

# Possibilities of Mathematical Modelling of Explosive Substance Aerosol and Vapour Dispersion in the Atmosphere

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**Abstract**—The paper deals with the possibilities of modelling vapour propagation of explosive substances in the FLUENT software. With regard to very low tensions of explosive substance vapours the experiment has been verified as exemplified by mononitrotoluene. Either constant or time variable meteorological conditions have been used for calculation. Further, it has been verified that the eluent source may be time-dependent and may reflect a real situation or the liberation rate may be constant. The execution of the experiment as well as evaluation were clear and it could also be used for modelling vapour and aerosol propagation of selected explosive substances in the atmospheric boundary layer.

**Keywords**—atmospheric boundary layer, explosive substances, FLUENT software, modelling of propagation

## I. INTRODUCTION

**I**N principle, the solution relating to the propagation of chemical substances in the atmosphere can be performed using a mathematical and physico-chemical approach. However, it is a complicated problem from both the mathematical and physico-chemical viewpoint. Individual problems are solved separately, i.e. either through the mathematical approach or through the physico-chemical approach. However, it proves very advantageous to solve individual problems using both approaches simultaneously and thus to combine the strengths of these approaches. The physico-chemical experiment provides mathematical modelling with basic information about the flowing fluid and chemical additions, the area, the definition of boundary conditions and the verification of results. The verification is feasible in selected point of the area. The mathematical approach is very advantageous, especially from the viewpoint of visualization of a given area with a flowing fluid. It enables the “inspection” of the fluid together with the calculation of all important physical quantities in the entire area of the current

field, see [1]. This method enables the use of an experimental simpler measuring device for solving complicated problems as well.

When verifying the utility of the experiment with respect to very low tensions of chemical substance vapours the modelling was applied to the propagation of mononitrotoluene to the open space. The transport of this mononitrotoluene was determined at different distances from the source of propagation. The experiment was performed in the military area by members of the University of Defence. The FLUENT 6.3 software was used for mathematical modelling of mononitrotoluene propagation. The final-volume method was used and the results were compared with the experiment. The developed methodology was applied to the propagation of other gaseous substances (e.g. chemical warfare agents or explosive substances) in the atmosphere to the same area in the first phase. The methodology can also be used in other areas.

## II. VIEW OF THE PROBLEMS

### A. Mathematical model of substance propagation in the atmospheric boundary layer

Mathematical modelling continues to become a more significant instrument for process modelling in the atmospheric boundary layer. With the current computing machinery it has been possible to solve equations describing turbulent flow which influences vertical profiles of meteorological quantities significantly in the atmospheric boundary layer and thus also the motion and dispersion of substances, e.g. pollutants. Therefore, the study of turbulence is absolutely fundamental for mathematical modelling of flowing in the atmospheric boundary layer [2]. The issues concerning the modelling of pollutant motion and dispersion in the atmospheric boundary layer are dealt with via numerical modelling in the form of two approaches different in quality.

The first one is the use of the “diffusion (Gaussian) model” which is based on the application of the “statistical theory of turbulent diffusion” and is used for fast obtaining approximate values of pollutant concentrations [3]. Taylor was the first designer of this model in the 20’s and after him Sutton continued developing the given problems in the 30’s and 40’s of the 20<sup>th</sup> century. In the course of time and due to technical development the diffusion models were modified in various ways and, currently, there is a whole series of them. They differ in their orientation and accuracy. In practice they are used especially for dispersion studies for the reason of

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availability and easy manageability. Another approach is represented by “dynamic models” which are based on the numerical solution of partial differential equation systems describing physical processes in the atmospheric boundary layer. These models enable acquiring much more detailed information about the current and concentration field of additions (pollutants) in the area than it is with Gaussian models; however they also require much more detailed definition of the calculation area, boundary and initial conditions and also more time for calculation. One of the characteristics of these models is also the fact that it is possible to define in detail e.g. the effect of terrain configuration and surface, physical properties of additions or the temperature of source and also the fact that it is possible to solve the time-dependent problems using these models as well [1].

Mathematical modelling of flowing and dispersion of pollutants in conjunction with solving ecological problems has still been in the stage of research and there has not been any specialized software yet which would be intended for solving ecological problems only. Nevertheless, for solving these problems interconnected with flowing the CFD (Computational Fluid Dynamics) codes [4], e.g. FLUENT, ANSYS – FLOTTRAN or FLOW 3D can be used with certain constraints.

