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**MATHEMATICS METHODS AND INFORMATION SYSTEMS IN CHEMICAL TECHNOLOGY**

**МАТЕМАТИЧЕСКИЕ МЕТОДЫ И ИНФОРМАЦИОННЫЕ СИСТЕМЫ В ХИМИЧЕСКОЙ ТЕХНОЛОГИИ**

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# The development of a decision support information-modeling system for safety in the chemical industry

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*The analysis of the urgency of developing a decision and support information-modeling system for safety in the chemical industry is carried out. The article also covers the main elements of this information-modeling system. Key normative documents backing up the knowledge base of such an information-modeling system are listed below. The algorithm of the safety decision supporting information-modeling system is proposed. A database model of the safety decision supporting information-modeling system is elaborated below. A production rule system is set forth to manage issuing recommendations on the robust decision support information-modeling system in the chemical industry based on a methodological document. An implementation plan is laid out for the robust decision support information-modeling system in chemical industry. It is a ready-made software package based on two-level (client–server) architecture of information systems. This article also contains recommendations based on a test case of a tank equipment total destruction. Results of the computational experiments' simulation in the TOXI$^{+Risk}$ software corresponding to the test selected values are available.*

***Keywords:*** *information-modeling system, industrial safety, database, client–server architecture, production model, software.*

# Разработка информационно-моделирующей системы поддержки и принятия решений по управлению безопасностью химических производств

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*Проведен анализ актуальности разработки информационно-моделирующей системы (ИМС) поддержки и принятия решений по управлению безопасностью химических производств. Приведены основные подсистемы структуры данной ИМС. Перечислены основные нормативные документы для заполнения базы знаний ИМС; предложен алгоритм работы и разработана модель базы данных ИМС. Разработана система продукционных правил для управления выдачи рекомендаций ИМС на основе методического документа. Приведена программная реализация ИМС, представляющая собой готовый комплекс программного обеспечения на основе двухуровневой (клиент–серверной) архитектуры информационных систем. Приведен вывод рекомендаций, полученных для тестового примера аварии полного разрушения резервуарного оборудования. Приведены результаты моделирования вычислительных экспериментов в программном комплексе ТОКСИ$^{+Risk}$ для заполнения тестовой выборки.*

***Ключевые слова:*** *информационно-моделирующая система, промышленная безопасность, база данных, клиент–серверная архитектура, продукционная модель, программное средство.*

## Introduction

Today, many chemical, petrochemical and oil and gas production facilities are located near residential or socially significant accommodations and public transport facilities. Because of this, the potential number of victims in possible accidents at these facilities increases.

One of the important research methods is emergency forecasting. Therefore, it is most effective to model accidents at a given facility of a chemical, petrochemical or oil and gas industry.

Currently, information and computer technologies have been widely used in the field of chemical process control, the environmental monitoring of chemical enterprises and industrial safety, both in Russia [1–5] and abroad [6–8]. There is a number of software systems for modeling and/or forecasting emergencies at hazardous production facilities (HPF), and a practical experience has been accumulated in using them in the chemical and petrochemical industries [9, 10].

However, in a real accident, it is impossible to model the unfolding situation in real time. Therefore, it is necessary to enact a procedure for modeling possible emergencies for the standard equipment and initial parameters for storing hazardous substances in advance. Upon obtaining the modeling results, the decision maker (DM) should immediately analyze the gathered data and make a management decision regarding enterprise personnel rescue and the mitigation of the severity of the consequences. However, this procedure takes up considerable time in the real situation.

To solve these problems, it is proposed to implement an information-modeling system (IMS) for the support and decision making in managing the safety of chemical plants based on production models. This system will allow one to select a pre-modeled accident scenario, most likely in the given situation, obtain information on the damage zones associated with various types of fires, explosions, hazardous matters dispersion, and then give recommendations on improving the safety of the recipients in the zone of damage.

## Developing a safety decision support IMS in the chemical industry

When creating an IMS, the two-level architecture of an information system was used. It is a client-server architecture, which uses only a server containing a database and a database management system (DBMS), and a client holding the level of data representation.

1. *Data presentation level.* At this level, the interaction of the system with the user is formed. It is executed in the form of a program for working with the user, containing the procedure and conditions for the reactions of the information system to user actions based on clear functions.

2. *Level of access to the data* (server). It provides for the functions of storage, deletion, modification, processing and selection of data in the database.

Structural element of IMS includes five subsystems (Fig. 1):

• *The subsystem of interaction with the user (User Interface)*. This subsystem is meant for the intuitive interaction of the user with the system.

