THE ANALYSIS OF THE USE OF MATHEMATICAL MODELING FOR EMERGENCY PLANNING PURPOSES

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Abstract

Mathematical modeling in the field of fluid mechanics counts among efficient methods of the prevention, solution, or retrospective analysis of large scale of emergencies regarding emergency planning, industrial safety and chemical terrorism prevention. In order to utilize this method with maximum effectiveness, several basic questions should be answered. The following are the most important: what can be modeled; when the modeling makes sense; how to model; how to verify the results of mathematical analyses; what are the most important common objectives of modeling in relation to the safety and emergency planning; etc. This article aims to these and other questions concerning primarily the specifics of various modeling tools. The statements are corroborated by several inland modeling studies and compared to the foreign ones.

Key words

CFD, emergency planning, mathematical model, pollutant, gas, statistical models, worst-case scenario.

1 Introduction

Mathematical modeling of physical phenomena in the area of fluid mechanics counts among advanced scientific disciplines whose procedures and results are widely applied in practice in many other fields.

In recent years, increasing attention has been paid to the application of advanced mathematical models in the area of major chemical accidents [1]. Specific attention has been paid to the modeling of heavier-than-air gas releases [2], [3]. Another area of study is the modeling of dispersion of flammable substances where the course of an accident much more depends on the surrounding area and obstacles [4]. Complex mathematical models are compared with large-scale tests [5] and physical models [6]. Attention is also given to the comparison of these tools between each other [7] or with less complex models [8], [9].

For the correct application and further advancement of epistemological knowledge in modeling it is essential to understand properly the mentioned procedures and results of mathematical calculations so that at least the major errors, mistakes and misunderstandings in practice could be avoided. Understanding of the used models, computer software tools and their results can then be reflected in a better communication with the public also in emergency planning. This paper aims to make at least a small contribution to the fulfillment of this vision.

2 Analysis of the modeling objectives

The fundamental key questions for each user (investigator, modeler) in the context of emergency planning needs in the vicinity of industrial enterprises are: what, why, when and how to model? We will attempt to give an answer to them.

Question 1: "What to model?" Answer: What is meaningful in real time and is technically feasible with the complexity and precision the investigator (ordering party) of the problem requires. In modeling, the general rule is to model the problem instead of the system. The emergency planning tasks relate primarily to public protection. It is therefore necessary to model threats to the population, e.g., the hazardous substance concentration and its evolution over time. It is important to know where, with what exposure, after what time and for how long the population will be exposed to the threat. To consider the feasibility of the model is equally important. There are tasks that cannot be reliably modeled, for example, at different scales (for details see [10]). The reasons for that typically involve problems with physical similarity of the modeled process or with technical limits of the measuring or computing equipment.

Question 2: "Why model?" The objectives of modeling for emergency planning can be three fold: to predict the situation, to understand better the characteristics and patterns of emergencies and, finally, to determine the current state during the course of an accident. Prediction is used for preparation, ability to anticipate and then to manage the consequences of emergencies, for planning measures and to determine necessary resources and personnel. Knowing the process characteristics can help predict the progress of the situation; modeling of past accidents provides more information about the system. Modeling is also used to validate and verify mathematical models. Determination of the current state is an important emergency planning tool as well as a complement to monitoring. Modeling of ongoing accidents has a certain advantage as some parameters (especially meteorological condition parameters) can be assigned according to the current state and are not subject to uncertainty. One more purpose of modeling in the context of major accident prevention can be mentioned: modeling of potential consequences of accidents in the framework of risk assessment to decide on the acceptability of risk and subsequent adoption of preventive measures to reduce it.

Question 3: "When to model?" The question connected with the purpose of model and with the question "why model?". Generally, information provided by a model is beneficial at a given moment when it can be used in practice. For the purpose of emergency planning and preparedness, we model *before an emergency situation* to predict and subsequently plan and get prepared, *during an emergency situation* to protect, and *before or after an emergency situation* so get to know the nature of the phenomenon.

Question 4: "How to model?" The answer is to use the tools that best serve the aimed purpose of modeling. This does not primarily consist in defining the system as precisely as possible but in giving the best answer to the question arising from the problem. If a simple model answers the question "well enough" then the use of complex computational models is not only needless and uneconomical, but it may also be misleading because a great number of (potentially unknown) parameters are required. Before a particular model is used, an assessment of available models with regard to their suitability for a given problem should be made.

