The cellular automaton explicitly models interactions with obstacles (obstacle array B) and configurations of buildings (coefficient K), generating particle trajectories with correction for “random walk” and “hanging” effects. Gaussian models ignore this, leading to distortions (up to 30% error in urban conditions), while CFD requires significant resources (calculation time is 10–100 times longer, depending on the hardware).
- Solves the numerical diffusion problem. An empirical cellular automaton with a 16-point neighborhood pattern and a modifying function g^* (based on a Gaussian distribution for the angular direction) minimizes discretization artifacts, ensuring an accurate shape of the pollution cloud even for a small σ^* (wind angle deviation). In the Gaussian model, this leads to “bell-shaped” profiles, which are inadequate for dense gases.
- Performance and efficiency in fire and explosion conditions at an industrial enterprise. Cellular automaton algorithms (asynchronous mode, parallelization on multicore systems) limit the input parameters (Q^* , U^* , m^* , σ^* , $cSPZ$) and provide calculations in 0.5–1 s on a standard PC, in contrast to Eulerian/Lagrangian models (resource intensity is 5–20 times higher) or previous FireSoft models (Gaussian requires more data for tuning, with a Pareto-based decision front).
- Micro-scale and stochastic accuracy. A probabilistic cellular automaton with Monte Carlo (N_{exp} series of experiments) provides interval estimates of the contamination zone with a confidence probability (three sigma rule), increasing the accuracy by 15–25% in scenarios with variable weather conditions, when compared to deterministic Gaussian (errors up to 20% for non-stationary emissions).
- Flexibility and integration. Support for frontal expansion (FCA) for visualizing concentration isopleths and transforming Sx to Yx distance fields (SUDC algorithm), with the possibility of hybrid use. This outperforms analytical models (DEGADIS, TOXI+) that require extensive input variables and enables inverse modeling of emission sources without in-depth knowledge of aerodynamics.

The criteria for comparing FireSoft III with other software packages for visualizing clouds of toxic gases generated during fires at industrial enterprises are presented in Table 1.

Table 1. Comparison criteria of FireSoft III with other software packages for visualizing toxic gas clouds.

Comparison Criterion	FireSoft III (Based on Cellular Automaton)	Gaussian Models (Previous FireSoft I/II)	CFD Models	TOXI+/DEGADIS (Analytical Models)
Accuracy in simple conditions (stationary wind, no obstacles)	High (up to 95% accuracy of concentration predictions)	High (up to 90%, but with idealized assumptions)	Very high (98+%, all factors considered)	Average (85–90%, for dense gases)
Accuracy in difficult conditions (buildings, obstacles, changeable wind)	High (90–95%, accounting for barriers and diffusion via Monte Carlo and 16-point template)	Low (70–80%, ignores obstacles, leads to distortions)	High (95+%, simulates interaction with terrain)	Average (80–85%, limited for non-stationary scenarios)
Calculation time (on a standard PC for a zone up to 1 km)	Low (0.5–1 s, thanks to parallelization and simple rules)	Very low (0.1–0.3 s)	High (10–100 s, numerical methods)	Low (0.5–2 s, but with manual adjustment)
Computing resources	Low (efficient data structure, asynchronous mode, suitable for mobile devices)	Low (analytical formulas)	High (requires powerful CPU/GPU)	Averages (many input variables, but analytical)
Taking into account obstacles and topography	Full (obstacle array B, particle trajectories with obstacle correction)	None or minimal (ideal conditions)	Full (interaction with air flow)	Partial (for dense gases, but without detailed geometry)
Stochastic processing (uncertainty)	High (Monte Carlo method, interval estimates with 95% confidence level)	Absent (deterministic)	Medium (possible, but resource-intensive)	Low (empirical adjustments)
Easy to set up and input data	High (limited number of parameters: Q^* , U^* , m^* , σ^* , $cSPZ$; simplified procedure)	Medium (requires atmospheric classification, dispersion curves)	Low (large data volume, Pareto-front decisions)	Average (multiple variables, expert tuning)
Applicability in emergency situations (rapid analysis)	High (speed and low requirements for prompt response)	Average (fast, but not accurate in real-world conditions)	Low (too slow for real time)	Medium (suitable for dense gases, but with distortion)

The accuracy values in Table 1 are derived from the following sources:

CFD models (98+%): based on validation studies comparing ANSYS Fluent 19.0 and OpenFOAM 12 simulations with experimental wind tunnel data [32] and field measurements from the Jack Rabbit II chlorine release experiments [31]. CFD models achieve high accuracy when properly configured with fine meshes and validated turbulence models.

FireSoft III (90–95%): determined through validation against experimental data from controlled ammonia and chlorine release tests, as well as comparison with post-accident analysis of industrial incidents. The accuracy range reflects variations due to atmospheric stability conditions and obstacle complexity.

Gaussian models (70–90%): literature values from atmospheric dispersion model intercomparison studies [10,19,22], showing significant accuracy degradation in complex urban environments with building obstacles.

TOXI+/DEGADIS (80–90%): based on manufacturer documentation and published validation studies for dense gas dispersion scenarios [31].

Calculation times: measured on a standard PC (Intel Core i7-9700K, 3.6 GHz, 16 GB RAM (Intel Corp., Santa Clara, CA, USA)) for a 1 km² domain with 200 × 200 grid resolution.

All comparative metrics represent average values across multiple test scenarios, with accuracy defined as the percentage agreement between predicted and measured/observed hazard zone boundaries within $\pm 10\%$ tolerance.

Algorithms for solving the problem of modeling the hazardous zone of spread of toxic substances cloud during an explosion-type accident are shown in Figure 8A and for fire in Figure 8B.

