

# The Use of Simulation Programs of Leakage of Harmful Substances for Crisis Management

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**Abstract**—The paper deals with simulation programs of spread of harmful substances. Air pollution has a direct impact on the quality of human life and environmental protection is currently a very hot topic. Therefore, the paper focuses on the simulation of release of harmful substances. The first part of article deals with perspectives and possibilities of implementation outputs of simulations programs into the system which is education and of practical training of the management staff during emergency events in the frame of critical infrastructure. The last part shows the practical testing and evaluation of simulation programs. Of the tested simulations software been selected Symos97. The tool offers advanced features for setting leakage. Gradually allows the user to model the terrain, location, and method of escape of harmful substances.

**Keywords**—Computer Simulation, Symos97, spread, simulation software, harmful substances.

## I. INTRODUCTION

THE sustainable development is a trend of advancement of human society which harmonizes economic, social and environmental components. Environmental component has been often underestimated until recently and it has been getting into awareness of people only in recent past. Environment is often polluted by releasing various contaminants into the water, soil, and air. This article concentrates on the modelling of the harmful substances release into the air and a possibility of the usage of the related outcomes of the programs used for making constructive simulation more accurate to be suitable for the practical training of the intervention of rescue units.

Legislation deals with the air protection in the Directive 2008/50/EC of the European Parliament and of the Council of 21 May 2008 on ambient air quality and cleaner air for Europe [1]. The aim of the directive is to improve monitoring and assessing the air quality together with providing information to the public.

In order to protect human health and environment as a whole, it is extremely important to fight against emissions of harmful substances at their source, establish, and execute the most effective measurements for their minimization on local as well as national levels. The same principle should be applied also when harmful substances are released as a part of emergency events and crisis situations.

As long as it is possible, techniques of modelling and simulation should be used as they enable to better interpret the data from individual areas from the point of view of

geographic distribution and concentration. This is the reason why this paper concentrates on the selection of the appropriate software support for modelling and simulation of the release of harmful substances into the environment and a possibility to implement the outcomes of these programs into the education as well as practical training of the intervening units during emergency situations [2].

Simulation is used in many contexts comprising modelling of natural or human systems with the aim to obtain knowledge about their behaviour. Other contexts comprise technological simulations for optimizing the performance, security engineering, testing, training, and educating. Simulation can be used for visualisation of possible real impacts, alternative conditions, and ways of acting.

## II. CLASSIFICATION OF SIMULATION APPROACHES

Currently, there are mainly used two types of models for simulation and leak modelling of hazardous and noxious substances into the environment [3].

### A. Statistical Modelling

More widespread are statistical models which cope better with time-consuming and costly calculation. They are more widespread thanks to the greater availability. Simplification of the solution is the result of major inaccuracies of model in the vicinity of emission sources and in rugged terrain. In the atmosphere there are ongoing random happens, in a statistical sense. Turbulence means in fact a condition in which the instantaneous velocity shows irregular, disorganized, random pulsations, so that practically can be examined and put into analysis of statistical properties. Statistical models can describe the actual flow in a simplified manner. Mathematically, the statistical models are based on solution of the diffusion equation where it is assumed the dominant advection transport in the wind direction. In the vertical and horizontal direction perpendicular to the direction of flow is then statistically described turbulent diffusion using the normal distribution. Examples of tools of this group is modelling program SYMOS'97.

### B. Dynamic Modelling

Dynamic models are based on the direct application of basic hydrodynamic and thermodynamic equations which are solved numerically. It seeks to express the status and timing development of the real boundary layer of the atmosphere. It is quite difficult due to the complexity and randomness of turbulent flow in the atmosphere. Systems of equations include certain simplifying of assumptions and empirically measured or estimated coefficients. Another problem in

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dealing with these difficult numerical calculations of systems of partial differential equations is considerable demands on the performance of computers and computation time. The mathematical model consists of a set of algebraic and partial differential equations, which is solved by finite volume method (or finite element method) [4]. Representative instruments of this group include Ansys Fluent, Star-CCM+ and Panache Panair.

