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OPEN BURNING AND OPEN DETONATION OF EXPLOSIVES. PREDICTION OF POLLUTANT EMISSIONS

The paper presents a complex analysis of the presence of various pollutants (CO_2, CO, NO, NO_2, CH_4, TNMH, C_6H_6) in the vicinity of sites intended for open burning and open detonation of explosives. Previously obtained data (measured field data on a representative sample) regarding the emission factors of pollutants originating from different types of explosives have been used. To predict the atmospheric dispersion of reactive agents, the ADORA and ALOHA models were used. Comparative analysis was performed with computational and experimental data on the emission of detonation products using regression analysis of the obtained emission coefficients. The overall results show satisfactory values of correlation coefficients. The prediction power of used methods increased as follows: ADORA (the smallest error), ALOHA *E*/*A* (0.43) and ALOHA *E*/*A* 0.67.

1. INTRODUCTION

There are large quantities of surplus, obsolete or unserviceable ammunition worldwide. Two years ago the United States military had a stockpile of nearly 400 000 t and almost 60 000 t are added each year to this quantity [1]. Developed countries have financial means to destroy the surplus explosives and ammunition or pay other countries to deal with this issue on their own. On the other hand, underdeveloped or developing states usually solve the problem in an environmentally unacceptable way – through open burning (OB) and open detonation (OD) – a way involving destruction and endangerment of the environment. This problem is relevant to the Western Balkans countries as well

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as the other states in the South-East Europe (SEE) region. However, the vast majority of citizens in both the developed and developing countries, as well as various organizations (in particular, environmental non-governmental organizations), are reasonably concerned about the short-term and long-term consequences to human health and environment caused by OB and OD activities [2].

Addressing the stated issues is not an easy task. One of the significant problems refers to the lack of knowledge needed to assess and evaluate OB and OD emissions data that apply to the situation at the field, and, also, lack of the skills needed to use the information to evaluate the true risk that OB or OD presents to the environment.

Various techniques for air pollution prediction, i.e., emissions of pollutants were used by various authors for various problems. Djebbri and Rouainia [3] predicted *the two pollutant concentrations (NO_x and CO) in industrial sites by a modified radial basis function (RBF) based neural network*, while Blagojević et al. [4] developed an *artificial neural network (ANN) model for predicting air pollution* in Serbia. In this study, the regression modelling is applied to data showing emission factors of various pollutants originating from OB and OD of explosives. The objective was to determine the regression equations that could allow the prediction of most common detonation products such as carbon dioxide (CO_2), carbon monoxide (CO), nitrogen oxide (NO), nitrogen dioxide (NO_2) methane (CH_4), total non-methane hydrocarbons (TNMH), and benzene (C_6H_6) which represented the surrogate for volatile organic compounds (VOCs). The ADORA (Atmospheric Dispersion of Reactive Agents) [5, 6] and ALOHA (Areal Location of Hazardous Atmospheres) [7] models were used to correlate, confirm or refute assumed interdependencies.

ADORA calculates the composition and dispersion of clouds that are the result of reactive chemicals being released into the atmosphere [6]. It only needs the composition of the reactants and the local discharge and environmental conditions as inputs for these calculations. Assuming that the shape of the cloud is known, it solves the preservation of the mass, momentum, energy, and type equations in the integral formulation.

2. EXPLOSIVES

An explosive might be defined as a quasi-stable chemical that rapidly changes from a solid or liquid to a gaseous state following activation or detonation. An extreme increase in pressure by gas evolution results in the explosion, with the energy released as a function of the explosives' thermodynamic properties. High-explosive molecules are often characterized by an aliphatic or aromatic structure with substituted nitro groups. These compounds have regions of greatly differing oxidation-reduction potentials so that, when detonated, they release a large amount of heat, form a shock wave, and release various gaseous products through rapid intra- and intermolecular oxidation reactions. The

activation energy needed for the detonation process can be supplied by high-pressure shockwaves, friction, electricity or heat.