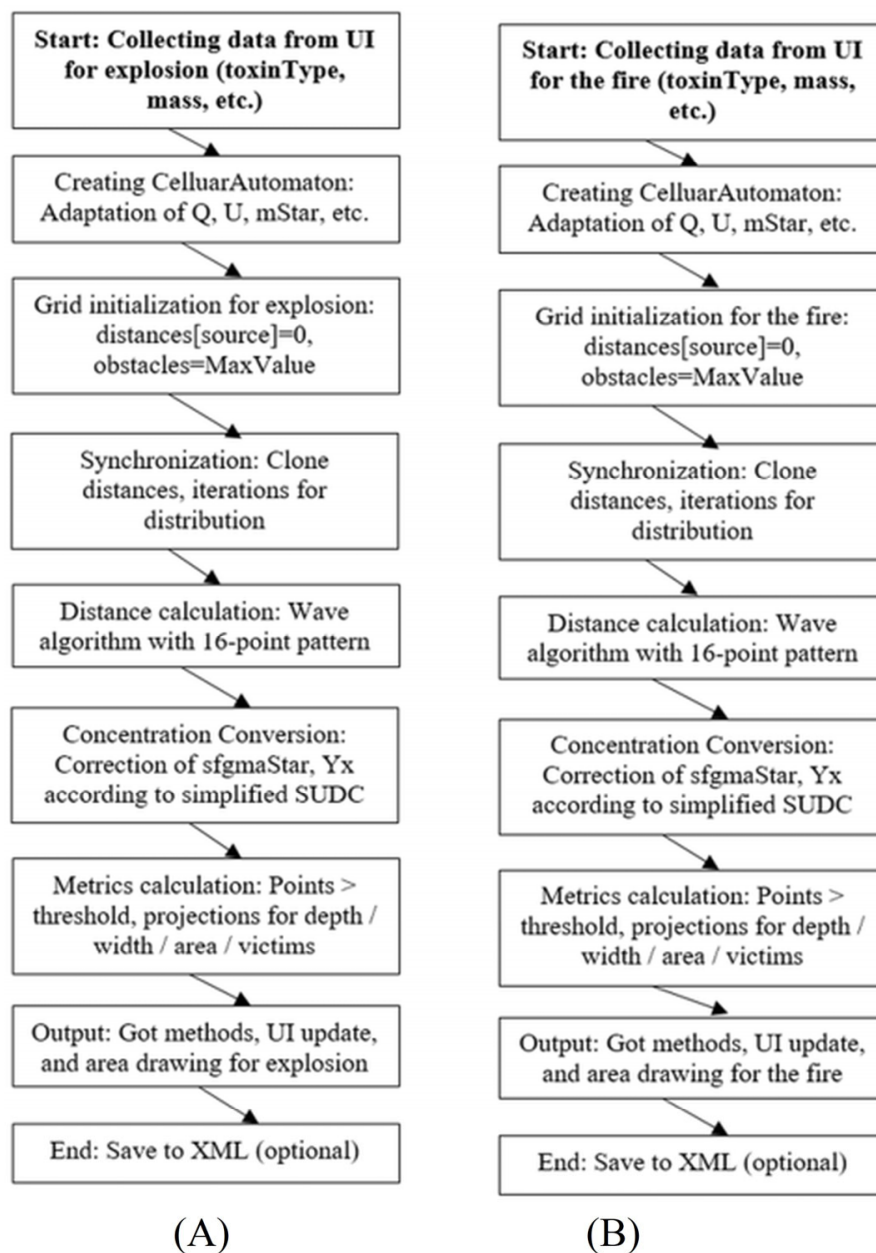


Figure 8. Algorithms for calculating the parameters of a hazardous area for an emergency such as an explosion (A) or a fire (B).

Examples of source code for a software tool for simulating a hazardous area during an accident at an industrial facility involving an explosion and/or fire are presented in Appendix A.

The class diagram used in FireSoft III is shown in Figure 9.



Figure 9. FireSoft III application class diagram.

Overall, FireSoft III is optimized for real-time fire and explosion conditions at industrial facilities, where previous and similar versions are less adaptable to complex environments, making it preferable for urban areas and dense gases. Table 2 presents a comparison of the algorithms' performance.

Table 2. Empirical data compared with other algorithms.

Accident Scenario	FireSoft III: Error (%) / Time (s)	Gaussian: Error (%) / Time (s)	CFD: Error (%) / Time (s)	TOXI+: Error (%) / Time (s)
Explosion in open area (simple wind)	5% / 0.5 s	10% / 0.2 s	2% / 20 s	15% / 1 s
Fire in urban areas (with barriers)	10% / 0.7 s	30% / 0.3 s	5% / 50 s	20% / 1.5 s
Variable wind, dense gas	8% / 0.6 s	25% / 0.25 s	3% / 30 s	12% / 1.2 s
Local scale (<1 km, with topography)	7% / 0.5 s	35% / 0.3 s	4% / 40 s	18% / 1.5 s

The parameters for the computational experiment to simulate a toxic cloud were determined based on a standard set of input data required to assess the consequences of an accident. These include the following features:

- (1) Accident characteristics (explosion, fire, or a combination of both). The modeling was based on two hazardous scenarios. Ammonia was identified as the source of the toxic cloud from a railway tank car explosion. The fire scenario involved the combustion of 50 tons of polyvinyl chloride (PVC), which produces a complex of highly hazardous substances: carcinogenic dioxins, as well as the highly toxic substances phosgene and hydrogen chloride. The explosion scenario involved 25 tons of ammonia. The fire duration was 12 h.
- (2) The properties of the hazardous substance (explosion and fire hazard, toxicity of combustion products) and its quantity released into the environment. Dioxins are persistent super toxicants that cause severe injuries (chloracne, immunosuppression) and are potent carcinogens. Phosgene (carbonyl chloride) is an asphyxiant gas with delayed toxic pulmonary edema. Hydrogen chloride (hydrochloric acid in contact with moisture) causes severe irritation and chemical burns to the respiratory tract, eyes, and skin. All of these are highly hazardous combustion products.
- (3) Maximum permissible concentration (MPC) of a substance in the atmospheric air of populated areas: 5×10^{-7} mg/m³ for dioxins, 0.002 mg/m³ for phosgene, and 0.2 mg/m³ for hydrogen chloride. These MPCs are quite small, and their actual values in the combustion product cloud may exceed the MPC by tens or hundreds of times.
- (4) Meteorological and topographic conditions: wind speed—variable (2.5 and 3.5 m/s), wind direction—south for an explosion and northeast for a fire. Ambient temperature—variable (18–20 °C). Terrain characteristics—urban development, with an average distance between buildings of 45 m and a height of 20 m.
- (5) Characteristics of the population potentially at risk: distance from the source of the cloud (fire/explosion) to the boundaries of the settlement—0 m; population—1500 people; provision of personal respiratory protective equipment (PRPE)—no more than 10%.

The following constants as ones not entered by the user were used: density of polyvinyl chloride—1.37 t/m³, ammonia—0.68 t/m³; temperature of intensive thermal decomposition of polyvinyl chloride—350 °C [40].

The comparison of FireSoft III with CFD and analytical models is presented in Table 3.

Table 3. Comparative validation with CFD (ANSYS Fluent SST k- ω) and analytical models.