For the training preparation, instructors can use various computer programs which enable better graphic visualisation of the solution, practice different ways of dealing with the different situations, and the way of command. What is more, they can represent a tool for the various roles in the process of solution of the emergency situation. The environment of these programs increases the effect of preparation, which results in being more realistic and the trainees will better memorise the trained actions [2].

### III. MODELING TOOLS FOR THE RELEASE OF HARMFUL SUBSTANCES

This chapter lists the most commonly used programs for the modelling of the release of harmful substances. Based on the analysis of the individual programs, their individual features, possibilities, and output formats were assessed for the use in the proposed simulation tool for the support of practical training in dealing with emergency or crisis situations.

#### A. Ansys Fluent

It is a computer program for modelling and simulation of the liquid flow, heat transmission and chemical reactions in complex geometry [5]. The tool provides advanced options for designing a flexible simulation network while it enables to solve the issue of flow simulation even with the non-structured network which can be generated with the relative size. Supported types of simulating networks comprise 2D triangular/quadrangular shape, 3D square/hexagonal/pyramidal shape or mixed (hybrid) shape of the network. Ansys Fluent also enables to make the used simulation net finer or rougher according to the specific features of the analysed flow [6].

Ansys Fluent enables parallel processing of the results which has impact on the speed of the simulation. Parallel processing is reached by division and distribution of the calculation between the hosting and other computing processes. The hosting process controls the calculation and at the same time integrates the obtained results from the calculation processes. All functions required for the calculation of the solution as well as visualisation of the results are accessible via clear and interactive interface [5].

#### B. Star-CCM+

Star-CCM+ is a relatively new product of the CD-Adapco company which is the same one which developed the Star-CD product. Star-CCM+ is known as the next generation of the software tool designed for calculation of the liquid flow dynamics (CFD), which is built on the latest software

technologies represented by the client/server architecture, object oriented programming, scalable parallel computing or the support of another platforms [7].

The tool provides techniques for the automated creation of the simulation network, wide range of physical models, great choice of the turbulence models and at the same time powerful tools for results evaluation. Based on its unique qualities, this tool can be directly incorporated into the CAD or PML environment e.g. SolidWorks. Extension Star-CAD serves this purpose.

Compared to other commercial tools, this program can be used intuitively via integrated user interface. After the geometry creation using the CAD tool, it can be transformed into Star-CCM+ and subsequently create a simulation network, select the required physical model as well as other features of the calculation. Presentation of interactive results together with the possibilities of their further processing is possible via the same Star-CCM+ tool [7], [8].

#### C. Panache – Panair

It is a diagnostic computer model designed for the simulation of atmospheric processes related to pollution and risks [3]. It uses 3dimensional methods for the calculation of the dynamics of the liquid flow, for the calculation of the wind flow over the whole terrain, for the spread of pollution, fire or explosion. If they are used together with other prognostic wind models as is MM5, they can be used for the analysis of the prognoses of both pollution and risks [9].

Fast development of the computer hardware and CFD methods enable people who are not experts in numeric modelling to create studies of the release on personal computers in the reasonable time. Panache uses physical models and deterministic techniques of solution which comprise less empiricism and are less sustainable to position, own scenario or the characteristics of the contaminants as Gauss models [3], [9].

Air can be modelled either with constant density or as a gas following the ideal gas laws. Atmospheric turbulences above the ground or around the obstacles, as are thermal effects, are modelled using 0-, 1- and 2- linear equation models. All the effects of the terrain topography (Fig. 1) as is the surface of the terrain, vegetation or town build-up areas are taken into account. Chemical reactions as is burning and production of secondary or tertiary contaminants is modelled according to suitable reaction mechanisms together with reaction speed controlled by kinetics, mixing or photolitically.

#### D. Symos97

Symos97 is the tool for quick forecasting of consequences and impacts of chemical materials leaks on the environment. Thanks to this program, it is possible to calculate and visualize the emission leaks and to model the consequences that resulted from contamination of the environment. The model includes connectivity to geographic information system for direct results display in the map. This software is easy to use members of crisis management [10].