Explosives are usually classified based on their velocity of detonation. There are low (propellant) and high (detonating) explosives. Low explosives (e.g., black powder, smokeless gunpowder, nitrocellulose, etc.) react slowly and burn rapidly instead of detonating. High explosives, on the contrary, produce extreme pressures by rapid detonation. They can produce peak pressure of 36 000–360 000 atmospheres in less than four microseconds. The detonation also produces a 2–10 s fireball. High explosives are more stable to detonation than low explosives; their detonation is initiated by exceeding higher activation energy through shock. These explosives are characterized by detonation rates as high as 6400 m/s, while low explosives have this value in the range of 80 m/s. In addition, high explosives are possible to divide into three groups as follows (taking into account their chemical structure): aliphatic nitrate esters (esters of nitric acid), nitramines and nitroaromatics. Examples of high explosives according to Watts [8], are: trinitrotoluene (TNT), RDX (1,3,5-trinitroperhydro-1,3,5-triazine – hexogen), composition B (CB, an explosive containing approximately 59.5% of RDX, 39.5% of TNT and 1% of wax) and PETN (pentaerythritol tetranitrate).

3. EXPERIMENTAL

The interdependencies of the obtained parameters of product emissions by the detonation of TNT and CB were examined. The process of chemical reaction, from the moment of initiation of explosives to detonation reaction, creates detonation products that expand in a gaseous, liquid or solid state. As a result, the rough detonation cloud appears. As the detonation process continues, the released products are deposited in the soil, water or remain in the air for some time. It is important to highlight that complete or incomplete detonation can occur and, therefore, different methods of calculating emission coefficients can be applied. Consequently, different mechanisms of explosives' decomposition lead to various volumes of decomposition products.

The field investigation was conducted based on arbitrarily selected samples of explosives and compositions for the conditional and constructive analysis of the obtained emission concentrations of chosen explosives. The prediction of toxic emissions by the detonation of explosives and selection of samples was carried out according to the methodology reported elsewhere [6, 9–14]. Comparative analysis of the obtained results with experimental data was achieved through the regression analysis.

The linear regression method allows a researcher to make predictions about one variable based on the information that is known about another variable. This method can be used in the case of two continuous variables – an independent variable and a dependent one. The independent variable is the parameter that is used to calculate the dependent variable or outcome.

On the other hand, a multiple regression model extends to several explanatory variables. Multiple regression is a statistical technique that uses multiple descriptive variables to predict a variable's response results. The objective of multiple linear regression (MLR) is to model a linear relationship between explanatory variables and a response variable. This type of analysis is a mathematical model that involves one independent and several dependent variables. Dependence testing and research require the drawing of a scatter chart, which represents the relationship (dependence) between the variables *X* and *Y*. The chart allows a visual representation of dependence between variables, i.e., emissions of products, their character and intensity.

4. RESULTS AND DISCUSSION

The results are expressed in the form of emission factors that define the ratio of the mass of the product in the cloud formed after detonation at the end of chemical reactions to the original mass of the explosive material. During each test, environmental conditions such as temperature, humidity, wind speed, altitude and atmospheric conditions were monitored, as well as the movement of clouds as a function of time. However, in this research, only the final emission coefficients (Table 1), obtained by reducing to ambient conditions, were the subject of analysis.

Table 1

Experimental and calculated emission coefficients of TNT and CB detonation products

Explosive material	Data source		Product						
			CO_2	CO	NO	NO_2	CH_4	TNMH	C_6H_6
TNT	measured value		1280	49	1.4	1.4	1.5	2.1	0.1
	ADORA		1260	58	2	1.2	1	0.85	0.14
	ALOHA	$E/A = 0.43$	920	280	0	0	0.19	0	0
		$E/A = 0.25$	1360	0	0.03	0	0	0	0
CB	measured value		870	31	0.8	1	0.6	1.2	0.062
	ADORA		980	48	1.7	1	1.7	2.3	0.18
	ALOHA[a]	$E/A = 0.67$	750	97	0	0	0	0	0
		$E/A = 0.43$	900	0	0.01	0	0	0	0

[a]E/A (entrained air ratio) are the coefficients for predicting the ratio of air in the detonation pressure and can range from 0.25 to 1.5, specifically for this research from 0.25 to 0.67.

Data on emissions of products were used for the regression analyses to determine the ratio and value of concentration levels for pure TNT and CB. The results were analyzed and a scale from the highest to the lowest value was formed as a function of the type of explosive substance. These data were used for the construction of the set of scattering diagrams presented in Figs. 1–7. The diagrams were arranged according to

the emission products of the detonation of TNT and CB. They also contain the equation and linear trend as well as the values of the coefficients R^2, which show the scattering of the obtained data. The highest value of the R^2 is obtained for CO_2 (0.9227), while the lowest value is determined for CO ($R^2 = 0.6643$). The scattering gradient from the highest to the lowest emission coefficients for analyzed products is presented in Table 2. One could claim that the R^2 values belong to the wider range, and, consequently, it is possible to consider various levels of reliability of test results.