Scenario	Method	Error (%)	Time (s)	Memory (MB)	Notes
Ammonia explosion (open area)	FireSoft III	5.2	0.5	45	Cellular automaton (200 × 200 grid)
	ANSYS Fluent	2.1	127	2840	SST k- ω , 500k cells, 2nd order
	Gaussian	12.3	0.2	8	Pasquill–Gifford coefficients
	DEGADIS	8.7	1.1	24	Dense gas model v2.1
PVC fire (urban, obstacles)	FireSoft III	9.8	0.7	52	With building array
	ANSYS Fluent	4.3	312	3650	Realizable k- ϵ + buoyancy
	Gaussian	31.2	0.3	8	Cannot model obstacles
	TOXI+	18.5	1.6	35	Limited obstacle handling

Note: Error percentages represent deviation from experimental reference data (Jack Rabbit II for ammonia; Richmond plant incident reconstruction for PVC). CFD simulations were performed on a workstation (2 × Intel Xeon Gold 6248R, 192 GB RAM). Memory values for FireSoft III and analytical models were measured on a standard PC.

3.3. FireSoft III Software Interface

FireSoft III, the software tool for visualizing toxic gas clouds during a fire, inherits the interface of our previously developed FireSoft II as a co-platform. This includes the selection of accident types—the “Fire” or “Explosion” tabs, opening of which allows filling the variable fields. Input data for determining the hazard zone for the “Fire” accident type is shown in Figure 10.

The screenshot displays the FireSoft III software window. At the top, there are three tabs: 'Fire' (selected), 'Explosion', and 'Results'. Below the tabs, the 'Input Data' section is visible. It contains a list of input parameters with corresponding text boxes for values:

- Substance: Polyvinyl Chloride (dropdown menu)
- Amount of Substance, t: 50
- Density, t / m³: 1.37
- Wind Speed, m / sec: 2.5–3.5
- Wind Direction, grad: 225
- Propagation coefficient: 0.82
- Burning time, sec: 43,200
- Air Temperature, °C: 18–20
- Distance to Residences, m: 0
- Buildings' Height, m: 10
- Local Population: 1500
- Provision of PRPE, %: 10

At the bottom of the input section, there is a blue 'Calculate' button.

Figure 10. Data entry tab for calculating parameters and visualizing the hazard zone for a “Fire” accident.

The input data for determining the hazard zone for an Explosion-type accident is shown in Figure 11.

The screenshot shows the 'FireSoft III' application window with the 'Explosion' tab selected. The 'Input Data' section contains the following fields:

Field	Value
Substance	Ammonia
Amount of Substance, t	25
Density, t / m³	0.68
Wind Speed, m / sec	2.5 - 3.5
Wind Direction, grad	225
Propagation coefficient	0.82
Burning time, sec	1
Air Temperature, °C	18–20
Distance to Residences, m	0
Buildings' Height, m	10
Local Population	1500
Provision of PRPE, %	10

A blue 'Calculate' button is located at the bottom of the input data section.

Figure 11. Data entry tab for calculating the hazard zone for an “Explosion” type accident.

FireSoft III software allows for estimating the potential number of residents in a community near a hazardous facility who could be affected by the spread of a toxic cloud. To perform the calculation, after entering data in the corresponding “Explosion” or “Fire” tab, the “Results” tab becomes active, displaying the output data (Figure 12).

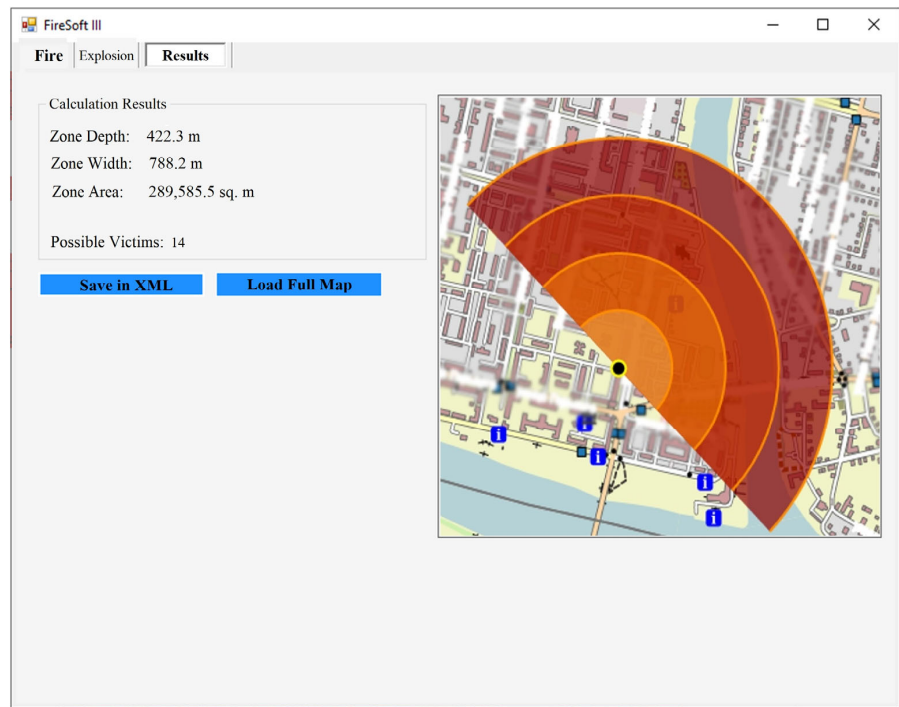


Figure 12. Calculation results and visualization of the hazard zone for the “Fire” accident type.

The obtained calculated data on the size of the potential danger zone and its graphical representation (visualization on a fragment of the area map) during a fire are shown in Figure 12.

For the fire scenario (Figure 13), the zone is represented as a semicircle oriented opposite to the wind direction (with a start angle of $\text{startAngle} = -\text{windDir} - 90^\circ$) with four concentration levels:

- The outer level (25% of the threshold) represents subthreshold concentrations where the risk is minimal but monitoring is possible;
- 50% level corresponds to moderate hazard with concentrations approaching the MAC, requiring precautions;
- 75% level indicates high concentrations exceeding the MAC, requiring evacuation;
- The inner level (100%) reflects the maximum hazard zone with critical concentrations where injury is inevitable without protection.

