THE MODELING OF FIRE EFFECTS ON THE ENVIRONMENT

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Abstract:
The industrial fires involving significant quantities of combustible liquids pollute the environment with smoke and toxic gases. In the paper are presented the original results of the authors concerning the modeling of such fires in open air. The results of the numerical modeling are processed, analyzed and interpreted, with emphasize on the value of polluting fire effluents.

Key words*: air pollution, fire effluents, modeling of fire effects, industrial fires*

JEL classification: *Q5, Q53*

1. Introduction

The researches on the fire consequences were focused mainly on the direct threats to the people in the closed areas to the fire and to the financial losses connected to fires, in aspects such as the damages over the buildings and infrastructure [1, 5, 7, 8, 16, 17]. However, the fires threaten also the environment, causing local effects on land and water biotopes, also being a significant source of persistent pollutants. The negative effects of fires over the environment were brought to the general public's attention after some major industrial fires occurred in the eighties. The most significant fire can be considered the one that occurred in Sandoz, Basel region, Switzerland, when a significant part of Rin was polluted by the contaminated water resulted from fire extinguishing activities. [7] these incidents had as effect the intensification of the research activity concerning industrial fires, mainly by applying for large research programs in Europe.

As one can see by analyzing the energy creating entities, about 80% of the world's energy support is provided by combustion of flammable liquids (such as gasoline and hydrocarbon fuels), solids (such as coal and wood) and gases (such as natural gas containing methane and small amounts of other hydrocarbons such as ethane, propane and butane). The other 20% are accounted from other energy sources such as nuclear or renewable energy [8].

The purpose of the paper is to underline the importance of industrial fires as pollutants, and on the other hand, the possibility to use computer simulations to minimize the effects of these fires.

Application of numerical simulation in industry has grown rapidly during the last decades. It complements the theoretical investigations where nonlinearity, high number of degrees of freedom, or lack of symmetry are of importance, and complement experiment where devices are expensive, data is inaccessible, or the phenomena very complex. For the study of combustion, numerical simulations improve our understanding of flame structure and dynamics [2, 10]. They are widely used in the design and optimization of practical combustion systems because, compared to experimental testing and prototyping, the development costs of numerical simulation are very low. Today, no real progress in design or optimization can be made without numerical simulations [8]. Following this idea, the paper below presents a fire modeling of an industrial fire, especially created to analyze the possible effects of a real fire, on the quality of environmental air.

2. Fire effects on the environment

Fire effects can be translated through the physical, chemical, and biological impacts of fire on ecosystem resources and the environment [9]. The abiotic effects of fire include its role in changing air quality, water quality, soil properties, and nutrient cycling. Biotic effects include altering vegetation and related impacts on wildlife. Fire effects are the result of an interaction between the heat regime created by fire and ecosystem properties. Fire effects on the environment cover effects on air, water, soil, vegetation, and wildlife.

2.1 Fire Effects on Air Quality

All fires emit air pollutants in addition to nonpolluting combustion products; but fires vary widely in what pollutants are emitted in what proportion.

The chemistry of the fuel as well as the efficiency of combustion governs the physical and chemical properties of the resulting smoke from fire. Although smoke from different sources may look similar to the eye, it is often quite different in terms of its chemical and physical properties. Generally, the emissions we cannot see are gas emissions and the emissions we can see are particulate emissions [3].

Ambient air quality is affected by: • the pollutants emitted to the atmosphere from fires; • the background air quality that has already been degraded by other sources; • the transport of the polluted parcels of the atmosphere and • dispersion due to atmospheric movement and turbulence, secondary reactions, and removal processes. [22]

2.2 The estimation of total emissions in the atmosphere

Although there are few standards that contain applicable data, concerning the toxicity of smoke, knowledge concerning this problem have been accumulated from the research activities that were developed in time. There is available information in the specialty literature concerning the production of the burn gases, especially the lethal ones, such as CO and HCN, but also concerning some no lethal organic compounds that, in some cases, can have bad long term effects. However, because of the complexity of the uncontrolled burning process and partially because of the high prices of the chemical detailed analysis, there are lots of aspects that need to be studied [21].

The majority of studies concerning the toxicity of the gases are based on the data obtained after the reduced scale fire modeling. However, these data can not be used to approximate, in general, the effects of smoke in real fire cases. One can observe the lack of quantitative chemical data referring to the effluents resulted after real fires.

3. The combustible liquid pool fires

The structure of the majority of pool fires can be classified as follows [20]: • *the combustible liquid*; • *an area of unburned combustible vapors,* situated above a liquid; • *an area of bright flames surrounding the vapors*; • *a combustion area* situated above the bright flames area, where there are obvious turbulences in the flame; • *the fire plume,* generally having an ascension and turbulent movement.