Table 2

Scattering gradient for the emission coefficients of analyzed products

Analyzed product	CO_2	CO	NO	NO_2	CH_4	TNMH	C_6H_6
Emission coefficient (R^2)	0.9227	0.9046	0.8822	0.8720	0.8614	0.8470	0.6643

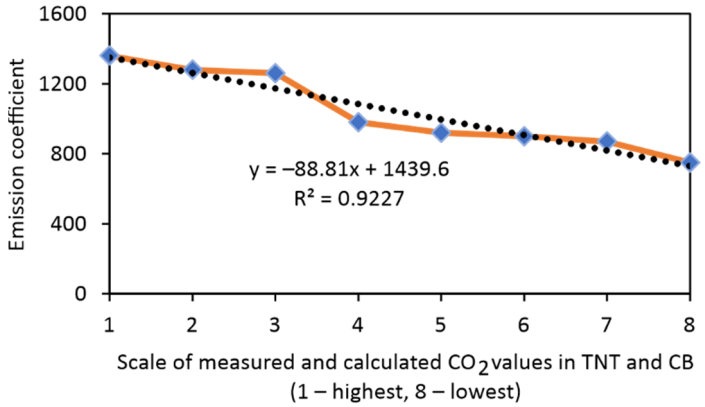

Fig. 1. Emission coefficient scatter diagram for CO_2

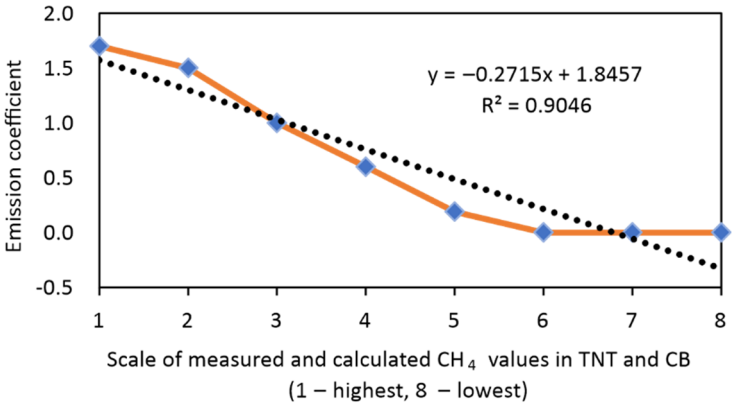

Fig. 2. Emission coefficient scatter diagram for CH_4

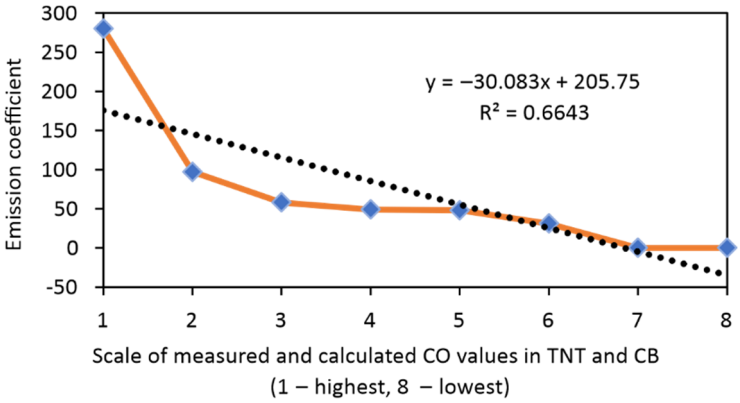

Fig. 3. Emission coefficient scatter diagram for CO

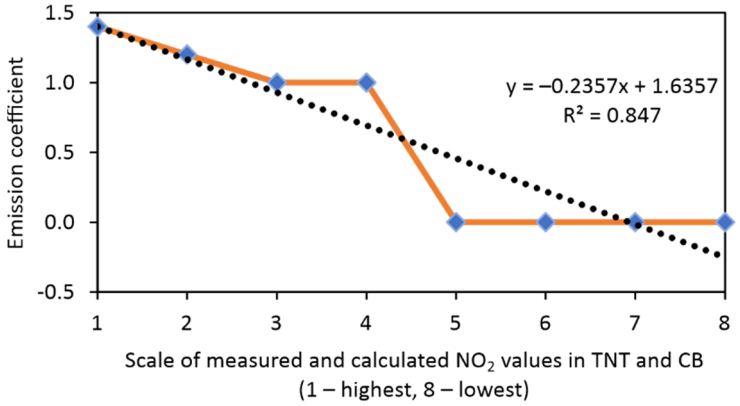

Fig. 4. Emission coefficient scatter diagram for NO_2

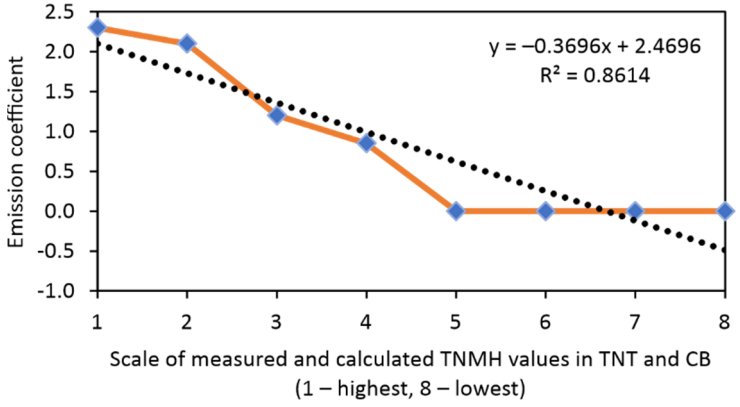

Fig. 5. Emission coefficient scatter diagram for TNMH

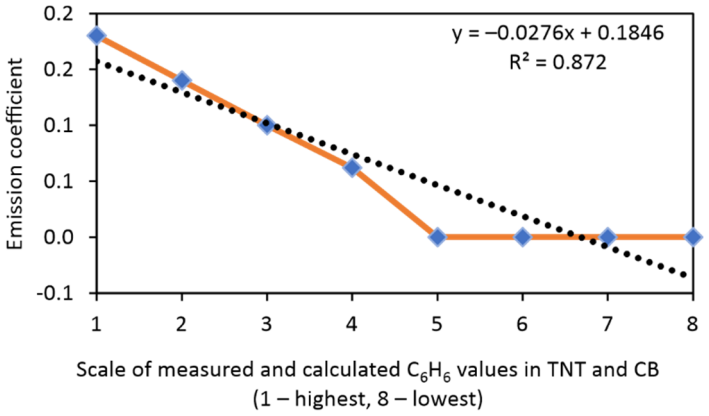

Fig. 6. Emission coefficient scatter diagram for C_6H_6

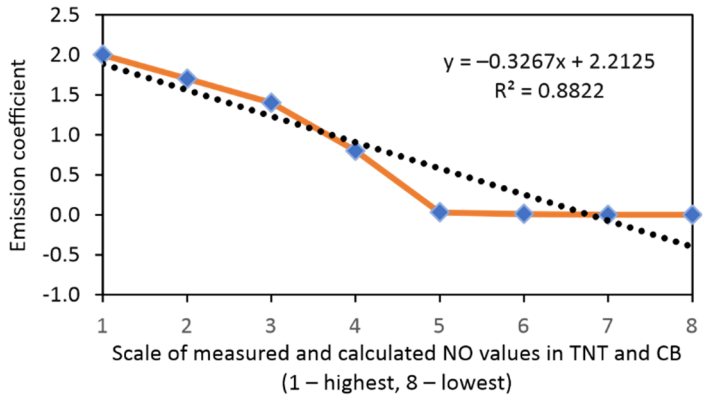

Fig. 7. Emission coefficient scatter diagram for NO

The results of calculations using ADORA and ALOHA models in the function of the measured coefficients and multicriteria regression analyses are shown in scatter diagrams in Figs. 8–13. Equations and linear trendlines are also presented on diagrams as well as the values of the coefficient R^2 for both methods of data acquisition – measurements (experimental) and calculations.

Figures 8–13 show the deviation of the calculated values from the experimentally measured emission coefficients. They also reveal a significant level of deviation in terms of the individual coefficient values. To cope with noticed deviations, it is possible to conduct a further clarification by the value scale together with a summary overview of multicriteria regression analysis.

The reliability of prediction of emission factors for various pollutants, applied in this study, by comparing different methods along with experimental ones, is quite appropriate. This approach is confirmed in several recently conducted studies dealing with the determination of emission factors (EFs) from various sources.