#### B. Approaches to mathematical modelling of the atmospheric boundary layer

If we consider the modelling of flowing in the atmospheric boundary layer, it is necessary to include “turbulence” in this process. We call the tool for modelling a real, i.e. turbulent, flow in the atmospheric boundary layer a “turbulence model”. It is a system of additional equations and empirical formulas which form an integrated solvable system of equations together with dynamic equations [1].

Mathematical models intended for modelling pollutant dispersion in the atmospheric boundary layer can be divided into two groups different in quality, i.e. statistical and dynamic models.

##### Statistical (Gaussian) model

These models are based on the application of statistical theory of turbulent diffusion. Substance propagation from a point source is described using a “diffusion equation” which is simplified and can be solved analytically. The turbulent diffusion is defined using the normal (Gaussian) distribution. Currently, this approach is a basis of practical models used for the development of dispersion studies as well as the assessment of emergency situations. The calculation in this approach is less time-consuming and costly. However, it shows inaccurate results in the vicinity of an emission source, in a broken ground and at low speeds of flowing (at the zero speed of flowing the diffusion equation has no solution) [1].

The distribution of pollutants from a point source can be described mathematically using the “diffusion equation” (1), according to the system of signs in the FLUENT handbook [3][3]:

$$\frac{\partial Y}{\partial t} = -u_j \frac{\partial Y}{\partial x_j} + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( \rho K_j \frac{\partial Y}{\partial x_j} \right) \quad (1)$$

where  $Y$  is “mass fraction of a pollutant”,  $u_j$  is “speed components” and  $K_j$  is “turbulent diffusion coefficients in the direction of axis  $x_j$ , for  $j = 1, 2, 3$ ”. Whereas the turbulent diffusion (dominant component of pollutant vertical distribution) is of random character, it can be described statistically according to the normal (Gaussian) distribution.

##### Dynamic model

Dynamic models are based on the numerical solution of partial differential equations which formulate physical laws of conservation of mass, momentum and energy in the flowing of a real fluid [1], [4]. These “balance equations” (2) can be defined in a simplified fashion in the standard form as follows:

$$\frac{\partial(\rho\zeta)}{\partial t} = -\frac{\partial}{\partial x_j} (\rho u_j \zeta) + \frac{\partial}{\partial x_j} \left[ \alpha_\zeta \frac{\partial \zeta}{\partial x_j} \right] + S_\zeta \quad (2)$$

The abovementioned equations include derivations in time and space and their solution requires the definition of “boundary conditions”. The boundary conditions enable the physical basis of processes to be introduced in the model and, therefore, they are very important for modelling processes in the atmospheric boundary layer.

Considerable demands for computer performance and the calculating time are disadvantage when performing these complicated numerical calculations; however, acquired final values are more accurate. The choice of a model is dependent on the characteristics of source which is to be modelled and on the requirements for the quality of results. The observance of pressure, temperature and density stratification in the atmosphere is a significant criterion [2].

#### C. Defining and modelling of point sources of gaseous and liquid media

Source parameters include the data on the type, size and position of the source in the area, and composition and quantity of discharged substances. It is necessary to define the position of the source in the Cartesian coordinate system, its volume flow rate, temperature, speed and its direction at the outlet from the source and the concentration (mass fraction) of individual additions at the outlet from the source. The source efficiency may be constant or may vary depending on time. In the case of accidental releases it is difficult to define the quantity and concentration of a substance which will occur in the given place in the instant of accident. First of all, it is necessary to identify and understand the processes that take place in the source itself, e.g. explosion, evaporation, concurrent escape of gas and liquid phase, etc. For calculating necessary parameters for different types of sources empirical formulas can be used. The source setting is enabled by defining the volume source elements of mass, momentum, energy, turbulence and other scalar quantities. It is also possible to define these sources as non-constant, dependent on time or, if need be, on other quantities [5].

In practical problems these types of sources occur most

commonly: point source (chimney), plane source and volume source. These types differ in geometric properties and in the definition of an addition coming out of the source. For instance, chimney represents a cylindrical vertical structure from which gaseous as well as solid additions are discharged. This type of source is appropriate if modelling the by-passing of chimney as an obstacle is the point of interest. As exemplified by the chimney all variants of the source definition (such as the usual inlet positioned on the plane defining the outlet from the chimney or on the boundary of the area and the volume source positioned inside the area) will be defined.