Two different pieces of software in terms of principles and visualization options will be presented in the following paragraphs. It will be demonstrated how different, yet principally correct, the results they produce can be and why.

3 Principles and visualization options of ALOHA 5.4.4 and ANSYS Fluent 13.0.0 software tools

Models incorporated in programs (software) that for the purpose of emergency planning use fluid mechanics physical laws can be primarily divided according to the principles into two groups: simplified (statistical) models and dynamic (CFD) models.

The group of simplified (statistical) models – e.g., mathematical models SLAB and DEGADIS (Dense Gas Dispersion Model), which is used in ALOHA – includes semi-empirical relations whose coefficients were set on the basis of data from field tests. Therefore, the configuration of the surrounding area, for example, is described only with a few parameters. The reliability of these models can be rather limited outside the area for which they were set. They use two types of models. The first model type is based on the application of the statistical theory of turbulent diffusion. Diffusion of pollutants from a point source is described by a so-called "diffusion equation" that is simplified and can be solved analytically. Turbulent diffusion is defined by normal (Gaussian) distribution. This approach is currently the basis for practical models used for elaboration of dispersion studies and assessment of emergency situations. The calculation procedure is less time-consuming and costly, but the results are imprecise for emission source vicinities, broken terrains, low flow velocities, and very short time intervals of modeled releases. At zero flow velocity the diffusion equation has no solution. A detailed description can be found in J. Casal [11]. The second model type applies to the modeling of heavier-than-air gas releases. These models operate with simplified equations of conservation of mass, momentum and energy. They are referred to as “box models”. The diffused gas is modeled as a cloud with blurred edges and with the same properties in all directions. The box models often display concentrations only in two dimensions (2D) [12]. In this article this model group is represented by the ALOHA 5.4.4 software tool [13].

The group of dynamical models – used for example in ANSYS Fluent, Fluidyn PANACHE, FLACS and ANSYS CFX software tools – is based on the numerical solution of systems of partial differential equations that express the law of conservation of mass (continuity equation), the law of conservation of momentum (Navier-Stokes equations) and the law of conservation of energy (energy equation - heat transfer by convection, conduction or radiation). This basic set of equations can be supplemented by additional equations that express species transport (gas, liquid or solid species). The system of equations is then solved with an appropriate numerical method; in this case, with the method of finite volumes. It is more sophisticated software; the calculations are more time-consuming and more expensive. In comparison with simpler software it produces more precise results in the vicinity of emission sources, in rugged terrains as well as at low flow velocities. An important specific feature of this group of models is the fact that their calculation algorithms take into account the effects of mechanical turbulence (due to the configuration of the terrain geometry) on the flow field. They allow modeling in both 2D and 3D geometries [12]. In this article this model group is represented by the ANSYS Fluent 13.0.0 software tool [14]. The visualization principles and options for the two groups of models depends on the software used and may vary considerably. Generally, more complex CFD tools operate with a greater number of calculated data that can be visualized in different ways. Simple tools often work well only for a simple prediction or overview of the situation, so among other things, they usually do not allow display of the situation progress over time. However, understanding them is the key to the correct interpretation of the results.

ANSYS FLUENT 13.0.0 calculates the concentration at each point of the examined area, and in the case of time-dependent tasks also for each time step. The estimation of the physical process is then usually visualized in preset time steps as the process develops. In contrast, in its basic “Display Threat Zone” ALOHA 5.4.4 displays the field of maximum concentrations during the entire course of the accidental release. It visualizes not the development of the emergency situation develops, but rather its overall impact regardless of its evolution over time. Modeling in ALOHA allows simulation of three different phenomena. A gas release can be modeled as a plume; the output being only final concentrations regardless of their changes over time (the model does not model the gradual emergence of the plume, only its steady state). A release can also be modeled as instantaneous that is based on the calculation of diffusion of a single gas or vapor cloud (puff) that is formed in the release area from the entire amount of the released chemical and disperses as it travels downwind. For this model it is possible to obtain a time course. The last modeled type of an accidental release is the time-dependent release for which there is no specific statistical model. In ALOHA it is calculated as a series of five finite-duration steady-state releases; each forming a cloud that does not interact with other clouds. Each cloud then contributes to the resulting concentration in each point and time of the thread zone [15].