The resulted fire is measured by a number of “quantifiable quantities”, among the most important of them: • *mass loss rate,* closely related to the heat release rate; • *the heat release rate*: the total amount of energy (in the form of heat), released by fire as a function of time; • *the temperature of the flames*; • *the height of the flames*; • *the production of soot and burning products* that is usually translated by the combustion fraction of the product (g/g); • *radiation*.

These measurable quantities are controlled by a number of *„physical characteristics"*, associated to the leakage, starting from simple parameters to the complex phenomena, including: • *the geometry of the pool fire*; • *the composition of the combustible*; • *the ventilation conditions*; • *the surrounding geometry*.

These physical features affects the burning behavior of the pool and are evaluated by using the measurable quantities.

In table 1 can be found the numerical values obtained by experimental determinations for the mass loss rate and for the heat release rate obtained from fire tests involving large diameter combustible liquid pools of different sources [4, 11, 18, 20, 21].

Table 1

The mass loss rate and the heat release rate for some combustible liquids

The combustible liquid	**Mass Loss rate** m''_∞ **[kg/(m^2·s)]**	**The net burning heat** Δh_n **[kJ/kg]**	**The heat release rate on the surface unit** Q'' **[kW/m^2]**	**Density** ρ **[kg/m^3]**	**The efficiency of combustion** χ_c
Metanol	0,017	20 000	340	796	0,955
Etanol	0,015	26 800	400	784	0,92
Heptane	0,101	44 600	4 504,6	675	0,93
Benzine	0,048	44 700	2 145,6	740	0,986
Kerosene	0,039	43 200	1 684,8	820	0,99
JP-4	0,051	43 500	2 218,5	760	1
Crude oil	0,022-0,045	42 500 ... 42 700	935 ... 1 921,5	830-880	-

The determination of the heat release rate is an essential aspect when it comes to fire modeling.

3.1 The combustion products

The production of soot in the fire plume is a very complex subject, because of the spatial formations that vary, because of the oxidation processes, of the influence of turbulence, depending on the temperature and fuel.

Table 2

The combustion products in ventilated fires, for some combustible liquids

The combustible liquid	**The chemical formula**	**The net burning heat** Δh_n **[kJ/g of burned combustible]**	**the effective burning heat** Δh_c **[kJ/g of mass loss]**	**The effective fraction of combustion [product in g / mass loss in g]**			
				CO$_2$	**CO**	**soot**	**Residual hydrocarbons**
Metanol	CH_3OH	20,0	19,1	1,31	0,001	-	-
Etanol	C_2H_5OH	26,8	25,6	1,77	0,001	0,008	0,001
Heptan	C_7H_{16}	44,6	41,2	2,85	0,010	0,037	0,004
Octane	C_8H_{18}	44,5	41,0	2,84	0,011	0,038	0,004
Kerosene	$C_{14}H_{30}$	44,1	40,3	2,83	0,012	0,042	0,004
Benzen	C_6H_6	40,1	27,6	2,33	0,067	0,181	0,018
Toluen	C_7H_8	39,7	27,7	2,34	0,066	0,178	0,018

These phenomena can lead to the appearance of some combustion products as a result to incomplete burning. For the fuels of type $C_xH_yO_z$ one expects, after the oxidation reaction, to result combustion products, (CO_2, CO, H_2O şi H_2,), soot (containing, usually, pure carbon) and other residual hydrocarbons (CH):

$$C_xH_yO_z + O_2 \rightarrow CO_2, CO, H_2O, H_2, \text{soot}, CH \qquad (1)$$

In table 2 is presented a report with test results [5, 20, 21] for some combustible liquids.

3.2 Large pool fires of combustible liquids

The large pool fires, separately from the general leakage fires, were subject of research for many years; however, the understanding of the different processes involved has not yet touched a maturity level. The main efforts today can be classified in two main groups: experimental efforts and modeling efforts. Both of them are imperatively needed, in order to obtain progresses in the field.

A serious work was realized by the Alabama laboratories in U.S.A., (fig. 1) [12], where detailed determinations were done to identify the production of soot, the flow fields and the mechanisms of the heat transfer in case of real pool fires.

Fig. 1. Image from the experiment of U.S. Coast Guard Fire and Safety Test Detachment, October 1994, Alabama, U.S.A.

Note: three fire tests each of 17,1 m^3 diesel fuel, in a tank with 15,2 m diameter and the deep of 0,61 m. The diesel fuel spilled over a layer of water of 0.5 m deep, in the tank.