#### *Source-inlet*

If it is not necessary to model the flowing in the chimney itself or the influence of the heat transfer through chimney walls, then its geometry is already designed in the pre-processor; then the top cross-section of S plane is defined as an inlet, chimney is not created geometrically at all. At the inlet the boundary conditions for the plane source are set at chimney height. They are: mass fraction of additions, temperature at the chimney outlet, speed at the chimney outlet and turbulent parameters (e.g. hydraulic diameter, turbulence intensity).

#### *Volume source*

If the chimney diameter is too small in relation to the area dimensions, it cannot be defined using "inlet" condition; it is better to replace it by the volume source. It can contain one cell only or a group of cells which, however, must form a separated zone. This can already be formed in the pre-processor during the preparation of the network or subsequently directly in the FLUENT medium using the tools of network adaptation and register creation.

### III. MATHEMATICAL MODELLING OF GASEOUS SUBSTANCE DISPERSION IN THE ATMOSPHERIC BOUNDARY LAYER USING CFD ANALYSIS METHODS

#### *A. Computation method*

The finite volume method is based on three basic points as follows:

- Division of the area into discrete volumes using the curvilinear network;
- Balance of unknown quantities in individual final volumes and discretization;
- Numerical solution of discretized equations.

In modelling the problem of gaseous pollutant dispersion in the atmospheric boundary layer using mathematical methods and CFD analysis tools it is necessary to [6]:

- 1) Select adequate software for a given type of problem solution;
- 2) Define the calculation area – its dimensional and shape parameters (GIS can be used too);
- 3) Select an adequate turbulence model for calculating;
- 4) Define initial and boundary conditions;

- 5) Define physical properties of air and particular pollutants;
- 6) Define parameters of pollutant source;
- 7) Select calculation parameters.

The selection of adequate software for calculating any physical problem is very important in consideration of practicability and especially accuracy of calculation. There is a lot of specialized software which is focused on various types of physical problems. Therefore, it is advisable to select the best software or at least to know real constraints of available software even if it is not the most suitable for the given type of the problem.

Calculation parameters can influence the solution accuracy, the execution phase and facilitate the problem convergence to be attained. The most important parameters are as follows [6]:

- Selection of a turbulence model and wall function;
- Selection of a differential scheme;
- Selection of an iteration method;
- Setting of relaxation parameters;
- Convergence criteria (calculation accuracy required);
- Selection of the time step and the number of iterations in a single time step (for a time-dependent problem).

#### *B. Calculation area*

At the beginning of any modelling process it is necessary first to define geometry of the calculation area and then to perform its networking or division into a certain number of cells. In the model, the calculation area is to illustrate a part of reality which is fundamental for the problem. The area is always defined by its shape and dimensions. The network which covers the area can be classified according to the number of cells and according to geometric shapes of individual cells (e.g. tetrahedrons, rectangular parallelepipeds and hexahedrons). In general, it can be said that the denser the network is the more accurate results are obtained. However, the number of cells is usually very limited by computer performance, i.e. it is often necessary to manage the network economically and to perform network densification only in the points where it is necessary for attaining quality results. It is essential that geometric shape of cells and their arrangement in space of the calculation area also affect the results of calculation.

Geometry of the calculation area and its networking can be performed either in the FLUENT program (with certain constraints) or in another program specialized for these operations, e.g. GAMBIT[6] [7]. The prepared networked calculation area created in another program than FLUENT can be imported to FLUENT (this possibility is relevant for a certain predefined range of programs).

#### *C. Initial and boundary conditions*

Setting "initial and boundary conditions" [1], [4], [7] contributes to defining the physical basis of a modelled process considerably. The "initial conditions" are given by physical quantities which define the initial situation conditions and change or update during the calculation together with each iteration. The "boundary conditions" express the conditions on

the boundary of the calculation area (i.e. at the inlet, outlet or walls of the calculation area), however, when compared with the initial conditions, they are given and don't change during the calculation. The boundary conditions can be divided into several types as follows:

- Condition for inlet and outlet – can be defined using pressure and speed;
- Wall conditions – the wall may be fixed or moving (e.g. rotating or sliding), with friction or without friction, smooth-surfaced or rough-surfaced;
- Symmetry conditions – zero normal speed and zero normal gradients of all sought quantities;
- Cyclic conditions – are used in the case when current formations repeat and can be of rotating as well as translational type;
- Periodic conditions – are similar to cyclic conditions; moreover, they enable hydraulic gradient in the direction of flowing fluid lengthwise the calculation area to be defined;
- Time-dependent boundary conditions.