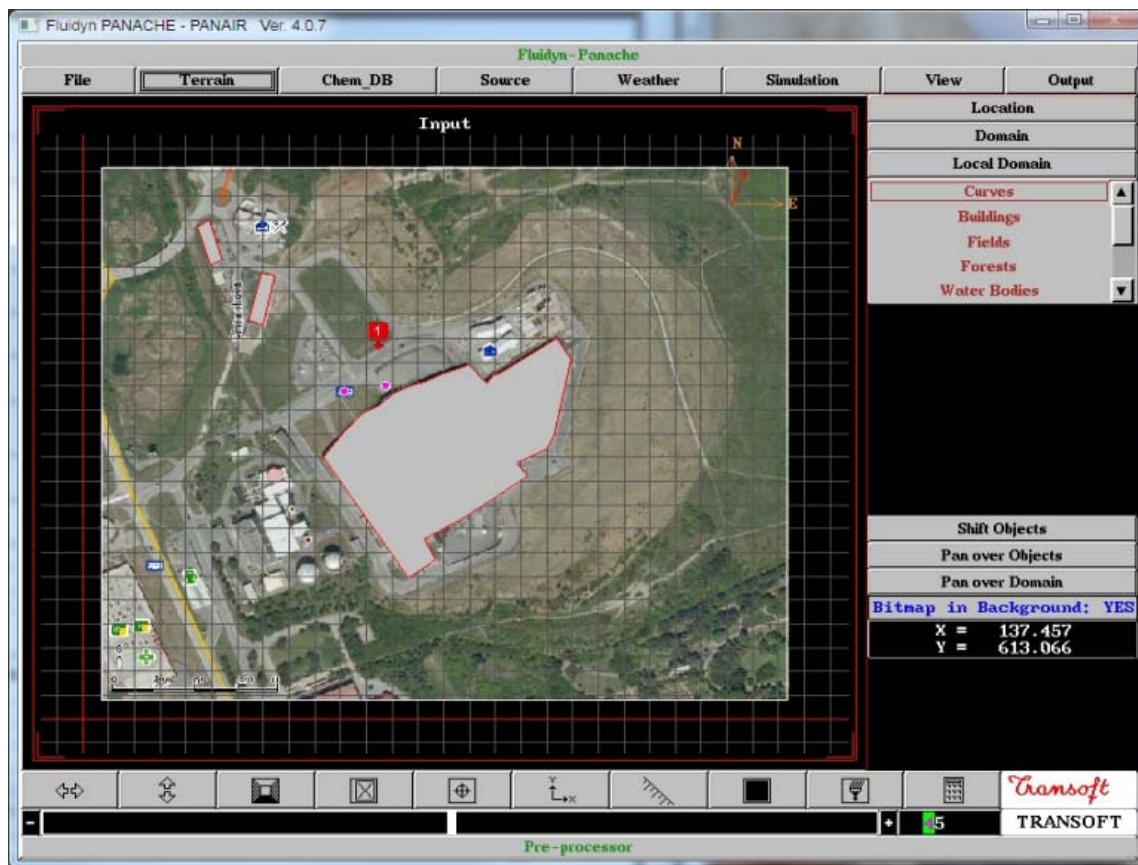


Fig. 1 Panache – Panair simulation

Methodology / SYMOS'97 software allows:

- calculation of air pollution gaseous substances and dust from point, line and area sources,
- calculation of the contamination from a number of sources,
- to identify the characteristics of pollution in dense geometrical network of reference points,
- to consider the statistical distribution of wind speed and direction relative to the stability classes layers of the atmosphere [10], [11].

Symos'97 calculation results are arranged in a very easy, comprehensive, and un-ambiguous format, which helps to make quick decisions. This effect is achieved by minimizing output items to important ones and by displaying results on the map (Fig. 2). They can create simulations and estimates of emissions in populated areas and forecasts the size of the concentration in the monitored area [12].