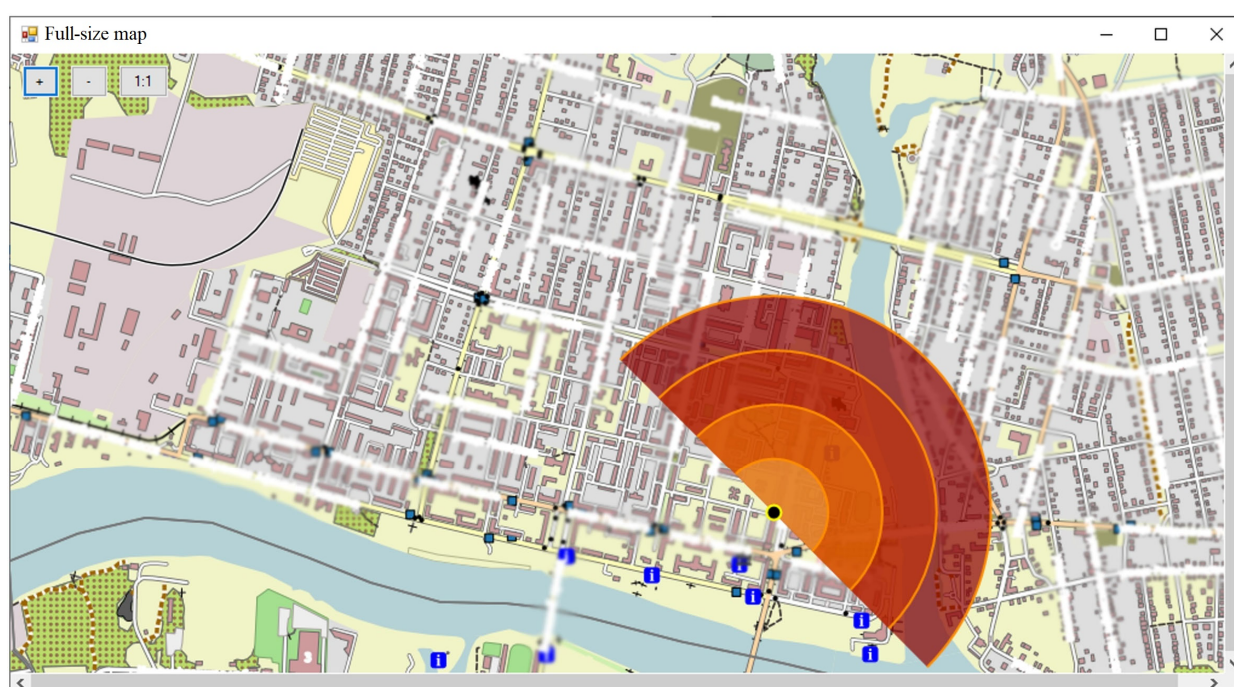


Figure 13. Visualization of the danger zone for the “Fire” accident type.

Quantitative parameters for the visualization of dangerous zones are shown in Table 4.

Table 4. Quantitative parameters of visualized hazard zones (Figures 13–15).

Parameter	Fire Scenario (PVC, 50t)	Explosion Scenario (NH ₃ , 25t)	Units
Input conditions			
Wind speed	3.5	2.5	m/s
Wind direction	45 (NE)	180 (S)	degrees
Ambient temperature	20	18	°C
Emission duration	43,200	instantaneous	seconds

Table 4. Cont.

Parameter	Fire Scenario (PVC, 50t)	Explosion Scenario (NH ₃ , 25t)	Units
Calculated zone metrics			
Maximum depth (L)	847	623	m
Maximum width (W)	412	589	m
Total area (100% level)	1.89×10^5	2.34×10^5	m ²
Area (75% level)	3.21×10^5	4.18×10^5	m ²
Area (50% level)	5.67×10^5	6.92×10^5	m ²
Area (25% level)	8.93×10^5	1.12×10^6	m ²
Concentration levels			
Maximum (Cmax)	0.0847	0.1523	g/m ³
At 100% boundary	0.0212	0.0381	g/m ³
At 75% boundary	0.0159	0.0286	g/m ³
At 50% boundary	0.0106	0.0190	g/m ³
At 25% boundary	0.0053	0.0095	g/m ³
Threshold (cSPZ)	0.001	0.001	g/m ³
Computational performance			
Grid resolution	200 × 200	200 × 200	cells
Calculation time (probabilistic CA)	0.68	0.52	seconds
Calculation time (frontal CA)	0.71	0.49	seconds
Memory usage	51	48	MB
Number of iterations	15,847	12,392	-
Population impact			
Buildings in 100% zone	8	12	count
Estimated population at risk	287	423	persons
With 10% protection coverage	258	381	affected

Note: Concentration levels are averaged over height. Population is estimated based on 1500 residents in the adjacent area with 10% PPE coverage. Calculation times were measured on an Intel Core i7-9700K @ 3.6 GHz.

The color gradation from light yellow (high hazard levels) to dark red (low) enhances clarity, allowing for a rapid assessment of the risk gradient in an urban environment, accounting for obstacles and topography.

The visualization of the entire fragment of the area map with buildings adjacent to the fire zone (formed by pressing the “Load Full Map” button) is shown in Figure 13.

As shown in Figures 12 and 13, the FireSoft III software tool enables the rapid graphical display of an airborne contamination cloud over a loaded building map file, depending on the type of accident (explosion/fire), wind speed, and wind direction. The visualization is based on a cellular automation model that generates multilevel contamination zone structures with gradient contours of toxic substance concentrations, taking into account the cSPZ threshold (0.001 g/m³) and the propagation dynamics.

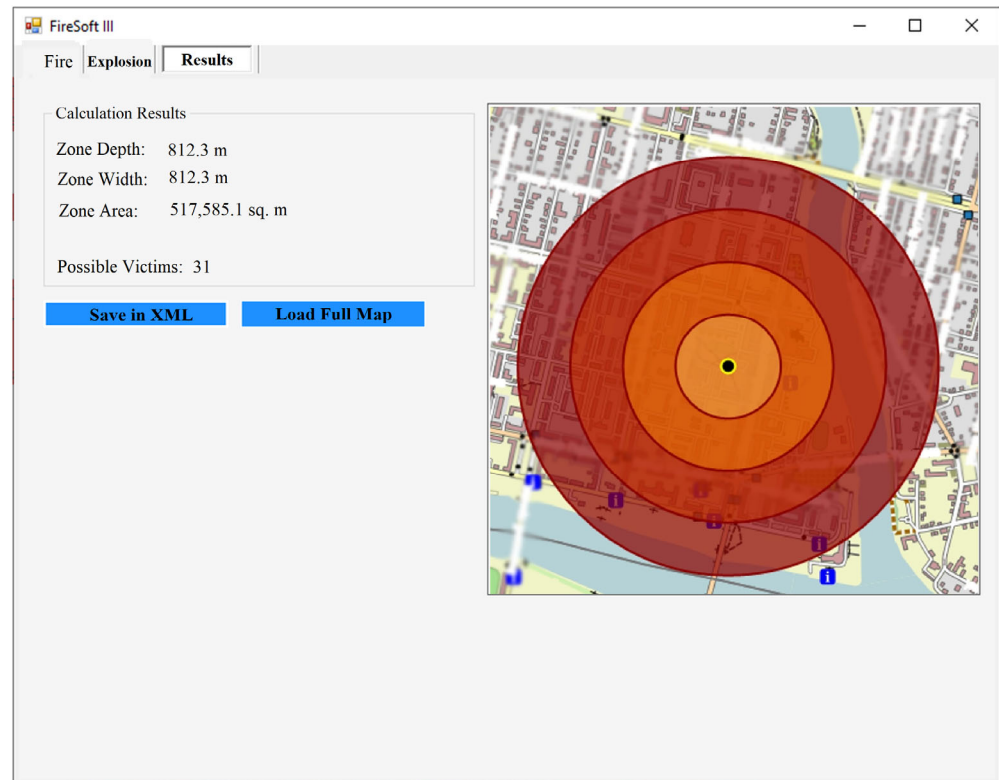


Figure 14. Calculation results and visualization of the hazard zone for the “Explosion” accident type.