• *Input data selection subsystem.* The selection of substances in the database (DB) by their properties (toxicity, inflammability), the selection of accident properties and screening equipment to set the input data for the calculation.

• *Data storage subsystem.* This subsystem consists of the following databases: the DB of hazardous substances and their properties; the DB of HPF standard equipment; the DB of computational experiments (CE DB).

• *Decision making support subsystem.* It is a knowledge base of recommendations which is composed of normative, normative-methodological and normative-technical documents, algorithms, methods, decision making models. An important part is also the unit of analysis and comparison of the obtained results. Production models of knowledge presentation are the basis of recommendations aimed at the reduction of the severity of the accident's consequences for personnel. The condition criterion is minimizing the number of victims and the injured at HPF.

• *The subsystem for issuing recommendations and visualizing the results.* The results are presented in the program's user interface [11].

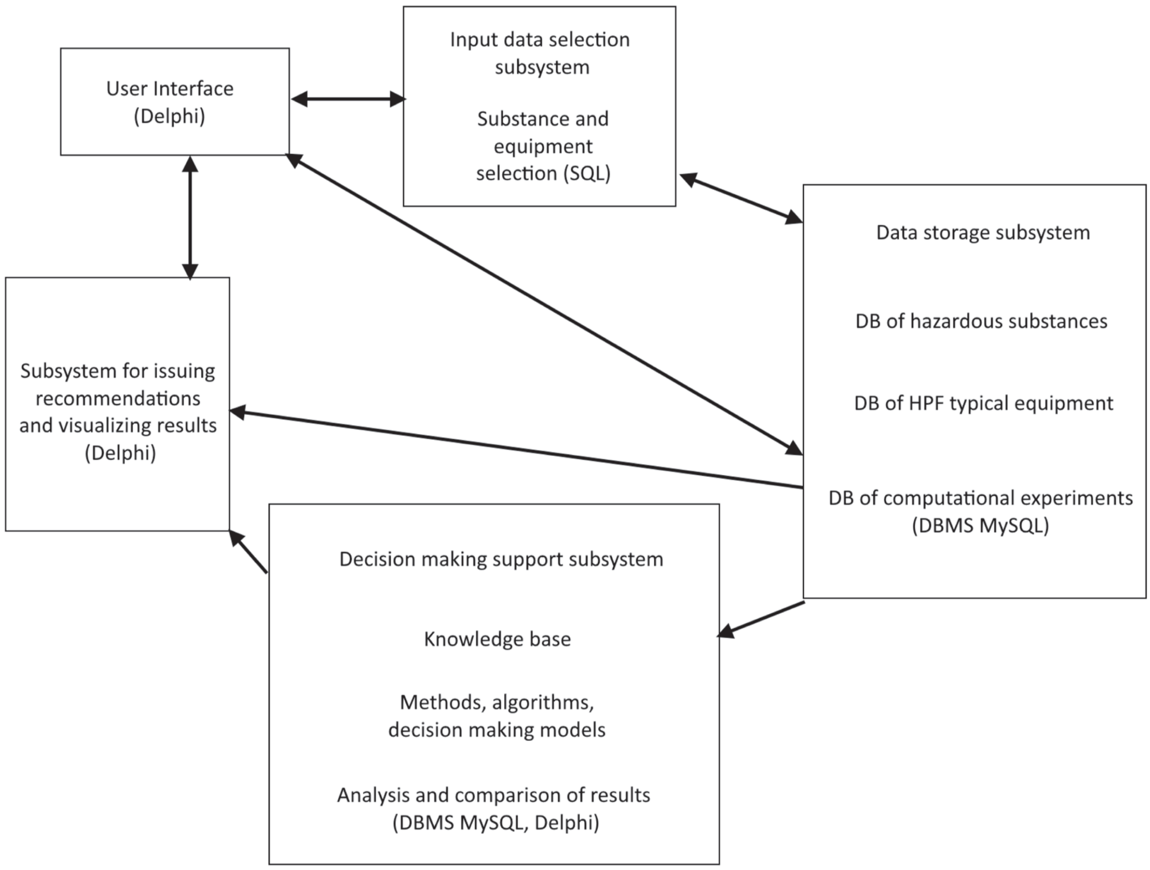


**Fig. 1.** IMS functional diagram.

Relevant information from normative documents in the knowledge base of recommendations is a guarantee of the effective use of the IMS. Below is a list of such documents (safety guides):

the methodological guideline for modeling the accidental releases[1]; the methodological guide for accident risk assessment at the oil and gas industry HPF[2]; the guide for assessing the consequences of accidents at explosive and fire hazardous chemical plants[3]; the methodological guideline for conducting hazard analysis and risk assessment for the accidents at hazardous production facilities[4]. These guides are based on the Federal Law[5] and federal norms and rules in the field of industrial safety[6].