The researches on large fires [12, 15, 19] identified that the production of soot (fig. 1), in large scale fires, is a key factor that controls their behavior. Comparing to the smaller fires, in which the flames are relatively without colors, and the soot appears only at the tip of the flame, while one advances to fires with larger diameter, the soot is produced in large quantities in the fire plume [12]. This aspect need the separation of the central regions of a pool fire in two well defined sections:

- „the luminous band" of the flame, right above the pool surface;
- the above part of the fire plume where, generally, the smoke hides the flames.

One discovered that the production of soot rises once with the diameter of the pool, reaching constant values (0,15 mass fraction) at diameters larger than 2 ... 3 m [15].

The area rich in combustible in the vicinity of the pool surface, can attenuate the irradiative flux of the combustible, keeping down the mass loss rate. This phenomena can be found often in the case of large fires of hydrocarbons in which an area of the emissive surface of the fire is covered in a thick and black smoke.

4. Fire computer simulation

As previously said, the practical CFD method to predict the generation of toxic gases in open fires presented below use local combustion conditions to determine the yield of carbon monoxide, carbon dioxide, soot and oxygen.

The Fire Dynamics Simulator (FDS) code is a computational fluid dynamics model for simulation of fire-driven fluid flow developed by the National Institute of Standards and Technology. It solves numerically a form of the Navier-Stokes equations appropriate for low speed, thermally-driven flow with an emphasis on smoke and heat transport from fires [6,13,14].

4.1. The description of the conditions of the simulations

The scenario used as a base for this study included a retention pan with a rectangular shape (37 × 65 m), with a surface of 2 400 m^2 containing two vertical cylindrical tanks with 16 m diameters.

The entry parameters, concerning the modeling, are as follows: • the surface of the pan, 2 400 m^2; • the combustible - benzine; • the mass loss rate, 55 $g/(m^2 \cdot s)$; • the ambient temperature, 15 °C; • the speed of the wind, 5 m/s; • the density of the air, 1,161 kg/m^3; • the relative air humidity, 70 %; • the radiative component of the burning efficiency, quantified by $\chi_r = 0{,}35$.

4. 2. Hypotheses and other preliminary considerations

The FDS three dimensional fire model takes into consideration also the existent atmospheric stratification that exists in nature. In the present scenario, the pressure induced by fire is a perturbation of the vertically stratified pressure, in a hydrostatic balance with pre established wind speed fields and temperatures. The environment and topographic characteristics implemented are justified by blocking some parts of the calculation domain to eliminate the flux through the solid delimitations. To solve the radiative transport from fire, one uses the finite volume method. The quantity of soot and burning products is calculated based on the combustion model. Also one takes into consideration the fact that the soot (modeled as Lagrangian particles) absorbs and reflects the radiation from fire [1,5,13].

A numerical network containing a number of 72 × 108 × 60 cells was used to create a cubic domain with the following dimensions: 288 × 432 × 240 m. The dimension of a cell is 4 × 4 × 4 m. As the numeric model was developed for rectilinear geometries and the fire scenario assumes that the burning develops only in the pan, the two tanks were implemented as two cuboids with the dimensions 14 × 14 × 8 m to keep the same surface occupied by the cylindrical vertical tanks (the surface of a disc with the radius of 8 m is equally to a square with side of 14,14 m). Each tank is situated under the level of the earth and is surrounded by an embankment of 3 m height.

A stratified wind profile of shape: $u(z) = u_0 \left(\frac{z}{z_0} \right)^p$, was imposed as a condition to the limit. The wind speed u_0 at the level of the embankment was of 5 m/s. The *p* exponent, a function of the surface rugosity, was of 0,15.

The temperature of the ambient atmosphere presumed to be uniform with the height (15°C).

The characteristics concerning the fire reaction of the burning fuel (benzine) were extracted from the third subchapter of the present article and implemented in the numerical program.

One presumed that the fire covers the whole area of the retention pan, in the initial moment of the simulation.

4.3. Results from the fire dynamic simulation

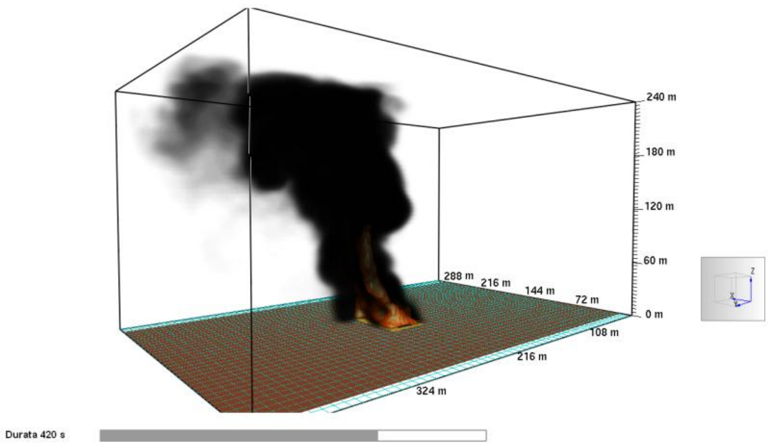

Fig. 2. Image of a simulation of a benzine fire, with a wind speed of 5 m/s above the retention pan and for time t = 420 s.