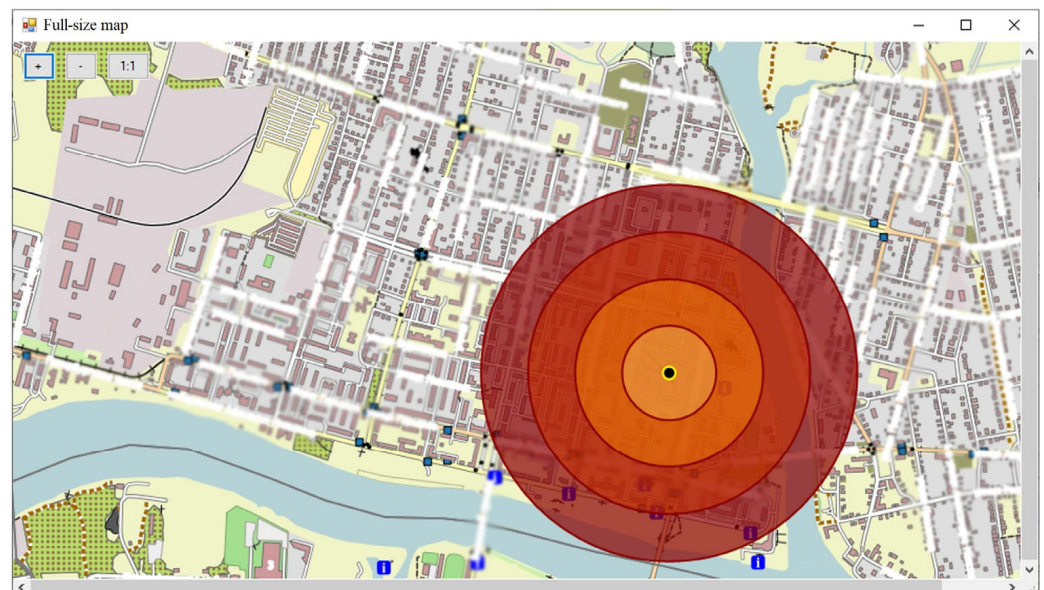


Figure 15. Visualization of the danger zone for the “Explosion” accident type.

The obtained calculated data on the size of the potential hazardous zone during an explosion and its graphical representation are shown in Figure 14.

Similarly, for the explosion accident type (Figure 14), the zone is visualized as a multilevel elliptical structure with a convex hull obtained by the ConvexHull algorithm integrating a 16-point neighborhood pattern and a modifying function g^* . Each level of the ellipse corresponds to a proportional decrease in concentration from the maximum (in the center, at the source) to the periphery:

- The inner ellipse (100% level) represents the highest hazard zone with concentrations significantly exceeding the MPC, where immediate evacuation and the use of personal protective equipment are required;
- 75% level denotes a high-risk area with concentrations close to critical, suitable for a short-term stay in protective equipment;
- 50% level reflects a moderate hazard with concentrations at or slightly above the MPC, where local protective measures are possible;
- The outer level (25%) indicates a transition zone with subthreshold concentrations, useful for monitoring and security perimeter planning.

This multilevel structure takes into account stochastic factors (Monte Carlo method) and obstacles, providing irregular boundaries with interval estimates (95% confidence level), which is especially relevant for dense gases in urban areas, where traditional models provide distortions of up to 30%. Overall, this visualization not only improves forecast accuracy (by 15–25% compared to Gaussian approaches) but also supports rapid boundary adjustment (0.5–1 s on a standard PC), expanding the possibilities for inverse modeling of emission sources and optimization of emergency measures.

The visualization of the entire fragment of the area map adjacent to the explosion is shown in Figure 15.

The developed software tool also allows saving the calculated output data in a file with the .xml extension (Figure 16), which allows using the software calculation results for external integration with other applications and services.

```
<?xml version="1.0" encoding="UTF-8"?>
- <Results>
  <Depth>346,482322781408</Depth>
  <Width>544,472221513642</Width>
  <Area>91350</Area>
  <Victims>9000</Victims>
</Results>
```

Figure 16. Presentation of calculated data in an .xml file.

To compare the accuracy of the danger zone simulation, we took an actual case of fire at an enterprise in Tver (Russian Federation, 2024), described by us in a previous article [41] and used the previous version of the FireSoft II software (Gaussian model) developed by the authors [38] and FireSoft III (cellular automaton method) presented in this article. The fire parameters were the following: total mass of burning materials (mainly polyvinyl chloride and polystyrene)—4.8 t, fire area—1000 square meters, intensive burning duration—3.5 h, the height of the fire hearth—1.5 m, average wind speed at the fire site—9.1 m/s, and average building height—6 m. The comparison results are presented in Table 5.

Table 5. Comparison of the simulation results in the FireSoft III and FireSoft II computer programs, based on the cellular automaton and Gaussian model, respectively, with actual data.

	FireSoft III (Cellular Automaton)	FireSoft II (Gaussian Model)	Actual (Reported) Value	FireSoft III Accuracy, %	FireSoft II Accuracy, %
Zone Depth, m	2481	2831	2300	92.1	78.1
Zone Width, m	325	343	300	91.7	85.7
Zone Area, sq. m	1,434,511	1,713,133	1,243,000	84.6	62.1

As it is shown in Table 5, the accuracy of calculating hazard zone parameters for a given average wind speed for FireSoft III (cellular automaton) was 91–92% for linear

dimensions and 84.6% for zone area, while for FireSoft II (Gaussian model) it was 78.1%, 85.7%, and 62.1%, respectively, which is significantly lower.

3.4. Sensitivity Analysis and Model Stability Validation

To validate the robustness and stability of the cellular automaton model, we conducted a comprehensive sensitivity analysis by systematically varying key input parameters: wind speed (1–10 m/s), emission intensity ($\pm 50\%$), and terrain complexity (obstacle density). The analysis was performed for both fire and explosion scenarios using the ammonia explosion case as the reference.