For the above system, an algorithm is developed, as shown in Fig. 2. The first two steps allow one to enter the input data into the developed system. The next step is the search for the selected data in the CE

[1] Safety guide "Methodological guideline for modeling the accidental releases of hazardous substances" (Ratified in the Rostechnadzor order dated April 20, 2015, no. 158).

[2]Safety guide "Methodological guideline for assessing the risk of accidents at hazardous production facilities of the oil and gas processing, and oil and gas chemical industries" (Ratified in the Rostechnadzor order dated June 29, 2016, no. 272).

[3]Safety guide "Methodological guideline for assessing the consequences of accidents at the explosive and fire hazardous chemical plants" (Ratified in the Rostechnadzor order dated April 20, 2015, no. 160).

[4]Safety guide "Methodological guideline for the hazards analysis and risk assessment for the accidents at hazardous production facilities" (Ratified in the Rostechnadzor order dated April 11, 2016, no. 144).

[5]Federal law dated July 21, 1997, no. 116-FZ (edition dated March 07, 2017) "On industrial safety of hazardous production facilities"(with additions and ammendments effective of March 25, 2017).

[6]Federal rules and regulations in the sphere of industrial safety "General requirements to justification of safety of hazardous production facility" (Ratified in the Rostechnadzor order dated July 15, 2013, no. 306).

database and the selection of the appropriate scenario. The processing of large amounts of data obtained as a result of modeling using specialized software is required in order to implement the request. If the input parameters and the CE database data are equal, the corresponding emergency modeling results are issued. Then the CE database results are compared with the criteria values in the normative documents, a list of recommendations aimed at localizing the consequences of the accident is elaborated and issued to the user.

It was decided to use a free relational database management system MySQL[7] to develop the IMS database.

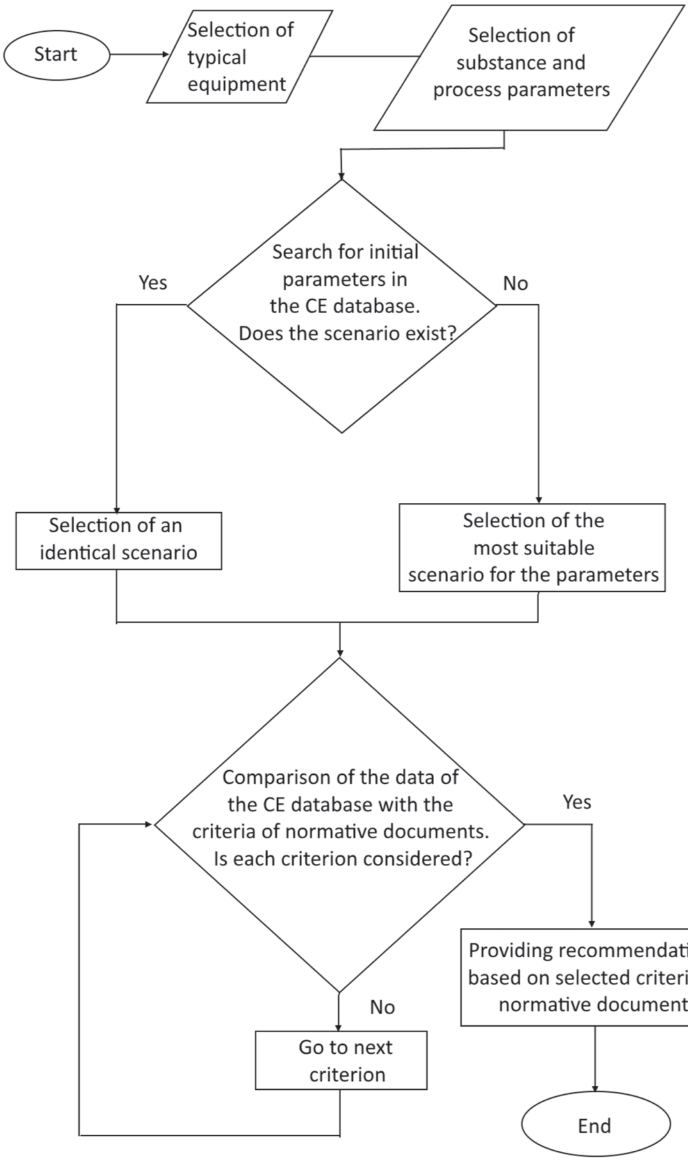


**Fig. 2.** The block diagram of the IMS algorithm.

The physical model of the database is presented on Fig. 3. A total of 10 tables were used in the current database. Each table has a primary key which characterizes a unique record number; for the table of substances, this is an identifier of a substance, for the table of stratifications—an identifier of stratifications, etc. The presence of external keys is clearly shown in the tables of input and experimental data. With their help, the tables of substances, stratifications and clutters are connected with the table of input data, and an outcome table (spill fire, fuel-air mix explosion, blowup fire, and dispersion), equipment and input data are connected with the table of computational experiments data.

