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Air pollution engineering for accidents with hazardous substances

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Abstract. **One of the challenges facing modern society is related to the dangers of industrial accidents and terrorist attacks related to the spread of fires and dangerous substances. In the present article, a systematic approach is proposed for organizing monitoring, creating possible development scenarios, modeling the spread of potential toxic-element pollution, comprehensive analysis and creating an adequate response to such severe situations. The assessment of the scale of pollution transport, dispersion, chemical transformation and the degree of danger is directly related to the correct registration of the basic accident, weather and environment characteristics and thoroughly monitoring of the dynamics of their change. The collection of the necessary data is carried out on the basis of heterogeneous sensor networks. The application of modern methods for the unification of disparate information scattered in space and time allows the accurate evaluation of the current state. Different development scenarios are generated on the basis of methodologies and corresponding mathematical models are applied. The risk assessment framework feeds these models with the unified sensor information and comprehensively examines them to provide a quantitative estimate of the possible critical levels of harmful pollution and predict the consequences. The paper's relevance is heightened by the growing threat of terrorism that targets industrial infrastructure and climate change that increase the frequency and severity of natural disasters, compounding the challenges of predicting and managing air pollution events. It contributes to the discourse on environmental engineering and disaster management by proposing a systematic methodology for real-time data collection, risk assessment, and the application of predictive models to inform effective response strategies. By tackling these issues, the paper aligns with contemporary priorities in environmental protection, public health, and safety regulations, making it highly topical for stakeholders in academia, industry, and government seeking to enhance resilience against air pollution disasters.**

Keywords: Air pollution engineering, accident modeling, dispersion of toxic substances.

I. INTRODUCTION

Air pollution is a dangerous phenomenon that threatens the lives of people and the planet as a whole by disrupting its eco-systems. Air pollution occurs most often as a by-product of industrial or other human activity, as a result of natural disasters (volcanoes for example) or as a result of industrial accidents or acts of terrorism. The last two ways of occurrence of air pollution are characterized by their sudden occurrence, in many cases impossibility of advance forecasting and monitoring, absence of a control strategy. The location of air pollution also cannot be easily predicted. In addition to the places of storage and pollutant production, such incidents can also occur during the transportation of dangerous substances, in the places of their application/use. This uncertainty about the realization of dangerous air pollution in time and space necessitates the creation of a new organization to reduce or eliminate the negative consequences of such accidents. In classic industrial air pollution, stationary stations usually monitor accurately the current state of air cleanliness closely. In contrast, pollution resulting from accidents requires rapid and large-scale deployment of sensor networks to collect data on the distribution and concentration of pollutants, collect local meteorological data on air currents and changes in the air environment that can affect the spread of the pollutants. This large

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volume of data must be normalized, tied geographically to the specific location of the accident, and carried out to a point in time. The general pollutant transport models must be also localized to the specific accident at the specific site.

The article is written to present a global picture of the most important components in air pollution engineering for accidents with hazardous substances. Secondly, the organization of effective information exchange and the choice and localization of the pollutant transport models are of major concern. The clear and concise understanding of these mandatory system attributes gives us the indispensable means to assess the magnitude of the disaster, predict its impact on people and the environment and plan the most effective actions to reduce or neutralize its harmful effects.

The paper is organized as follows: Section 2 reviews the current state of research for air pollution engineering. In the third section the main tasks of disaster management are revealed and the crisis headquarters information system is proposed. Section 4 presents the methodology of modeling and data analysis. A short review of mathematical models is given in Chapter 5 and a chosen model is described in details. In the last part of the text the most important conclusions and contributions are summarized.