ALOHA does not implicitly allow visualization of the accident course in time steps. With the "threat at point" option it is however possible to display the time course of the concentration in selected points of the field outside the buildings and an estimate of the concentration inside the buildings which can be applied in making decisions on the acceptability of risk.

A fundamental mistake is made when experts attempt to interpret results of the two above-described software tools as comparable. This would be possible only if ALOHA made possible to display the process evolution depending on time or if ANSYS Fluent visualized maximum concentration values of the released chemical in each point. Such maximum concentration values should be averaged for similar periods of time as in ALOHA. This could be done by using a task with a so-called "monitoring points". Such a task and its preparation is rather difficult and is rarely applied in practice.

4 Mathematical simulation example

To demonstrate the principles discussed above, an accidental gas ammonia release from an ice stadium into a complex urban area was chosen for an example of mathematical simulation.

The input data for calculation with ALOHA 5.4.4 were defined from meteorological data provided by the Czech Hydrometeorological Institute (CHMI) [16]. The data represent mean values of meteorological variables measured over the period 2006–2011. The parameters for accidental release (source) of ammonia were based on a qualified estimate derived from documents provided by the ice arena safety/facility technician. The calculation was performed for the wind velocity of 2 $m.s^{-1}$ from the direction of 45^0 (northeast), the temperature in the environment of 0 ^0C (due to the rapid evaporation of ammonia and selecting the source type as DIRECT it was not appropriate to set this temperature as the temperature of the source to -16.55 ^0C), the atmospheric stability class D (according to Pasquil-Giffort scale) with no inversion present, and the mass flow rate through the ammonia source of 0.586 $kg.s^{-1}$ (release of pure ammonia with no air as in ALOHA it is not possible to model ammonia-air mixture), for 5 and 10 minutes of continuous release from direct source. It was left to the model to choose between light and heavy gas dispersion under given conditions; after verification, the Gaussian model of light gas dispersion from a point source was automatically chosen; the software notified the user that verification was necessary with both available approaches).

The input data for calculation with ANSYS Fluent 13.0.0 were also defined from meteorological data provided by the Czech Hydrometeorological Institute (CHMI) [16]. The parameters for accidental release (source) of ammonia were also based on a qualified estimate derived from documents provided by the ice arena safety/facility technician.

Cuboid-shaped geometry with the width of 800 m, length of 800 m and height of 150 m was created from maps obtained from the Cadastral Office of Ostrava (Czech Republic) [17] with the DesignModeler program [14]. The grid of the geometry was created with ANSYS Meshing [14] software tool. The total number of grid cells was approximately 1.6 million.

Boundary conditions for the geometry were defined by atmospheric pressure of 101 325 Pa, the wind speed profile, the turbulent kinetic energy profile, the turbulent dissipation velocity profile and the air temperature profile according to [14] and [18]. Specific formulas for the profiles and other details of the problem are described in [19].

The gas ammonia source boundary conditions were defined by the source temperature of 256.6 = - 16.55 ^{0}C (ANSYS Fluent made possible to take account of the progress of the rapid changes of temperature: from the temperature of the source over the temperature of the evaporating two-phase release – ammonia pool – to the ambient temperature) and the mass flow of 1.58487 kg.s^{-1}. The pollutant was defined as a mixture of air with mass fraction of 0.63 and gas ammonia with mass fraction of 0.37 released from an area source with the width of 1.4 m and length of 2.4 located at the height of 6 m above the ground.

The air flow field was modeled using the RNG k-ε model of turbulence and Species transport model was used for species (pollutant) motion and dispersion modeling.

The ALOHA 5.4.4 results were exported in KML-format into Google Earth [20] where they were implemented onto orthophoto maps of the target area as iso-lines of gas ammonia concentrations (see Fig. 1). The orange iso-line represents the thread zone border for chosen ERPG-1 acute toxicity value (concentration of 25 ppm); the red iso-line represents the thread zone border for ERPG-2 acute toxicity value (150 ppm).