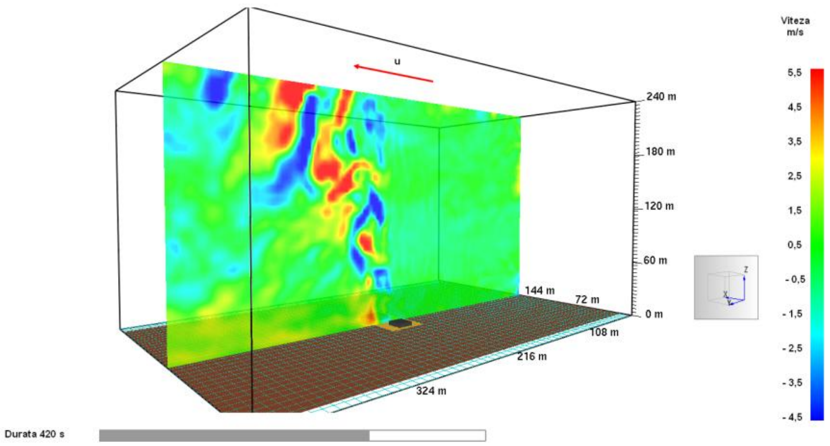

Fig. 3. The profile of the speed, in the calculation domain, on the direction parallel to the *Oy* axe, at x= 144 m, in the positive sense of *Oy* axe and for t = 420 s.

4.4.Processing, analysis and interpretation of results

The duration of a fire in limit conditions was established at 600 s. the simulations were developed on a computer having an Intel Core 2 Duo processor: 2400 MHz and 1024 MB memory DDRAM. The duration of the numerical calculations processed by the computer was of 23 hours, being performed 6.514 iterations.

All dynamic results are sequentially presented in 4 moments in time: 60 s, 120 s, 240 s and 420s from the beginning of the modeling. Having in mind reasons easier to understand, there cannot be presented modeling results every second out of the 600 s of simulation. These 4 "key" moments were chosen after repeated visualization and analysis of the entire simulation. Also, the "zero" moment (the initial moment) of the simulation is not the same with the moment of fire initiation. Due to restrictions on spreading of the article, there will only be presented numerical simulation at moment t = 420 s.

Figure 2 represents visualization – at the pre-established moment – of the tri-dimensional dynamic simulation of the turbulent cone of the burning in the conditions of the present fire scenario. One can observe that the direction (perpendicular on *zOx* plan) and the wind speed (5 m/s) influence the bearing of the turbulent cone, fact that is in full accordance to the experimental researches (see fig. 1) regarding large pool fires of combustible liquids. Simulations also show the correct "mapping" of large pool fires of combustible liquids (see fig. 1), meaning that the "luminous band ring" of the flames can be very well distinguished, right over the surface of the spill and the upper area of the cone where flames hide the flames.

In the calculation domain, the profiles of the speed contours on the parallel direction on axe *Oy*, at x = 144 m, in the positive momentum of axe *Oy* at moment t = 420 s is presented in figure 3. Although it may seem odd, there also appear areas with negative values of the speed taking into account that the wind has a 5 m/s speed in direction *Oy* with a layered environmental profile. This is because of eddies that appear due to the turbulent nature of the fire cone of large fires.

5. Conclusions

The research is presenting a new approach of modeling and simulation of environmental pollution from combustible liquid fires having as basis the modern concepts of chemical thermo-dynamics theory (thermo-dynamics, fluid dynamics, heat and mass transfer) and applied mathematics on fire calculations.

Dynamic and tri-dimensional simulation of industrial fire effects – with an accent on producing, development, transportation and spreading of combustion products into atmosphere, in different environmental conditions – was developed using a dedicated program.

The study illustrates the complex interaction between the topography, the environment and fires dynamics. Taking into consideration the easiest configurations chosen for this study, there are many factors that strongly affect the results of fire dynamics. Winds and temperatures play an equally important role as smoke dissipation into environment. Natural topography characteristics near the tanks will further modify the patterns of spills followed by modifications of transportation and dissipation of smoke from hydrocarbons fires.

Arbitrary pre-established environmental conditions could be replaced with local meteorological simulations which are based on data bases and computer modeling used by experts drawing up whether forecasts. The result will consist of the simulation ability that could be used in predicting fire effects on systems and outdoor industrial installations caused by natural disasters or man made in real world.

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