II. Materials and methods

Related works: When some substances in the air at concentrations higher than their normal ambient levels lead to significant effects on humans, animals, vegetation or materials we are talking for air pollution [1]. The main source of toxic air pollutants is the economic, industrial and population growth, although there are also various natural disasters (wind-blown dust, volcanic eruptions and fires, for example) that also contribute to air pollution. Different technical disciplines deal with the study of air pollution. They are usually combined into more general one – air pollution engineering. In the scientific literature on air pollution issues, there is no consensus on what is meant by air pollution engineering. Some authors understand by this concept the study of the generation and control of air pollutants [2]. Other authors consider within this terminology only preventive measures and air pollution control techniques for removing or reducing harmful gases, vapors and particulates from industrial process emissions [3]. In this article, the emphasis in air pollution engineering falls on the organization of monitoring and establishing the specific values of air pollution in the disaster/accident area, the construction of a realistic mathematical model for the pollution spreading over time and the taking of appropriate measures to reduce the adverse consequences resulting of pollution. Issues of preventive control, which are extremely important for stationary sources of air pollutants, are of secondary importance here. In most cases, they are regulated by various state legislative acts for control the handling of dangerous substances, their transportation and the prevention of terrorist acts.

In [4], the authors examine air pollution for various disasters, citing specific examples of such situations. Among those considered as consequences of natural disasters are floods [5], drought [6], wild fire [7], [8], earthquake [9], [12] tsunami [10] - [12], volcanic eruption [14] - [17], epidemics [18], [19], extreme temperature [20], insect pest infestation [21], mass movement (landslide, avalanches, earthquake) [22].

Air pollutions due to anthropogenic disasters are listed separately and include those resulting from wars, conflicts and fire accidents. Anthropogenic disasters can be initiated by careless treatment of the working environment or poor organization of work or be purposefully carried out in the case of terrorist acts and civil conflicts with the aim of causing significant physical damage, loss of life or impact on the environment. Risk assessment [23] and optimum risk management is usually sought to reduce the consequences of such disasters. Risk assessment includes (1) hazard identification; (2) exposure assessment; (3) dose-response assessment and (4) risk characterization. Optimal risk management deals with the actions that must be taken within the framework of laws and regulations in place to minimize the possibility of hazardous air pollution in accidents and to respond as quickly as possible to such accidents in order to reduce damage and preserving the life and health of people [24], [25].

Disaster management: The disaster management activity is diverse and has the main purpose of: 1) Identifying potential hazards and assessing the risks associated with them and selecting appropriate organizational actions to prevent such accidents or reducing the possibility of occurrence to an acceptable level; 2) Organization of the activities of various services and bodies to establish the extent of the accident, create teams to assist the victims and restore the critical infrastructure, predict the possible future impacts on people, the environment and the infrastructure and guarantee their safety; 3) Planning and organization of activities for full recovery from the impact of the accident (Fig. 1).

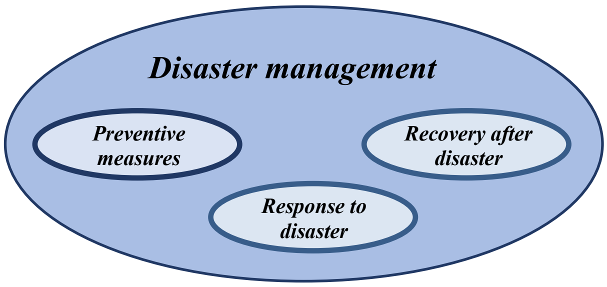

Fig. 1. Main disaster management components.

In 2005, the first international (agreement of 168 governments) framework program for building the resilience of nations and communities to disasters (2005-2015) was created in Hyogo [26]. Later in Sendai, this framework program was further developed for the period 2015-2030 as the Framework for Disaster Risk Reduction 2015-2030. The main goal remains the same - reducing existing risk and preventing the creation of new risk [27].

The preliminary preparation of society to deal with disasters and accidents is a complex and multidimensional process related to the relevant legislative and regulatory activity, creation of specialized bodies, services and commissions, material provision for action, determination of areas that are subject to increased risk for such disasters and accidents, creating action plans for various disasters.

These activities cannot always prevent disasters from occurring, but they can certainly reduce economic loss, damage to critical infrastructure, prevent or minimize human casualties, and enable recovery in a short period of time.