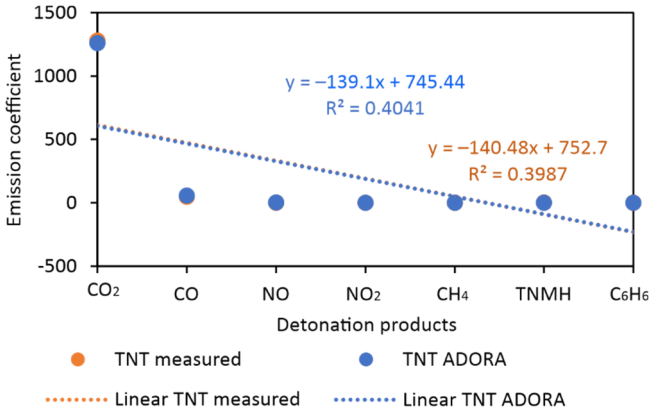

Fig. 8. TNT emission coefficients measured and calculated (ADORA)

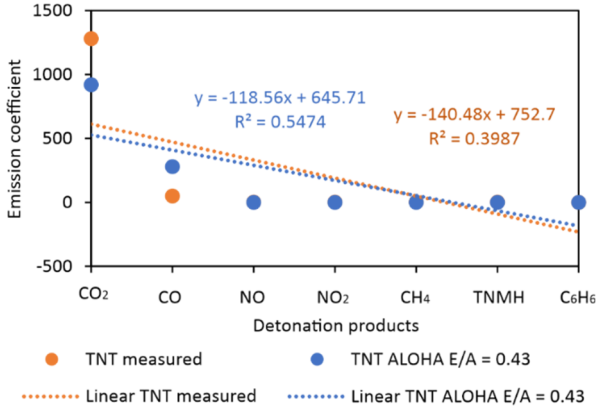

Fig. 9. TNT emission coefficients measured and calculated (ALOHA $E/A = 0.43$)

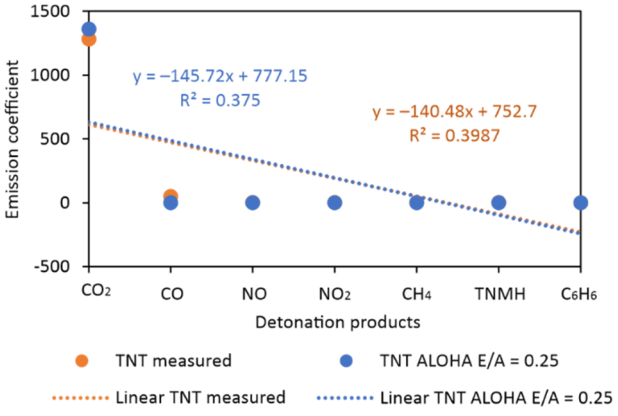

Fig. 10. TNT emission coefficients measured and calculated (ALOHA $E/A = 0.25$)

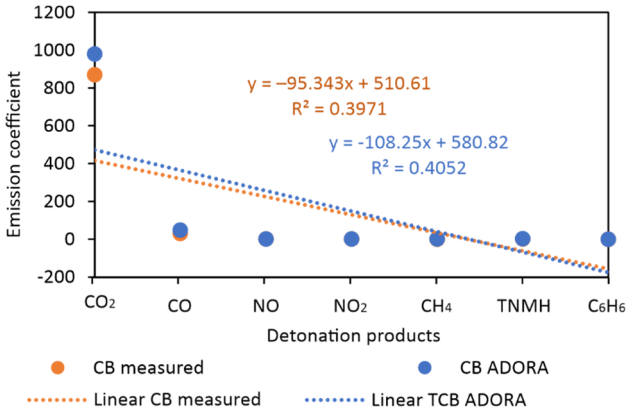

Fig. 11. CB emission coefficients measured and calculated (ADORA)

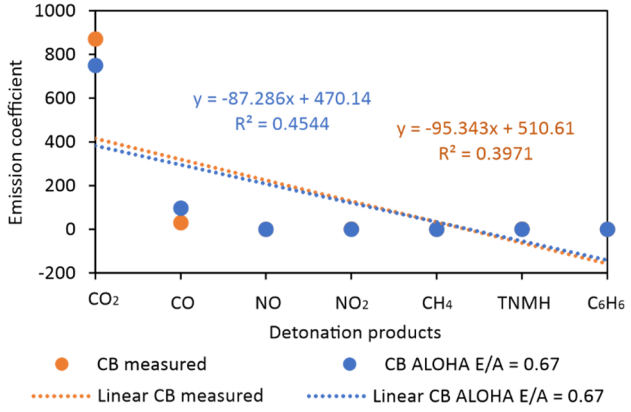

Fig. 12. CB emission coefficients measured and calculated (ALOHA E/A = 0.67)