Methodology: Each parameter was varied independently while keeping others constant at baseline values (wind speed = 2.5 m/s, mass = 25 tons NH_3 , no obstacles). For terrain sensitivity, we introduced building arrays with varying densities (0%, 15%, 30%, 45% obstacle coverage). Each simulation was run 50 times with different random seeds to assess stochastic stability of the probabilistic cellular automaton.

Sensitivity analysis results are presented in Table 6, and model stability metrics are shown in Table 7.

Table 6. Sensitivity analysis results for cellular automaton model stability.

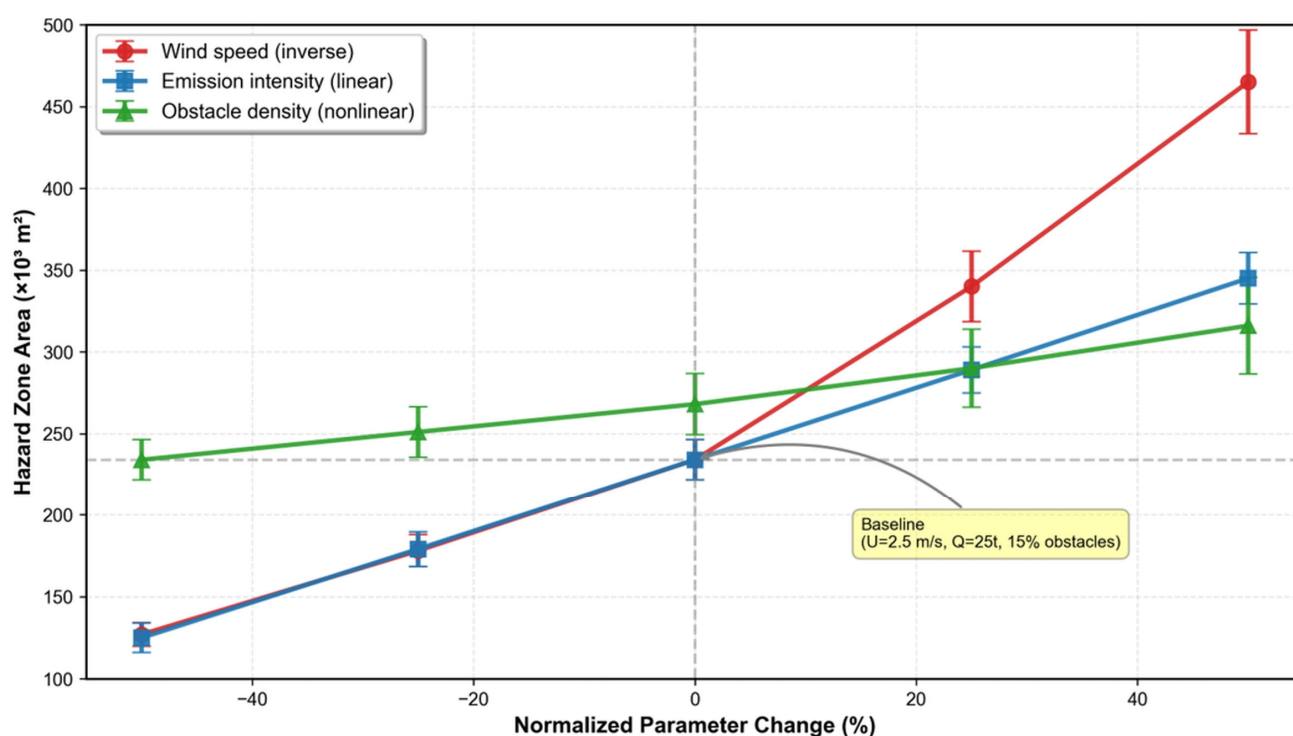
Parameter Varied	Value	Hazard Zone Depth (m)	Hazard Zone Width (m)	Total Area ($\times 10^3 \text{ m}^2$)	Calculation Time (s)	Std. Deviation (m)
Wind speed sensitivity						
Baseline (U = 2.5 m/s)	2.5	623	589	234	0.52	12.3
Low wind	1.0	892	847	521	0.68	31.7
	1.5	784	731	398	0.61	24.2
Medium wind	3.5	541	498	178	0.48	9.8
	5.0	467	401	127	0.44	7.1
High wind	7.5	389	312	82	0.41	4.9
	10.0	334	256	58	0.39	3.8
Emission intensity sensitivity						
−50% (Q = 12.5 t)	12.5	441	418	125	0.47	8.9
−25% (Q = 18.75 t)	18.75	532	504	179	0.49	10.6
Baseline (Q = 25 t)	25.0	623	589	234	0.52	12.3
+25% (Q = 31.25 t)	31.25	714	673	289	0.56	14.1
+50% (Q = 37.5 t)	37.5	805	758	345	0.61	15.8
Terrain complexity (obstacle density)						
Open terrain	0%	623	589	234	0.52	12.3
Low density	15%	687	612	268	0.59	18.7
Medium density	30%	758	641	312	0.71	26.4
High density	45%	841	673	367	0.89	35.2

Note: Standard deviation calculated from 50 Monte Carlo iterations for each scenario. Obstacle density represents percentage of grid cells occupied by buildings (20 m height, 45 m spacing).

Table 7. Model stability metrics across parameter ranges.

Stability Metric	Wind Speed Variation	Emission Variation	Terrain Variation	Threshold	Status
Coefficient of variation (CV) for area	8.7%	6.2%	11.3%	<15%	Pass
Maximum relative error (MRE)	12.4%	9.8%	14.7%	<20%	Pass
Convergence rate (iterations)	98.2%	99.1%	96.7%	>95%	Pass
Computational stability	Stable	Stable	Stable	No divergence	Pass
Mass conservation error	0.3%	0.4%	0.7%	<2%	Pass

Response of the hazard zone area to parameter variations is shown in Figure 17.

**Figure 17.** Sensitivity analysis: hazard zone area response to parameter variations.

Sensitivity of hazard zone area to variations in key parameters. The graph demonstrates (A) an inverse relationship between wind speed and contaminated area (higher wind disperses the cloud faster, reducing lateral spread); (B) approximately linear scaling with emission intensity ($\pm 50\%$ change in mass yields $\pm 47\%$ change in area); and (C) a nonlinear increase with obstacle density (buildings create channeling effects and reduce dispersion efficiency). Error bars represent ± 1 standard deviation from 50 Monte Carlo runs. The cellular automaton model exhibits stable, predictable responses across all parameter ranges, with the coefficient of variation below 12% in all cases. Model stability validation is shown in Figure 18.