The consequences of disasters and accidents often remain for years to hamper the population and the countries that suffered them. One such telling example is the consequences of the Fukushima earthquake, which up to this day, 13 years later, remain very serious. In such severe disasters, the main focus of remediation is on health care and rehabilitation of victims and repair of damage to infrastructure. Although not paramount, disaster analysis is needed to plan and implement better policies and practices to avoid or mitigate similar events in the future.

The third component of disaster management differs from the other two in the need for all actions to be performed in a very short period of time and coherently in time and space. This can only be accomplished in the conditions of a highly organized society, equipped with the necessary services, provided with sufficient equipment and opportunities for quick orientation in the situation, establishing the main parameters of the disaster and making adequate informed decisions.

Accidents related to air pollution are somewhat more insidious than other destructive incidents because they may go unnoticed by people initially at their impact. The activities of rescue, relocation, provision of decontaminated food and water depend to a large extent on the precise identification of hazardous substances and the extent of their spread. The type of airborne contamination also determines the way of providing emergency medical assistance and quality protection of the medical teams in action. The above-mentioned features of accidents related to air pollution require to a greater extent the development of an information subsystem to deal with such situations.

In Fig. 2, the architecture of such a system is proposed, the main purpose of which is to support the informational work of the crisis headquarters.

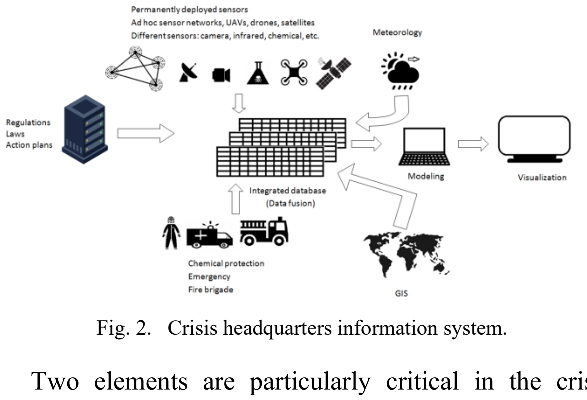

Fig. 2. Crisis headquarters information system.

Two elements are particularly critical in the crisis information flow diagram shown above. The first of these concerns the unification of information from multiple sensors and documents. Some of the information is permanent, but another part is tied to a specific place and refers to a specific moment in time. Bringing the information to a given time and obtaining dense coverage of the data in a given area requires not just interpolation/extrapolation of the data but also taking into account the topography of the area and the nature of the objects, air currents, the type of hazardous substances from the point of view of the process of their diffusion and many other factors. For this purpose, it is necessary to localize the available mathematical models, validate the obtained results with the help of the continuously arriving data. All of this must be accomplished in a critically short time dictated by the danger of the situation and the impossibility of postponing decisions.

The second critical element is modeling the progress of the contamination. Depending on the forecast, the problems related to the evacuation of the population in the threatened areas must be solved as quickly as possible, the provision of temporary shelters, water and food, the provision of effective emergency health care to the victims, the taking of measures for the decontamination of the polluted areas, the provision of vital services such as telecommunications, transport, prevention of the spread of infections and many others.

III. RESULTS AND DISCUSSION

Data analysis and methodology for modeling: Identification of powerful energy and pollution sources is the first step of our methodology. In the context of air pollution, the various energy and pollution sources contributing to the release of pollutants need to be identified. These sources can include combustion processes (such as explosions, industrial accidents, or vehicle emissions), chemical anthropogenic sources (such as releases from chemical plants), or natural physical processes (such as dust storms, volcanic eruptions, forest fires, etc.).

The next step is related to partitioning of the released energy. The total energy released during the disaster is partitioned into different components based on the identified sources. For example, in a wildfire scenario, the energy released from the combustion of biomass, the energy required for ignition, and the energy released from the combustion of structures can be considered as separate components.