The boundary conditions can be set as constants or as functions of three-dimensional coordinates or, if need be, as functions of time in the form of polynomial function, function in parts of linear and periodic functions of time. For modelling pollutant flowing and dispersion the boundary conditions are of great significance because they enable meteorological parameters typical for concrete “stable conditions” in the atmosphere to be introduced to the problem solved [8]. Defining the boundary conditions also includes defining parameters of the pollutant source in the calculation area.

#### D. Source modelling

In FLUENT the inlet of gaseous medium to the calculation area can be performed by three basic methods as follows [6]: In the first method the given calculation area will comply with the requirements for the problem setting, i.e. network refinement in the point of gaseous medium inlet to the area will be performed. The network will be refined to the extent that in the end it will contain the cells, the size of which will be adequate to the size of the given inlet (e.g. chimney) in real conditions with regard to the dimensions of the entire area. One or several cells refined in this manner will then be chosen from geometry and indicated as an inlet defined by a cell. Admittedly, such a procedure is possible and provides relatively accurate results, but it is very demanding in terms of time and practice especially if it concerns the creation of suitable network, but also the choice of a suitable mathematical model. Unlike both following methods for the source setting this method is not too suitable for modelling random pollution sources. Another method is based on a similar principle of the source setting using a cell, however, it differs – the given calculation area does not adapt so substantially by form of network refinement and attention is paid to setting boundary conditions instead. Certainly, this strategy can be used rather in the cases when the size of an unchanged cell does not differ from the size of the source set by the problem. Final values should not differ too much from the values obtained in the abovementioned

procedure. The third method concerns the use of inlet defined in FLUENT as “injections” which enables defining point or plane sources. The advantage of this form of setting is the possibility of modelling the discrete phase, e.g. drops, bubbles, sprays or particles. However, this procedure does not enable modelling additions. It is limited as to the real defining of the entire situation but in some cases it can be the most ideal for modelling a random pollution source.

#### IV. MODELLING OF MONONITROTOLUENE PROPAGATION

The military area where the measurements of mononitrotoluene propagation have been performed recently was used for the modelling of mononitrotoluene vapour propagation. This area is suitable for these experiments as the terrain is relatively flat and, therefore, there is not considerable turbulence owing to the by-passing of terrain unevenness.

##### A. Mathematical model

Mononitrotoluene vapour propagation was modelled using the FLUENT 6.3 software. First of all, the calculation area in the GAMBIT software, Fig. 1, was created and networked. The number of cells was 1 736 411. The networked area was exported from GAMBIT to FLUENT where the problem was solved using model  $k - \epsilon$ .

The physical properties of air and mononitrotoluene were as follows:

air  $M=29 \text{ kg.kmol}^{-1}$

mononitrotoluene (MNT)  $M=137 \text{ kg.kmol}^{-1}$

The density of mixture of both substances will be determined using the state equation; the specific heat, thermal conductivity and viscosity will be determined using rules of allegation based on kinetic energy or the state equation. At the inlet (in the place where the wind blows) the initial condition (velocity-inlet) was set together with the wind velocity profile and wind direction. Mononitrotoluene vapours circulated at the speed of  $19 \text{ m.s}^{-1}$ .

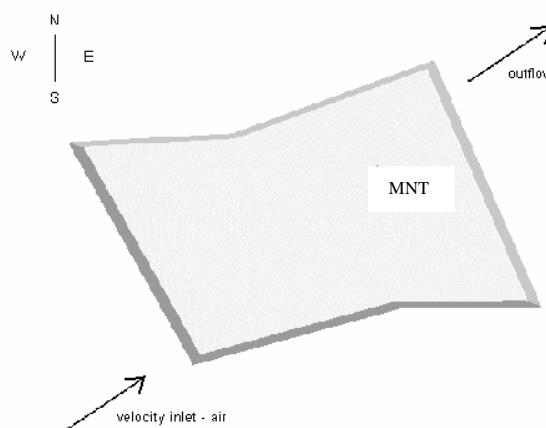


Fig. 1 Calculation area

##### B. Results

Numerical experiment proves the ability of mathematical modelling to describe mononitrotoluene vapour propagation

under given meteorological conditions. The result is distribution of basic hydraulic quantities, i.e. atmospheric pressure and velocity vector. On the ground it is possible to evaluate the distribution of mononitrotoluene concentration or, if need be, isosurface of concentrations of a given value as spatial areas. In selected predefined points gaseous substance concentrations can be evaluated and compared with the values measured during the experiment.