Input data needed to calculate air pollution can be divided into the following categories:

- Details of the sources;
- Meteorological and climatic bases;
- The data on the topographical distribution of data points in which the calculation is performed, information on the height and location of buildings in the area of interest;
- The data on air pollution limits and allowable concentrations of pollutants.

The required input data for simulation are further varied by source of danger type (point, area, road, cooling towers, etc.) and conditions in the atmosphere modeled calculation (calculation under normal conditions or still air). The most commonly used coordinate system used to describe the location of a resource or reference nodes, the rectangular system, the X axis pointing to the east, the Y axis pointing to the north and the Z axis pointing to the zenith and represents the altitude or height of buildings [11].

#### E. TerEx

TerEx is the tool for quick forecast of chemical materials and tripwire explosive systems impacts and consequences. Damage of society integrity is often the main goal of terrorist misuse of hazardous materials. The software model includes connectivity to graphic information system for direct results display in the map (Fig. 3).

TerEx is aimed mainly for flexible use by rescue units during the operation to quickly determine the range of area under risk and to manage measures to protect inhabitants. It is possible to use TerEx by the operation commander directly at place or by operation officer in Command and Control Center. TerEx is also very effective for planning and risk analysis. The model works even when not all input data are available. It is an advantage for use in stress situations [3].

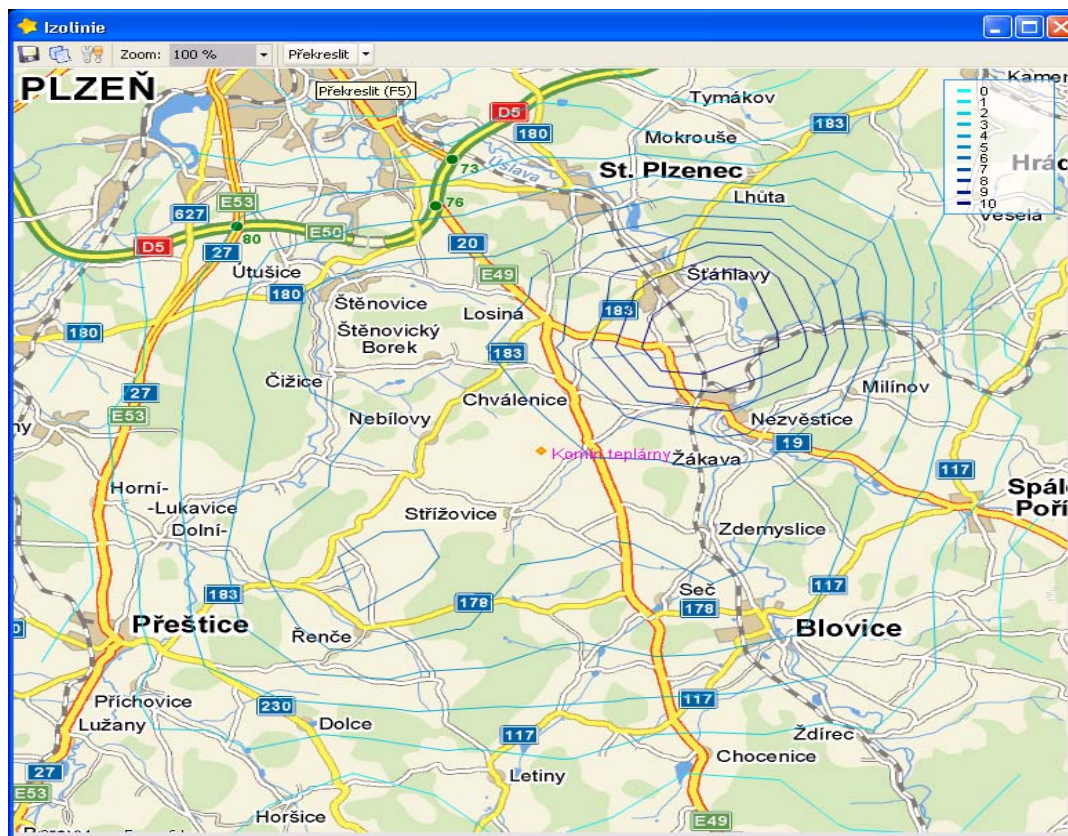


Fig. 2 Symos97 – displaying results on the map

The impacts and consequences forecast are based on conservative forecast. In practice, it means that the results correspond to such conditions where maximum possible impacts and consequences to the environment occur, i.e. the worst possible variant.