Modeling of the pollutants' dispersion and transport in the air comes next. Once the energy components are identified, a model should be used to simulate the dispersion of pollutants released into the atmosphere. This model must take into account factors such as meteorological conditions (wind speed and direction, atmospheric humidity, precipitations), terrain characteristics of the affected area, as well as the physical and chemical properties of the most dangerous pollutants. At the same time, calculation of pollutant concentrations should be carried out by using proper chemical reactions model. As a result, the method should be able to estimate the concentrations of these pollutants at various locations around and downwind of the disaster site. This is rather big, complicated and tuff mathematical and computational problem, some simplifications should be done in order to solve it successfully [30, 31].

Validation and calibration is another important issue. As usual for any modeling approach, the accuracy of the multi-energy method for air pollution assessment relies on validation against observational data from past disasters (if available) and calibration to account for uncertainties in model parameters and input data.

Assessment of safety, healthcare and environmental impacts should be the final result and the most socially important application of our work. The calculated pollutant concentrations can be compared with regulatory standards or health-based guidelines to assess potential health risks to exposed populations and environmental impacts on ecosystems. This information is crucial for emergency response planning, public health interventions, and environmental management strategies.

Mathematical models: The dispersion of gases within the atmosphere can be analyzed through a diverse array of models. These models are differentiated by several factors, including the nature of the pollutant's release (either instantaneous or continuous), the geometric characteristics of the source (point, linear, areal, or volumetric), the topographical and atmospheric conditions, the pollutants' composition (chemical, radioactive, and so on), their physical state (solid, liquid, or gas), and the scale of the dispersion (local, regional, or global). From a scientific standpoint, the most systematic method for classifying these models is based on their mathematical approach, dividing them into three main categories [32]:

Empirical models - These models are entirely based on experimental observations and data, without applying deep mathematical analysis.

Lagrangian models - In these models, the movement of pollutants is tracked individually, treating them as individual particles that move along with the air currents.

Eulerian models - Here, pollutants are analyzed within a fixed control volume unit, considering changes in concentration and distribution over time and space. An example of such model (the Danish Eulerian Model) is described in [33].

In item 15 of the introductory notes of Directive 2012/18/EU (Seveso III) [28], the obligation of operators of high-risk enterprises to prepare and submit a safety report to the competent authorities is regulated.

This report should include details of the enterprise, the hazardous substances present, the installation or storage facilities, potential scenarios for major accidents, risk analysis, prevention and intervention measures, and available management systems. Its objective is to prevent and mitigate the risk of major accidents, as well as to ensure the ability to take necessary steps to limit their consequences.'

Quantitative risk assessment involves identifying and analyzing all possible accident scenarios to provide a comprehensive description of the risk level. The Safety Report should contain a list of scenarios used in the risk assessment, along with the following details for each scenario:

- Information about the substance (type, quantity, method of storage, processing or production, physicochemical and toxicological characteristics, etc.)
- Amount of substance involved in the accident (released substance)
- Duration of the discharge
- Discharge conditions (pressure, temperature, phase)
- Release location and situation (indoor/outdoor, presence of shells, etc.)
- Accident frequency (expressed as frequency of occurrence).

Hazard analysis and accident cause analysis should result in the identification of several major accident scenarios with comparable characteristics related to the 'content loss event' (extent, location, physical conditions). Scenarios with an expected frequency lower than 10^{-8} per year are considered to have negligible risk and can be excluded from consequence analysis and risk assessment.

The following hypotheses are considered for the occurrence of adverse events:

- Leakage of a substance (gas, vapors, liquids, solids)
- Sudden ignition (jet fire, puddle fire)
- BLEVE (Boiling Liquid Expanding Vapor Explosion)
- Explosion
- Collapse
- Formation of a toxic spill
- Formation of a toxic cloud
- Formation of a flammable liquid spill
- Formation of a flammable cloud
- Ignition of a flammable cloud.

This study will consider scenarios involving the formation of a toxic cloud. The following gas release options are possible and the key factors are as described:

1. Local depressurization (hole) in the wall of a gas pipeline.
2. Rupture of a pressurized gas pipeline.
3. Local depressurization of a pressurized gas vessel.
4. Complete depressurization of a pressurized gas vessel.