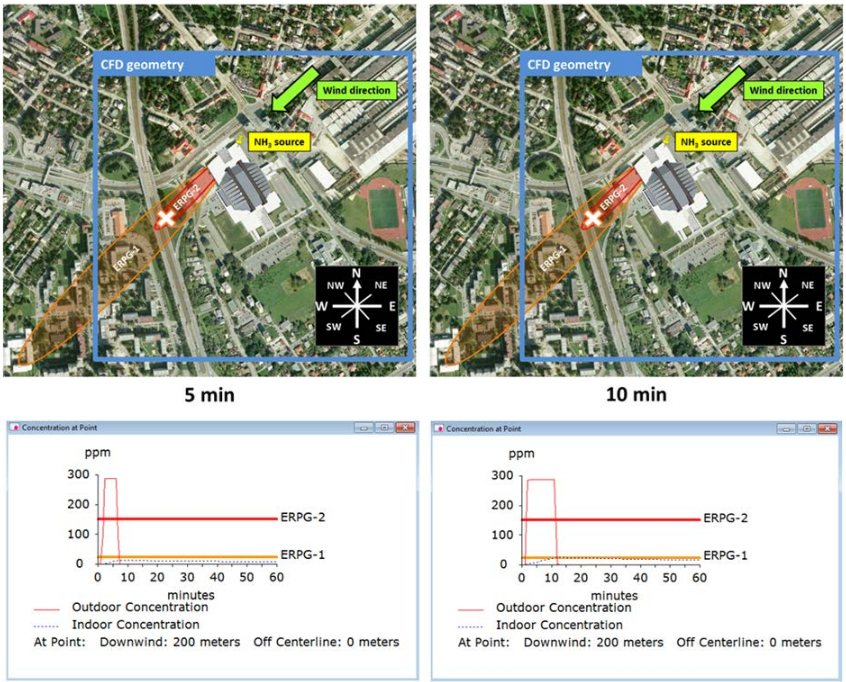

Fig. 1
Gas ammonia toxic thread zone for ERPG-1 and ERPG-2 acute toxicity values and five and ten minute variants of an accidental release – ALOHA 5.4.4

These results are probably overestimated for the following reasons. Overestimation stems primarily from the purpose of ALOHA. The objective is not to predict exact concentration distribution, but rather the area where the population is potentially threatened. Also application of the acute toxicity value according to ERPG can play an important role in the overestimation as it is determined for one-hour exposure whereas the required exposure time estimation in ALOHA for the solved task is around 5–15 minutes. This overestimation is reflected in the modeling using CFD if the same toxicity values are used. However, CFD tools may allow better integration of more detailed dose-effect models (see e.g. [21]). Another influencing factor is the fact that in ALOHA 5.4.4 gas mixtures cannot be defined, or more precisely, components of such mixtures cannot be separately evaluated. It is therefore necessary to define proportional quantity of pure media in the source, which in turn has an influence on its dispersion. Another fact is that it is not possible to model specific influence of the surrounding structures on the diffusion and dispersion of the pollutant plume.

The ANSYS Fluent 13.0 results (see Fig. 2) were visualized as filled contours of species (ammonia) concentration fields in 2D cut planes of 3D geometry at a height of 1.5 m above the ground (breathing zone). ERPG-1 and ERPG 2 acute toxicity values were again used for evaluation. Unlike ALOHA 5.4.4, ANSYS Fluent 13.0 makes possible to define gas mixtures and observe the mix components separately. It also contains turbulence models that take into account the effects of mechanical turbulence from surrounding buildings on the motion of the gas pollutant plume.