TerEx is characterized by high comfort and easiness in use. It is possible to select parameters from menus. TerEx Wizard enables to achieve highly reliable results both for specialist and for the person who is not an expert in chemistry or pyrotechnics (e.g. crisis manager). Via simple questions and menus, the user is guided to accurate and unambiguous specification [2].

#### F. Aloha

Areal Locations of Hazardous Atmospheres (Aloha) is a computer program designed to model chemical releases for emergency responders and planners. It can estimate how a toxic cloud might disperse after a chemical release—as well as several fires and explosions scenarios.

Aloha is designed to produce reasonable results quickly enough to be of use to responders during a real emergency. Therefore, Aloha's calculations represent a compromise between accuracy and speed. Many of Aloha's features were developed to quickly assist the responder [2], [12].

For example:

- Minimizes data entry errors by cross-checking the input

values and warning the user if the value is unlikely or not physically possible.

- Contains its own chemical library with physical properties for approximately 1,000 common hazardous chemicals so that users do not have to enter that data.

Program Aloha has an option to show drawings of various geographic information systems. Its use increases export freeware online map Google Earth.

These programs are suitable for creation of input data for initiation of the situation of emergency event with the release of a harmful substance or in the case of release which can be added into already running scenario of the emergency event. However, for the practical training and cooperation of the intervening units, it cannot be used [13], [14].

#### IV. EVALUATION OF SIMULATION PROGRAMS

From the model programs which were analyzed in detail it seems that tools concentrating on the accidental release of harmful substances as a source of input information are especially suitable. From the evaluation of the results as can be seen from Table I, it is clear that right these programs are suitable as input information into the simulator for the practical training of the solution of emergency events due to their variability and format of outputs.