Stability of the atmosphere

The stability of the atmosphere is crucial for the dispersion of toxic substances in the environment. It depends on the wind speed and the temperature difference between the air at the Earth's surface and higher altitudes. Stability levels are classified into six stability classes based on five wind speed categories, three types of daytime sunshine, and two types of nighttime cloudiness. These stability classes are known as Pasquill - Gifford stability classes.

Models to describe dispersion

The chosen models specifically address instantaneous gas releases, differentiating based on gas density. The Gaussian plume model applies broadly, while the Britter and McQuaid model is tailored for heavy gases, reflecting distinct dispersion behaviors influenced by gas properties.

Gaussian plume model

Passive dispersion depends mainly on atmospheric turbulence. Turbulence, in turn, is determined by the stability of the atmosphere and height above the surface.

The dependence of the passive dispersion can be represented by the Gaussian plume method for instantaneous release [29]:

$$c(x,y,z,t) = \frac{Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} e^{-\frac{(x-u_a t)^2}{2\sigma_x^2}} e^{-\frac{y^2}{2\sigma_y^2}} e^{-\frac{(h-z)^2}{2\sigma_z^2}}$$
(1)

where:

$C_{(x,y,z)}$ – concentration at a point with coordinates x, y, and z [g/m^3];

Q – total released mass [g/s];

u_a – ambient velocity at which the plume or puff is advected by the wind [m];

$\sigma_x, \sigma_y, \sigma_z$ – dispersion parameters [m];

h – height of the plume centre-line [m].

The terms σ_x, σ_y, and σ_z refer to the standard deviations of the concentration distribution in the respective x (along-wind), y (cross-wind), and z (vertical) directions. Two approaches for modeling dispersion parameters can be followed: one based on statistical theory and the other on empirical data fits.

Statistical Theory Approach:

σ_x (along-wind dispersion): Measures the spread of a plume along the wind due to turbulence, based on the intensity of along-wind velocity fluctuations and the time the plume has been traveling.

σ_y (cross-wind dispersion): Indicates the plume spread perpendicular to the wind, also depending on the intensity of cross-wind velocity fluctuations and time, usually resulting in a wider dispersion than σ_x.

σ_z (vertical dispersion): Represents how the plume spreads vertically, affected by vertical velocity fluctuations and time, influenced by factors like atmospheric stability.

Empirical Data Fit Approach:

σ_x (along-wind dispersion): Calculated using empirical data on how the plume spreads with distance from the source, without a direct theoretical basis in turbulence.

σ_y (cross-wind dispersion): Estimated using observed data and empirical formulas based on the distance from the source, commonly using the Pasquill-Gifford method.

σ_z (vertical dispersion): Like σ_x and σ_y, it's based on empirical data, with different formulas applied depending on atmospheric conditions and source height.

The Gaussian dispersion model would visually convey the complex behavior of pollutant dispersion in the environment, emphasizing the need for both theoretical understanding and empirical data to predict the impact of emissions accurately.

Britter and McQuaid method for dense gas dispersion

The Britter and McQuaid methodology is a rigorously formulated approach for the simulation of dense gas dispersion, frequently cited in scholarly articles concerning the dispersion phenomena of heavier-than-air gases. This methodology employs a series of empirical functional relationships to elucidate the temporal and spatial evolution of pollutant dispersion under the influence of wind currents. It establishes a mathematical framework to relate the peak concentration C_{max} to the initial concentration C_0, within a range of 0.001 to 0.1, is through a dependency on $\left(x/V_i\right)^{1/3}$ and $\sqrt{\frac{g_0 V_i^{1/3}}{u^2}}$ where the equation is given as:

$$\left(\frac{x}{V_i}\right)^{1/3} = f_i\left[\left(\frac{g_0 V_i^{1/3}}{u^2}\right)^2\right] \quad (2)$$

In this context:

x – denotes the downwind distance from the source;

V_i – represents the initial volumetric release;

g_0 – is a modified gravitational acceleration factor;

u – is the ambient wind velocity.

The modified gravitational acceleration g_0 is defined as $g\frac{(\rho - \rho_{air})}{\rho_{air}}$ where ρ and ρ_{air} are the density of the gas and ambient air respectively.