Several types of data were used during the model creation. Each identifier field has a whole number format —an integer. Text data are presented as a varchar (30) type, which allows for input of 30 characters per line. All variable values which are used in recording the rest

[7]Free relational database management system “MySQL”, 2018. URL: https://www.mysql.com/ (accessed March 22, 2018).

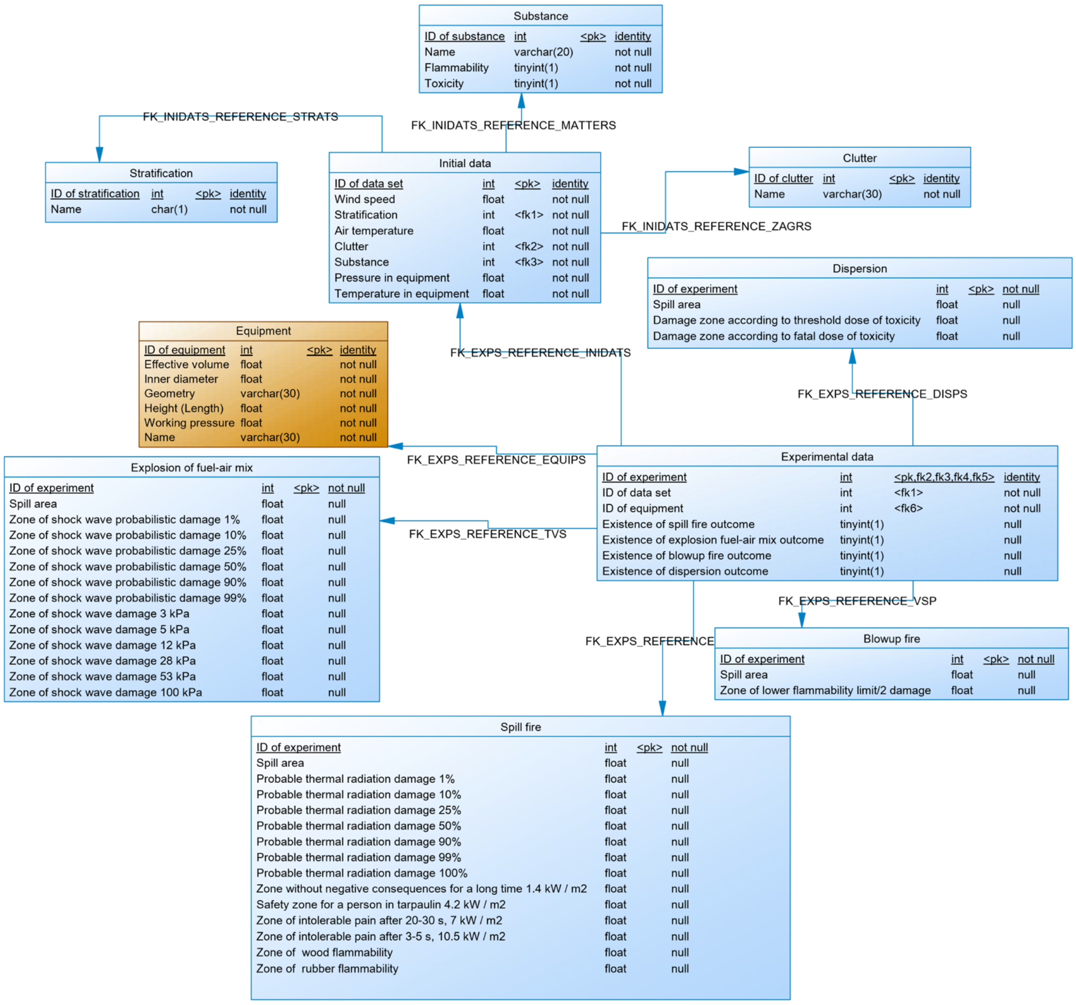


**Fig. 3.** The physical model of the database.

of the data have the format of floating numbers—float. It should be noted that, in the stratification table, there is a unique column which contains a record of the names of stratifications consisting of one letter, and it has a char (1) format. Another unique type is a tinyint (1), which is used to mark the presence of a certain outcome in a given computational experiment in the table of computational experiments, called a "flag".