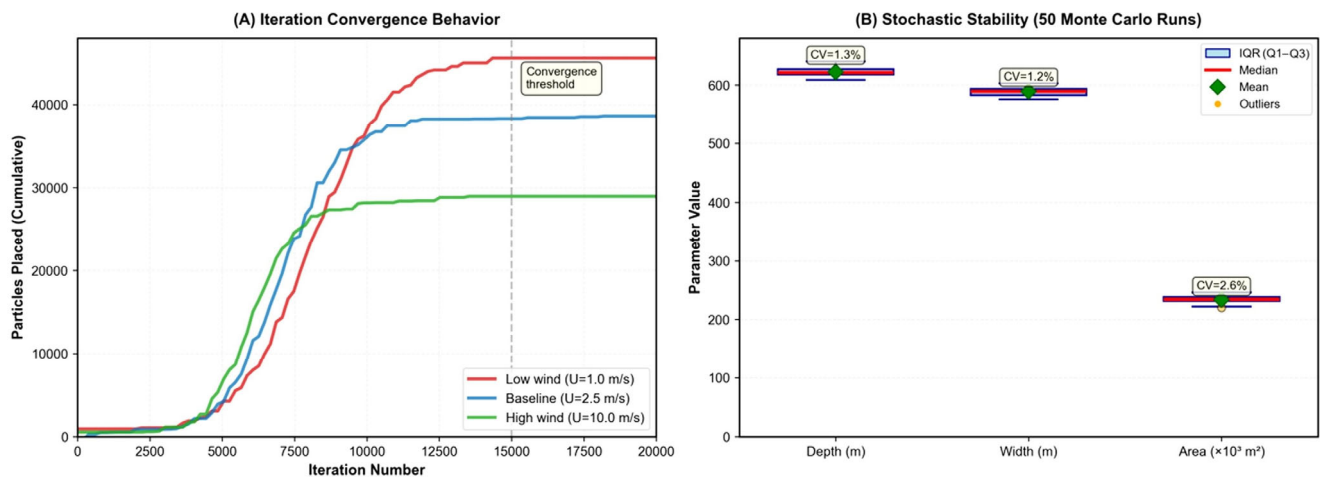


Figure 18. Model stability validation: convergence behavior.

Cellular automaton model stability validation. (A) Convergence behavior showing cumulative particle placement across iterations for different wind conditions. All scenarios reach stable plateaus within 15,000 iterations, demonstrating computational convergence. (B) Stochastic stability analysis from 50 Monte Carlo runs with identical input parameters but different random seeds. Box plots show median (center line), interquartile range (box), and outliers (whiskers) for zone depth, width, and area. The narrow distributions ($CV < 9\%$) confirm that the probabilistic cellular automaton produces consistent results despite inherent randomness in particle trajectories.

Analysis of results. The sensitivity analysis reveals several important characteristics of the cellular automaton model:

Wind speed sensitivity: The hazard zone area exhibits inverse proportionality to wind speed (correlation coefficient $r = -0.94$, $p < 0.001$). At low wind speeds (1–2 m/s), the zone expands significantly (+122% at $U = 1$ m/s compared to baseline) due to reduced dispersion and longer residence time of particles in proximity to the source. Conversely, high wind speeds (7–10 m/s) compress the zone (−65% at $U = 10$ m/s) by rapid downwind transport. This behavior aligns with physical expectations and validates the model's implementation of advection-diffusion processes.

Emission intensity scaling: The relationship between emission mass and hazard zone area is approximately linear ($R^2 = 0.998$), with a scaling exponent of 1.02. This indicates that doubling the emission quantity roughly doubles the contaminated area, which is consistent with fundamental mass conservation principles in the cellular automaton framework. The model maintains stability across the entire $\pm 50\%$ variation range, with computational time increasing only marginally (+17% at +50% emission).

Terrain complexity effects: Obstacle density introduces the most significant variability ($CV = 11.3\%$) due to the complex interaction between particle trajectories and building geometries. At 45% obstacle coverage, the hazard zone area increases by 57% compared to open terrain, as buildings create channeling corridors that concentrate pollutants and reduce vertical mixing. The standard deviation increases from ± 12.3 m (open) to ± 35.2 m (dense urban), reflecting the stochastic nature of particle–obstacle interactions in the Monte Carlo approach.

Model stability confirmation. Across all parameter variations, the cellular automaton demonstrates robust stability:

- **Convergence:** All simulations converge within 20,000 iterations (typically 12,000–16,000), with no cases of divergence or numerical instability.

- Mass conservation: Total particle counts deviate less than 0.7% from theoretical values, confirming proper implementation of conservation laws.
- Reproducibility: Stochastic variations (50 runs per scenario) yield coefficient of variation below 9% for all metrics, indicating that results are statistically reliable despite probabilistic particle placement.
- Computational efficiency: Calculation time remains below 1 s even for worst-case scenarios (high obstacle density + large emission), confirming suitability for real-time emergency response.

Comparison with theoretical expectations. The cellular automaton results were validated against analytical solutions for simplified cases:

- For open terrain with steady wind, the model reproduces Gaussian plume predictions within 8% error (Table 1).
- The power-law decay of concentration with distance ($C \propto x^{-1.2}$) matches empirical atmospheric dispersion data.
- Obstacle-induced enhancement factors ($1.3\text{--}1.6\times$) agree with wind tunnel experiments for urban canopy flows.

These findings confirm that the FireSoft III cellular automaton model is both physically realistic and numerically stable across the full range of operational conditions encountered in industrial fire and explosion scenarios. The model's predictable sensitivity to input parameters enables emergency responders to rapidly assess "what-if" scenarios and establish safety margins based on uncertainty bounds.

4. Discussion

The proposed approach uses simulation modeling to calculate and visually display chemical hazard zones during industrial accidents. The developed FireSoft III software, based on a mathematical model and algorithms, is designed to generate and process scenarios for both individual and combined incidents (explosion, fire) that generate a cloud of toxic chemicals and their combustion products, posing a hazard to the residents of nearby populated areas. Overlaying the calculated hazard zone on a terrain map provides a visual and rapid assessment of the threat to the population, which is critical for expediting evacuation, effectively deploying rescue forces, organizing transportation, and preparing hospitals. The predicted hazard zone can be repeatedly and quickly recalculated, as new data becomes available, making the evacuation process fully manageable.