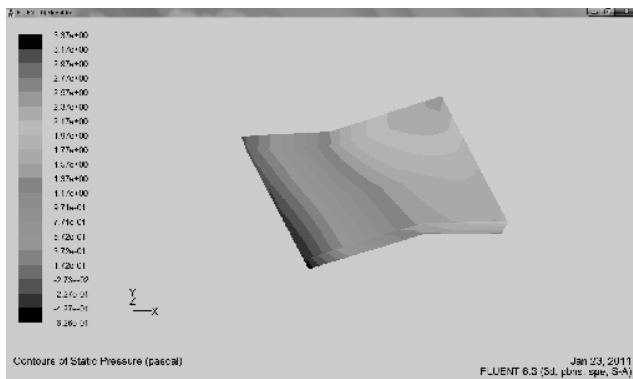


Fig. 2 Distribution of pressure on the ground during the air flow

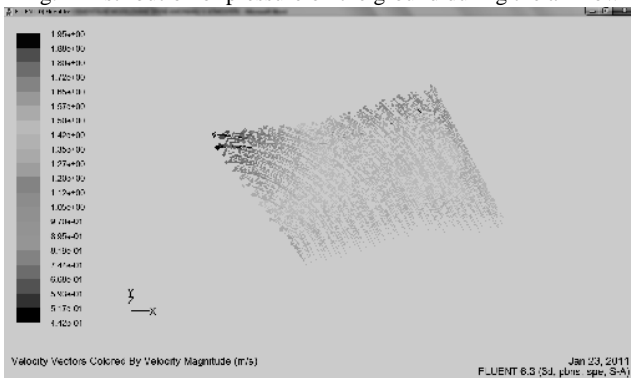


Fig. 3 Velocity vectors in the plane limiting the area from above (the change in direction due to not completely plane area can be observed)

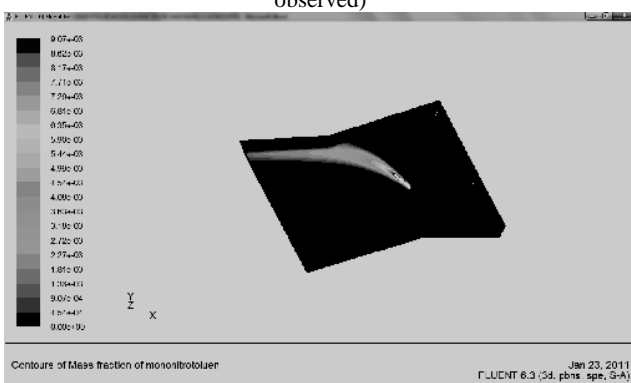


Fig. 4 Distribution of mononitrotoluene mass fraction on the ground; the diffusion of the substance and the drift in the direction of wind

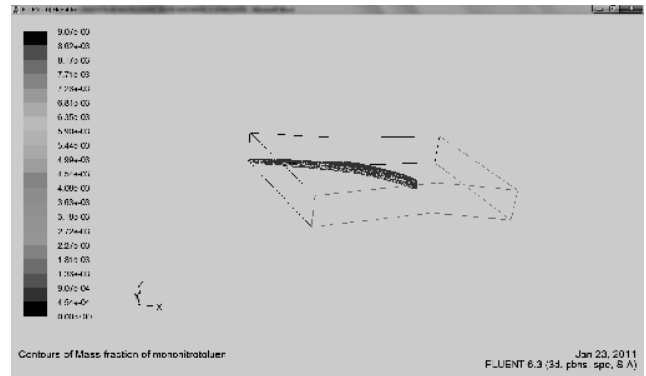


Fig. 5 Illustration of spatial isosurface of mononitrotoluene mass fraction of the constant value of 0.0009

## V. CONCLUSION

The modelling of explosive substance vapour propagation is possible in the FLUENT software. Both constant and time-dependent meteorological conditions can be taken into account. The source can be time-dependent as well and thus follow a real situation. The evaluation is clear but for the comparison with the prospective experiment it will be possible to use the record of concentration values in a given measuring point. Further, the modelling of propagation of dangerous gaseous substances can continue in testing areas and subsequently in the real atmosphere considering meteorological conditions. In the future, the work will be extended by the possibility of evaporating liquid substances and propagation of drops, vapours and solid substances (e.g. explosive substance particles) using the FLUENT software. At the same time, calculations for other explosive substances can also be performed.

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