Since the parameters are entered by the user to search for scenarios, for the sake of correctness they cannot have gaps. Therefore, the fields of the source data tables should not have NULL values (gaps) in their cells. At the same time, there is no such requirement for the tables which contain the data of computational experiments (except identifiers), so they do not need the Mandatory (not NULL) property.

The tables for the input of initial data allowing for the assessment of the scale of an accident are the two main tables with initial parameters.

The data table "Input data" contains data on the substance and its storage parameters, meteorological conditions. It is also connected with the tables "Substance", "Stratification", and "Clutter", which are filled with the values used in combining input data. The "Substance" table has 25 records of various substances, the "Stratification" table – only 6 records, and the "Clutter" table – 4. The data table "Equipment" is filled with the data on standard pieces of equipment and their properties.

The CE database contains the data obtained during modeling in TOXI$^{+Risk}$ [1]. The scenarios of hazardous outcomes may group the accident data. In this paper, the accidents occurring on stand-alone units of equipment (tanks) are considered. Groups of criteria collected into each outcome are divided into deterministic and probabilistic.

The client part was created using the Borland Delphi[8] 7 programming environment based on a structured Delphi object-oriented programming language.

Edit type fields, which allow one to input parameters, are used to input numerical data. Other values are entered into the Combobox drop-down boxes.

[8]Software tool «Delphi». Company Embarcadero, 2018. URL: https://www.embarcadero.com/ru/products/delphi (accessed March 22, 2018).

When one clicks the "Select Scenario" button, a similar scenario is searched for in the database of computational experiments. The selected scenario will be displayed in the Memo field ("white square" on Fig. 4). If such a scenario does not exist, the program will select the scenario with the most matching parameters.

When one clicks on the "Damage zones" button, the values of the damaged zones of the hazardous outcomes are displayed.