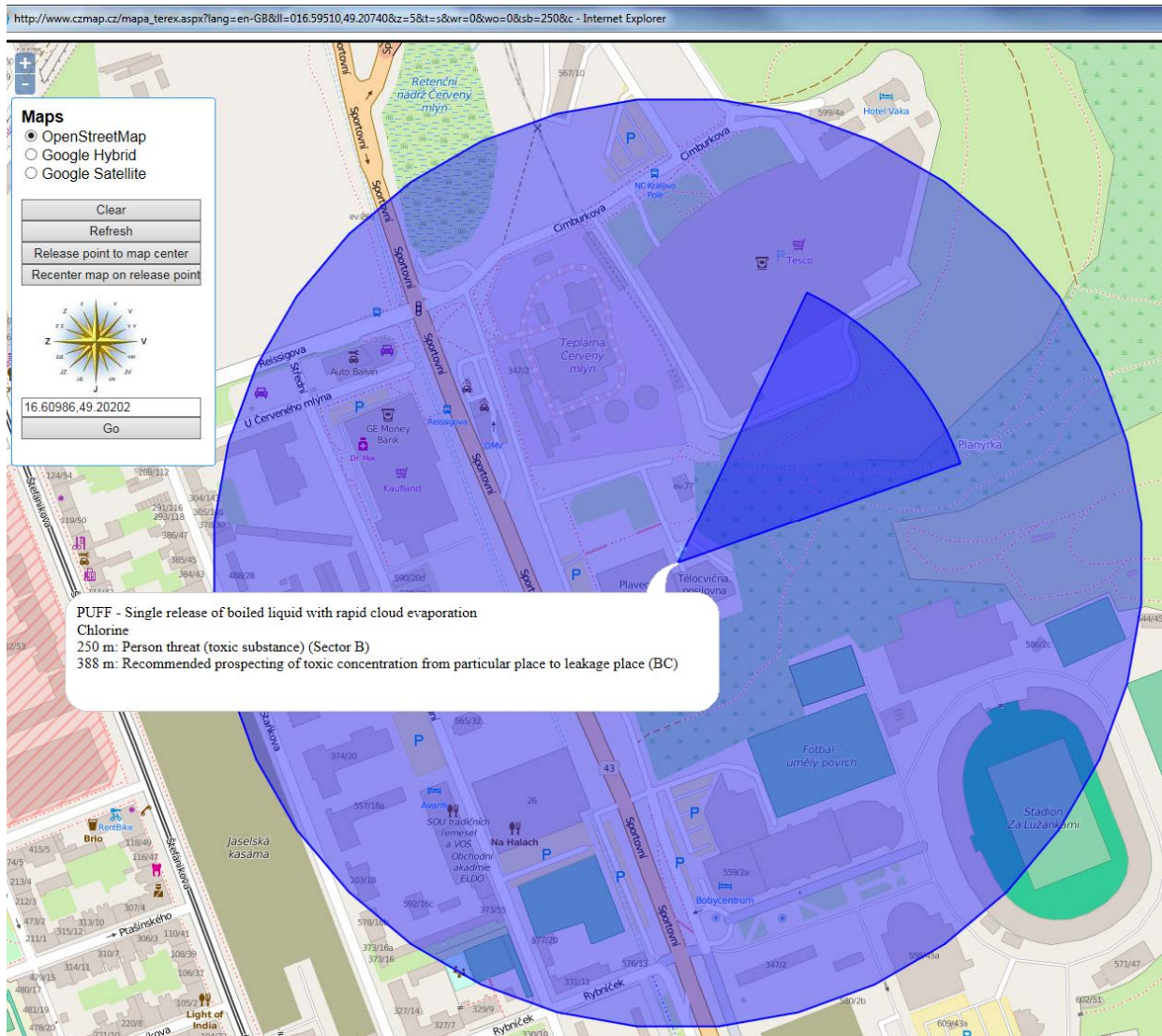


Fig. 3 TerEx – Export to Map

TABLE I  
EVALUATION OF SIMULATION PROGRAMS PROPERTIES

Simulation programs	Detectable by Inputs	Practical Exercises	User Friendly	Communication Interface	Data Output Multiple Formats	Output to Geographic Information System
Ansys Fluent	YES	YES	YES	NO	NO	NO
Star-CCM+	NO	YES	NO	NO	NO	YES
Panache – Panair	NO	NO	YES	NO	YES	YES
Symos97	YES	YES	NO	YES	NO	YES
TerEx	YES	YES	YES	YES	YES	YES
Aloha	YES	YES	YES	NO	NO	YES

The basic criteria were functionality, usability in solving emergency events, practical training, user friendly, and possibility of implementation of outputs from other tools. During the analysis of available simulation tools, some criteria were reconsidered and complemented with other characteristics which were required from the simulation tools. These added characteristics specified in more detail the choice of suitable simulators and made the original characteristics

about what the simulator should meet, more accurate.

## V. CONCLUSION

During the detailed analysis of the simulation programs, it has been found out that any of the producers does not provide a testing version of his simulator for verification of all its characteristics and functionalities. The only exception is

National Ocean Service, Office of Response, and Restoration Company which provides a modelling program ALOHA for free. Therefore, it was very difficult to carry out the evaluation of practical as well as utility characteristics of individual applications. Information was taken from both the sources provided by the producers of individual simulators and from the publications and evaluation provided by the users using the given software.

For the implementation of the outputs from the simulation tools of the release of harmful substances, it is possible to create editor of scenario in the majority of programs. It enables to create both static emergency event and dynamic one in relation to the internal running time of the simulation.

Based on the evaluation of the available possibilities of simulation of the release of harmful substances, the development of the simulator in the frame of SIMEX project should make use the outputs of the simulation programs for emergency simulations. Of the rated instruments are programs Terex and Aloha.

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