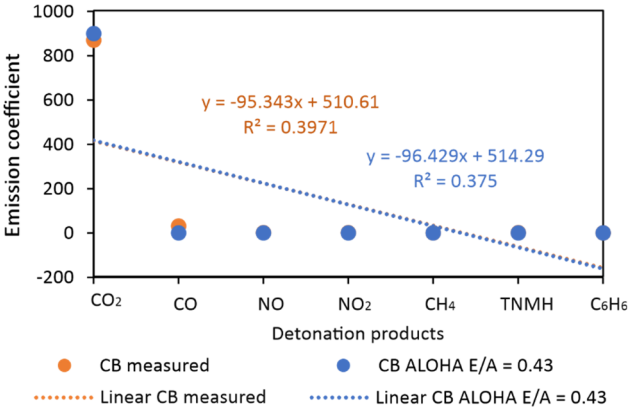

Fig. 13. CB emission coefficients measured and calculated (ALOHA E/A = 0.43)

Aurell et al. [12] determined EFs from three sources: open detonation (OD), open burning (OB) and static firing (SF) of obsolete military munitions. The samples were collected using an aerostat-lofted sampling instrument manoeuvred into the plumes with remotely controlled tether winches. It is important to note that this study was the first attempt to determine emission factors, among other pollutants, of particulate matter ($PM_{2.5}$) for OB and surface OD. Furthermore, PM emission factors were higher for soil-covered than surface detonations. Namely, the $PM_{10}/PM_{2.5}$ ratio for covered detonations was approximately 30:1 while this ratio for the open detonation of CB was about 1:1. This significant difference is attributed to the large amounts of soil ejected during the detonation and entrained into the plume. Yuen et al. [15] introduced the hybrid optical remote sensing (hybrid-ORS) method in their determination of EFs of particulate matter with aerodynamic diameters < 10 mm (PM_{10}). This method is based on the measurement of range-resolved PM backscattering values with a micro pulse light detection and ranging (LIDAR, MPL). The results obtained by hybrid-ORS method for the determination of EFs were 13% higher for OB and 174% for OD compared to previously reported results in [14] and [11], respectively. In comparison with concurrent field measurements by EPA [16], EF values obtained by hybrid-ORS method were 37% higher for OB and 54% for OD. Concerning TNT, no statistically significant changes of the EFs were noticed during the detonation of 22.7 and 45.4 kg of this explosive. This confirms the fact that the total amount of detonated mass in this range does not have an effect on the EFs for OD of TNT. The research conducted in 2018 demonstrates the prediction and measurement of emissions from explosions and combustion events caused by metal (Mg and B) containing TNT formulations [17]. These additives were chosen because Mg/B can overcome thermodynamic limitations on realizing full-combustion enthalpy for B on detonation timescales. The TNT:Mg:B composition (80:4:16 by weight, stoichiometry approximately MgB_2) allows to study pollutant emission by explosions that release carbonaceous particles, metal additives known to combust when formulated in explosives (Mg), and metal additives (B) for which full explosive performance has yet to be realized. The simulations could predict solid and gaseous chemical species produced by explosive events. The experimental work was carried out in such a way to allow the measurement of gases and particles emitted during testing TNT.

5. CONCLUSION

Air quality protection requires reliable and up to date information about the polluting factors to ensure an efficient decision-making process for the protection of human health and the environment. The resulting decisions must be optimized for daily supervision of air pollutant levels but also risk situations related, among other things, to various military activities including those dealing with open burning and open detonation of explosives.

Analysis like the one presented in this paper might be very useful for identifying air pollution patterns during the burning or detonation of explosives based on the interactions between pollutants and meteorological factors. Some sophisticated techniques, as described in the paper, can provide comprehensive classifications of the monitoring sites, supporting source apportionment and the optimization of the monitoring operations.

The results dealing with emission factors, obtained for different pollutants and reported in this study, indicate that all methods used for these purposes inherently involve some uncertainties. They can be quantified with more specific measurements. In the meanwhile, until such measurements are made possible, there are some measurements and emission estimation which allow the determination of emission factors of numerous pollutants from explosives and other military munitions.

ACKNOWLEDGMENTS

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