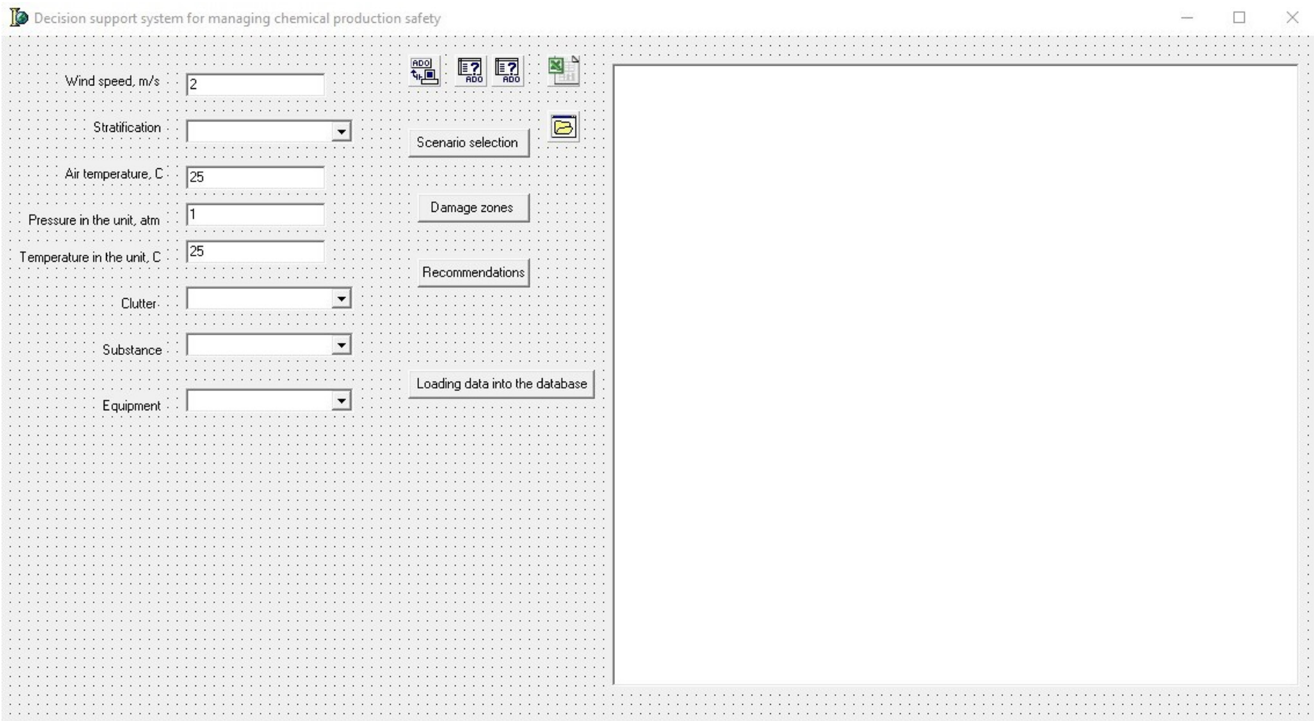


**Fig. 4.** The screen form of the interface of the decision support system.

On Fig. 5 the scenario is displayed under the unique identifier 23. It has labels of different outcomes. In the presence or absence of this outcome, the value varies from 1 to 0 respectively. In this example, the substance "Butane" is located in standard equipment "LPG tank 15-1200-02" (EQUIP_ID=15) at the pressure of 20 atm. The results of a computational experiment were obtained for the scenario including a wind speed of 1 m/s, stratification F, temperature in the apparatus equals to the ambient temperature – 25 °C, the location is heavily cluttered (all of the above data on the process parameters are included in the initial data set INIDAT_ID = 15). Toxic damage is absent, EXP_RAS (Dispersion) label is 0.

SELECT * FROM disserdb.exps WHERE EXP_ID=23 | Enter a SQL expression to filter results (use Ctrl+Space)

| | EXP_ID | INIDAT_ID | EQUIP_ID | EXP_PROLIV | EXP_TVS | EXP_VSP | EXP_RAS |
|---|---|---|---|---|---|---|---|
| 1 | 23 | 15 | 15 | 1 | 1 | 1 | 0 |

**Fig. 5.** Scenario No. 23.

Having identified the presence of certain outcome marks, the software starts to display the values of the recorded criteria from the database for the user (Fig. 6). As one can see, the scenario of toxic damage from the "Butane" substance is absent.

Having received these values of the damage zones, the user must be given recommendations on the actions in case of an accident. After analyzing a number of safety guides, it was decided to use the guide "Methodological guideline for the hazard analysis and risk assessment for the accidents at hazardous production facilities" (see Footnote 4 on page 61), as it clearly indicates the criteria for safe locations and fatal injury. On Fig. 7, recommendations for the above butane scenario are presented. The recommendations are derived based on production rules. The criteria described in the manual mentioned above are checked. If a specific criterion in the CE database exists, the user will be presented with its description in the form of a recommendation based on the text of the document. For the user's convenience, recommendations are presented in the form of a system of production rules, the main components of which are shown in the table.