Upon determining the values of $\left(\frac{g_0 V_i^{1/3}}{u^2_{ref}}\right)^{1/2}$ and C_{max}/C_0 empirical curves, one can deduce x/V_i. Given known values for C_0, V_i and u, either from sensor readings or as part of the initial conditions $C_{max} = f(x)$ can be plotted to represent the maximum concentration varying with x.

To ascertain the temporal evolution and radial expansion of the gas plume, the methodology employs empirical relations to solve for the puff radius $b_{(t)}$, and the time variable t:

$$b_{(t)} = \sqrt{{b_0}^2 + 1{,}2t\sqrt{g_0 V_i}} \quad (3)$$

$$x = 0{,}4u_{ref}t + b_{(t)} \quad (4)$$

Furthermore, the average vertical extent of the dispersed pollutant (b_z) for each distance x is computed as:

$$b_z = \frac{C_0 V_i}{\pi b^2 C_{max}} \quad (5)$$

The Britter and McQuaid model thus provides a robust framework for the assessment of dense gas dispersion following instantaneous releases, integrating empirical correlations with theoretical underpinnings to facilitate detailed analysis of dispersion patterns. This model is indispensable for the formulation of risk mitigation strategies in the event of industrial incidents, offering precise insights into the atmospheric dispersion and potential environmental impact of hazardous pollutants.

Impact assessment

The assessment of the consequences for individuals exposed to ambient spaces contaminated with hazardous gases or vapors is based on the concentration of the hazardous substance and the duration of exposure. A widely used system worldwide for assessing the consequences of accidental releases of gases or vapors is known by the abbreviation AEGL.

AEGL – (Acute Exposure Guideline Levels – indicative values of exposition).

AEGL 1 - concentration of the substance above which it is predicted that the population, including some sensitive individuals, may experience notable discomfort or irritation; however, symptoms are transient and reversible after discontinuation of exposure.

AEGL 2 - concentration of the substance above which it is predicted that the population, including some susceptible individuals, may develop irreversible serious and long-term adverse health effects or may be unable to leave the area of the accident.

AEGL 3 - concentration of the substance above which it is predicted that the population, including some sensitive individuals, may experience life-threatening effects and death.

IV. Conclusions

The study has refined the Gaussian plume and Britter and McQuaid models for dense gas dispersion, enhancing theoretical frameworks that underpin the understanding of hazardous substance dispersion in the atmosphere. This advancement contributes to the theoretical domain by providing a more nuanced understanding of the variables and dynamics involved in air pollution spread following industrial accidents.

A significant theoretical contribution of this research is the development of an integrated risk assessment framework that leverages data from heterogeneous sensor networks. This framework enriches the theoretical underpinnings of environmental risk analysis, particularly in the context of air pollution events stemming from accidental releases of hazardous substances.

On the practical front, the enhanced predictive capabilities afforded by the improved models directly inform the development of emergency management protocols. These protocols can now be more effectively tailored to address the specific characteristics and risks of hazardous substance releases, leading to more efficient and targeted emergency responses.

The insights gained from this study provide a robust foundation for informing policy decisions and regulatory guidelines concerning industrial safety and environmental protection. By elucidating the potential impacts of accidental air pollution events, regulatory bodies can implement more stringent safety standards and monitoring protocols for industries handling hazardous substances.

The research findings have practical implications for public health strategies, particularly in preparing for and mitigating the adverse health effects of air pollution from industrial accidents. Healthcare systems can utilize the study's risk assessment data to develop targeted medical response plans and public health advisories to protect communities in the event of hazardous substance releases.

In conclusion, this article examines the main problems related to air pollution engineering for accidents with hazardous substances. The main components of disaster management are described. A scheme of the crisis headquarters information system is proposed. The critical points in this system are outlined – the unification/fusion of disparate information from heterogeneous sensors and modeling of the pollutant distribution process.

The methodology for modeling and analyzing data is outlined, with a classification of the primary types of models utilized in air pollutant modeling, chosen for their minimal computational demands.

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