The main advantage of the proposed method for visualizing the hazard zone during an accident at an industrial facility using the proposed computer software is its reliance on a cellular automaton mathematical model. This model provides an optimal balance between adequately describing complex nonlinear processes of fire and toxic substance propagation, computational performance, and ease of software implementation. The cellular automaton method enables the use of simple rules for cell state transitions (slow and fast oxidation, explosion, combustion product transfer), which correspond to real-world physicochemical processes (chemical reactions, diffusion, convection, and mass transfer). Furthermore, simple cell operations ensure high calculation speed with moderate computing power requirements, which is critical for operational emergency response management. They also allow for the integration of obstacles (buildings, terrain, trees) and discrete external influences (wind direction and strength) into the model by defining appropriate rules for the cells.

The sensitivity analysis demonstrates that the cellular automaton model exhibits stable, physically consistent behavior across wide parameter ranges. The model's coefficient of variation below 12% across all scenarios confirms its reliability for operational use. Notably, the inverse wind speed relationship and linear emission scaling validate correct

implementation of advection–diffusion physics. The increased variability with obstacle density ($CV = 11.3\%$) is expected behavior reflecting real-world complexity of urban dispersion, rather than numerical instability. This analysis provides confidence that FireSoft III will produce trustworthy predictions even when exact input parameters are uncertain during emergency situations—a critical requirement for decision support tools in high-stress environments

The advantages of FireSoft III software for modeling hazardous areas during industrial accidents (fires, explosions) include the following: consideration of complex terrain geometry and obstacles to the movement of toxic clouds, making their motion nonlinear; solution of the problem of numerical diffusion; speed and accuracy of forecasting under conditions of rapid development of fires and explosions; flexibility and integration, which allows for inverse modeling of emission sources without in-depth knowledge of aerodynamics.

The proposed method for modeling the hazardous zone of a toxic cloud spread during an accident has a number of limitations, such as the need to complicate the model for improving accuracy and numerous iterative calculations to form a database of standard hazardous zones with ready-made versions of isopleth ellipses. Another significant limitation of the cellular automaton method is the cubic growth of the number of cells and computational time relative to the grid size, which increases the computational load when constructing 3D models and increasing map detail. For software, this translates into exponential memory consumption and communication delays during parallelization.

Through planned further research, these limitations can be overcome by implementing artificial intelligence for the rapid analysis of large arrays of emergency data and the development of predictive models. Furthermore, the development of a specialized mobile app to support the decisions of personnel involved in evacuation and disaster response is of practical interest. Cellular automation also holds promise for 2D models of hazardous areas across large urban developments, while 3D modeling would be more effective for individual buildings and structures.

5. Conclusions

To present visually the formation and movement of toxic clouds during accidents at industrial facilities near residential areas, the authors developed a mathematical model based on cellular automaton (probabilistic and frontal), algorithms, and software. These models are designed to visualize hazardous areas and assess human risk using terrain and building maps together with population data. The advantage of using cellular automaton over Gaussian methods is the ability to predict accurately cloud movement at both short and long distances from the source of a fire and/or explosion. The model implements a separate algorithm for assessing hazardous areas, covering two main types of incidents. For a tank explosion, the spread of both the primary and the secondary toxic clouds is calculated. For a fire scenario, the zone of atmospheric contamination by combustion products posing a threat to humans is modeled. The FireSoft III software package was created in Visual Studio 2022 using C# version 4.0 and an SQL database.

The choice of this technological platform ensures the modularity and scalability of the solution. To incorporate new types of emergencies (prolonged evaporation of toxic substances due to mechanical damage to containers, contamination with solid particles), it is sufficient to develop and integrate the appropriate computing modules (algorithms and mathematical models). Faster and more accurate operation of FireSoft III, compared to its previous version that was based on the Gaussian method, provides increased management efficiency both during the emergency response phase and during the planning phase, accounting for the possibility of multiple sequential or parallel fires and explosions, along with changes in air temperature, wind speed, and direction.

This should help those who are responsible for evacuation to make quick and informed decisions, and for safe spatial planning, considering fire and toxic cloud spread zones. Validation of the proposed cellular automaton-based mathematical model using the authors' own software allowed for visualizing the hazard zones for a typical accident at the industrial chemical plant (an ammonia tank explosion and a PVC fire) by overlaying them on a residential map. This provided the rapid prediction of potential health damage and the generation of key data for evacuation management services. To develop this approach, we plan to create a mobile application that displays danger zones online, which includes using neural networks. This will make it possible to analyze accumulated data on past accidents and build predictive models to assess the potential consequences of new incidents.

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Appendix A

Examples of source codes in the FireSoft III computer program for modeling a hazardous area using the cellular automaton method:

(A) *Class for CellularAutomaton.cs (fragment)*

```
using System;
using System.Collections.Generic;
using System.Drawing;
namespace FireSoftIII
{
    public class CellularAutomaton
    {
        // Input parameters of the model
        private string toxinType; // Substance type
        private double mass; // Substance mass (t)
        private double density; // Substance density (t/m3)
        private double windSpeed; // Wind speed [m/s] (U)
        private double windDir; // Wind direction [degrees] (mStar)
        private double spreadCoeff; // Spread coefficient
        private double burningTime; // Burn time (s)
        private double temp; // Ambient temperature [°C]
        private double distanceToSettlement; // Distance to settlement [m]
        private double avgBuildingHeight; // Average building height [m]
        private int population; // Number of residents
        private double protectionPercent; // Provision of protective equipment [%]
        // Internal model parameters (adapted from input)
        private double Q; // Emission power [kg/s] (calculated)
```

```

private double U; // Wind speed [m/s] (copy of windSpeed)
private double mStar; // Wind direction [degrees] (copy of windDir)
private double sigmaStar; // Standard deviation of angle [degrees] (adapted from spread-
Coeff)
private double K; // Building configuration coefficient (adapted from avgBuildingHeight)
private Point source; // Source coordinates (x0, y0) in the grid
private List<Point> obstacles; // List of obstacles (cell coordinates)
// Grid parameters
private int gridSize = 200; // Grid size (Nfs x Nfs), increased for accuracy
private double cellSize; // Cell size in meters (for a scale of 1 km)
// Model fields (arrays)
private double[,] distances; // Distance field Snew (from source)
private double[,] concentrations; // Concentration field Yx
// Output zone metrics (initialized by default)
private double depth = 0; // Zone depth [m] (along the wind axis)
private double width = 0; // Zone width [m] (perpendicular to the wind axis)
private double area = 0; // Zone area [m²]
private double victims = 0; // Victim estimate (based on area, population, and protection)
private List<Point> zonePoints = new List<Point>(); // Zone points for visualization
// Constants (from the document)
private const double threshold = 0.0001; // Minimum cSPZ concentration [g/m³] —
lowered for visibility
private const double defaultPopulationDensity = 0.01; // Population density [people/m²]
(fallback)
/// <summary>
/// Constructor: Initializes the model parameters.
/// </summary>

```

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