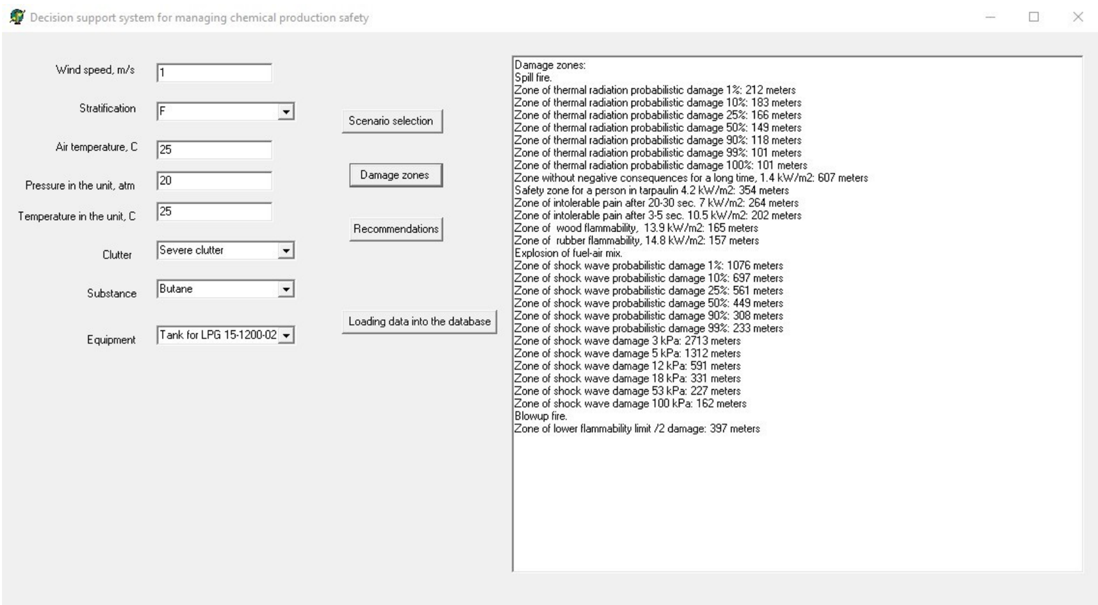


**Fig. 6.** Damage zone interface.

Recommendations:
Document SAFETY GUIDE "METHODOLOGICAL GUIDELINE FOR ANALYZING HAZARDS AND RISK ON HAZARDOUS INDUSTRIAL FACILITIES".
Spill fire.
When using probit functions the damage zones where the probit, function indicators reach the value corresponding to 90% probability are taken for the zones of 100% damage. Leave the 118 meter damage zone immediately.
The damage zones where the value of the probit function reaches the value corresponding to 1% probability are taken for the zones safe from the standpoint of the impact of damaging factors. For your safety, reach 212 meters from the equipment unit.
Blowup fire.
For a blowup fire it shall be assumed that the conditional probability of damage of a person who appeared in the zone of exposure to high-temperature combustion products of a gas vapor/air cloud equals 1. Outside of this zone, the conditional probability of a person being damaged is assumed to be 0. Leave the 397 meter damage zone from the radiation of the blowup fire of the fuel-air mix cloud.
Fuel-air mix explosion.
The value of excess pressure at the front of the shock wave P = 5 kPa is accepted as safe for humans. In order to reach a safe area, your distance from an equipment unit should be 1312 meters.
Impact on a person with a shock wave with P > 120 kPa excess pressure at the front is recommended to consider as a lethal damage. It is necessary to leave the 162 meter zone of complete destruction of buildings.

**Fig. 7.** IMS recommendations for scenario No. 23.

The main components of the system of production rules for managing the issuance of recommendations developed by the IMS based on the methodological document

| Parameter | Title |
|---|---|
| Pr | Spill fire outcome |
| Vs | Blowup fire outcome |
| Tv | Fuel-air mix explosion outcome |
| Di | Dispersion outcome |
| $Pr_1$ | Zone of thermal radiation probabilistic damage 1% |
| $Pr_{90}$ | Zone of thermal radiation probabilistic damage 90% |
| $Vs_{LFL}$ | Zone of lower flammability limit/2 damage |
| $Tv_5$ | Zone of 5 kPa shock wave damage |
| $Tv_{120}$ | Zone of 120 kPa shock wave damage |
| $Di_p$ | Damage zone according to the threshold dose of toxicity |
| N | Presence |
| P | Leave |
| D | Reach |

For the selected document, the production rules of the system take the following view:

If Pr=N, then P, $Pr_{90}$; D, $Pr_1$;

If Vs=N, then P, $Vs_{LFL}$;

If Tv=N, then P, $Tv_{120}$; D, $Tv_5$;

If Di=N, then P, $Di_p$.

Pressing the “Load data into the database” button allows one to upload new data modeled with the TOXI$^{+Risk}$ software package to the database of computational experiments.

To fill the database of computational experiments, the TOXI$^{+Risk}$ version 5.2 [1] software package was used. Computational experiments were carried out for various substances. Nine substances were used for the current test database: gasoline, chlorine, ammonia, methanol, butane, hexane, chlorine cyan, benzene, diesel fuel. They were selected in order to vary the event trees that characterize the possible outcomes of the scenario. Fig. 8 presents the HPF with one equipment unit (the star), as well as the calculated damage zones for the scenario under identifier No. 23.