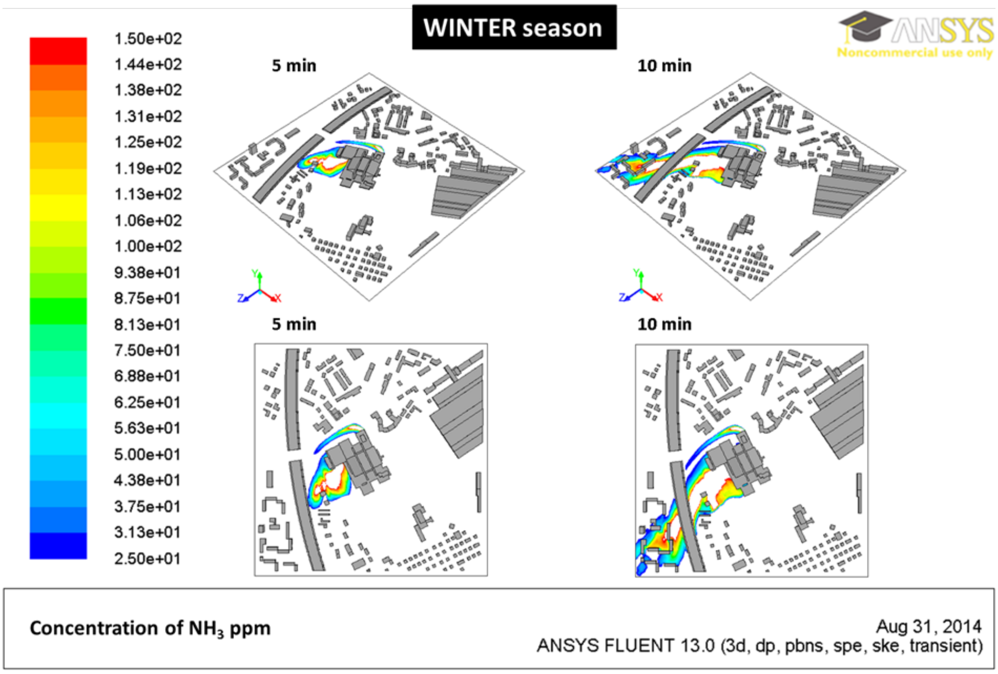

Fig. 2

Gas ammonia toxic thread zone for ERPG-1 and ERPG-2 acute toxicity values and five and ten minute variants of an accidental release at a steady state – ANSYS Fluent 13.0.0

The output results from both software tools – ALOHA 5.4.4 (see Fig. 1) and ANSYS Fluent 13.0.0 (see Fig. 2) – are distinctively different, which is not caused by any error in any of the software tools. The results of ALOHA 5.4.4 evaluated for 5-minute and 10-minute accidental release of gas ammonia are not different from each other whereas ANSYS Fluent 13.0.0 results clearly illustrate the dynamic evolution of the plume. Why is it so?

The answer can be found in Section 2 of this article (see above). In the context of ALOHA 5.4.4 results (see Fig. 1) is evident that the total area of the terrain affected by the pollutant does not increase after dispersion to a concentration limit lower than 25 ppm at an accidental release longer than 5 minutes. That means that even if the accidental release of the pollutant were continuous and of unlimited duration (infinite), under the given conditions the area affected with this concentration would not increase any more.

In contrast to ALOHA 5.4.4, ANSYS Fluent 13.0.0 (see Fig. 2) results show the instant state of the emergency situation at 5 and 10 minutes after the onset of the pollutant accidental release. ALOHA can only display the total field of maximum concentrations of the released pollutant over time period e.g. 5 or 10 minutes (more suitable time period for displaying the results in this software tool is the accidental release duration of 10 to 60 minutes).

Comparison of the result from both software tools also shows that in contrast to statistical models where the highest concentrations are always found in immediate vicinity of the source, the CFD model was capable to capture situations where the flow around obstacles cause dangerous concentrations found farther away from the source (depending on the terrain and buildings).

5 Conclusion

The article summarized basic points of mathematical modeling in the context of emergency planning, the possibilities and distinctions of groups of mathematical tools and specifics of the interpretation of their results. In summary, the following statements can be declared.

The larger is the spatial scale of the geometry and of the process occurring within it, the smaller become the differences of results, or their precision, in statistical and dynamic models. Simple and statistical models are primarily focused on estimating the adverse consequences of emergencies, depending on the limits (e.g. of toxicity) used. Dynamic models are primarily focused on spatio-temporal details. It can be said, though, that with their use it is possible to equally well define also the general trend of development of an emergency situation, as with statistical models.

Currently, the development trend in mathematical modeling tends to study single details of various emergency situations and also to integrate specialized modeling tools into one complex unit. This results from the growing need to model more complex physical processes in more complex terrains and urban areas. The ability to evaluate the influence of buildings and surrounding terrain is on the biggest advantages of CFD tools. Simple and statistical models in this context work well only for an initial estimate of the development and effects of emergencies or as a quick screening of emergencies during their course. If a detailed knowledge of the situation for better understanding of its course, planning and preparedness is required, it is advisable to employ detailed CFD modeling tools. This trend is also reinforced by the increase in performance and availability of computer technology. The goal has always been, is, and will be an effort to obtain comprehensible, adequate and, according to the purpose, precise results; that is, to help provide the best possible assistance to people.

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