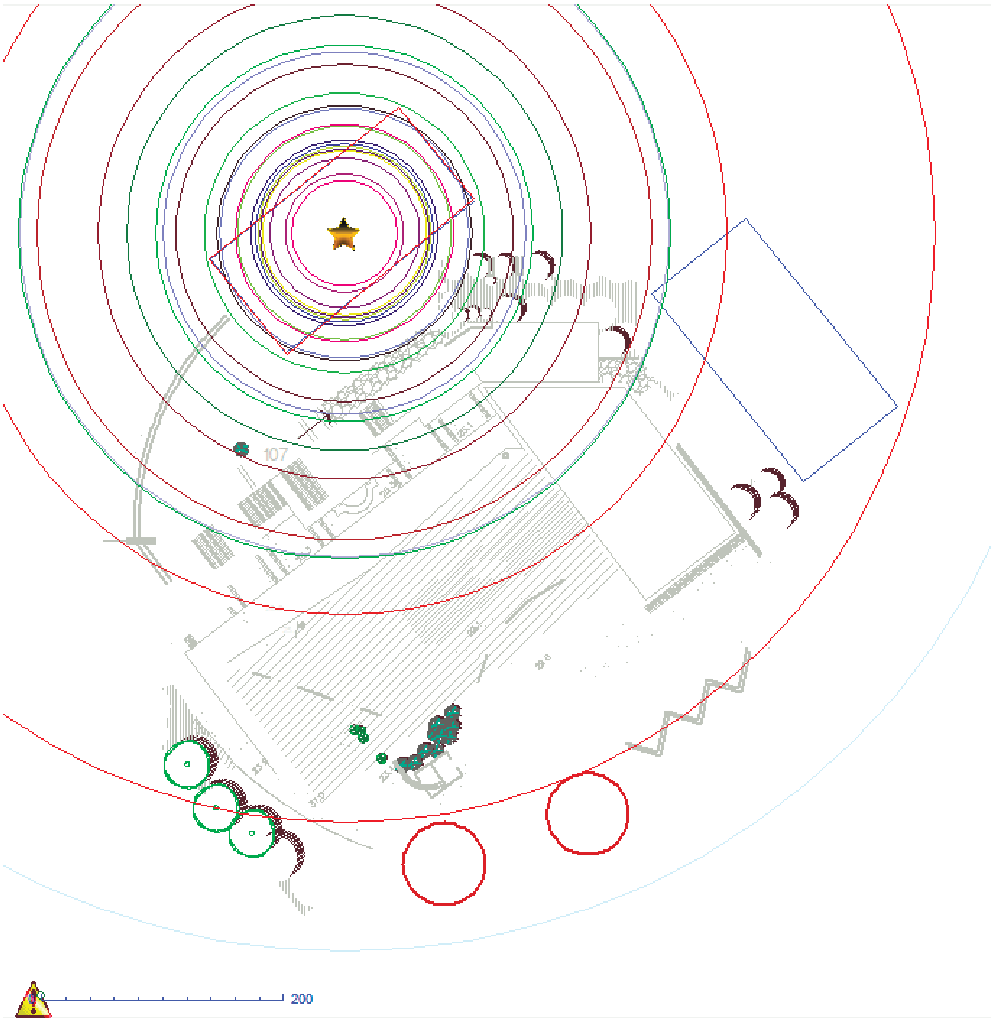


**Fig. 8.** Calculated damage zones for the selected scenario.

At this stage, the initial data must be input: meteorological parameters, equipment, properties of a hazardous substance, and the choice of an accident development tree. Upon the completion of the input of the initial parameters, the damage zones are calculated for the selected criteria.

After modeling, a file is generated with the results of the scenario of complete equipment destruction (Fig. 9). The criteria for each outcome are divided by page and split into deterministic and probabilistic.

**Blowup fire (Ministry of Emergency Situations method)**

| Site object | Equipment | Status | Hazardous substance | Meteo | Spill area, m2 | Hole area, m2 | Mass involved in the formation of hazardous factors, kg | Radius of the lower flammability limit/2 zone, m |
|---|---|---|---|---|---|---|---|---|
| new areal facility | Tank for LHG 15-1200 -02 | Operating status 1 | Butane | NE, 1m / s, F, 25 deg. C | 7934,31 | Complete destruction | 0 | 396,54 |

**Fig. 9.** The tab “Blowup fire” for obtaining the file with the results.

As a result, a file with the damage zones was obtained for various criteria of the calculation methods for entering data into the database of computational experiments. Each page of the file represents the results of a particular outcome. The current system includes 51 test experiments with various initial parameters.

## Conclusions

1. Analysis was carried out of the relevance of IMS development and the current state of specialized information technologies in Russia and abroad.

2. The functional structure of the IMS was developed. The utilization of this system allows the user to receive recommendations for improving the safety of recipients.

3. The algorithm for the operation of the IMS, schematically representing the order of interaction with the system, is presented.

4. The physical structure of the IMS database was developed; the interactions between the associated tables of the system data were clearly displayed.

5. A system of production rules was developed for managing the issuance of IMS recommendations based on a methodological document.

6. The software implementation of the IMS based on the client-server architecture of the information network was carried out; an example of the system's operation was presented.

7. Scenarios for the total destruction of equipment with various initial parameters were modeled using the TOXI$^{+Risk}$ software package to fill in the server part of the IMS.

In perspective, it is planned to implement scenarios of equipment depressurization to include the flare outcome, add new production rules from other normative documents and fill the CE database with new modeled results.

*The authors declare no conflict of interest.*

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